Two-body P-state energies at order α^6

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We present an analytical calculation of the complete α^6 correction to energies of nP levels of two-body systems consisting of the spin-0 or -1/2 extended-size particles with arbitrary masses and magnetic moments. The obtained results apply to a wide class of two-body systems such as hydrogen, positronium, muonium, and pionic or aniprotonic helium ion. We found an additional α^6 correction for nP levels of positronium, which was previously overlooked. Our results are also relevant for light muonic atoms, whose accurate theoretical predictions are required for extracting the nuclear charge radii.

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I. INTRODUCTION

Two-body systems, such as hydrogen and hydrogen-like ions [1], muonic hydrogen [2], muonic helium ion [3], positronium [4], and muonium [5], play a crucial role in testing quantum electrodynamics (QED), determining fundamental constants, and searching for physics beyond the Standard Model. All these tasks require accurate theoretical predictions for energy levels of these systems. If the mass ratio of the two constituent particles is small, as, e.g., in hydrogen, one can use the Dirac equation as a starting point and use the QED perturbation theory to account for the recoil and QED corrections. For systems like positronium and light muonic or antiprotonic atoms, however, the masses of the particles are equal or comparable, and the Dirac equation is no longer a good approximation. Thus, one has to rely on the QED formalism from the very beginning in their description.

The QED theory of light atomic systems is based on an expansion in the fine structure constant α and the derivation of the expansion coefficients as expectation values of various effective Hamiltonians with the nonrelativistic wave function. Specifically, the energy of a bound system of two particles with masses m_1, m_2, charges e_1, e_2, spins s_1, s_2, and g-factors g_1, g_2 can be expressed as an expansion

$$E(\alpha) = E^{(0)} + E^{(2)} + E^{(4)} + E^{(5)} + E^{(6)} + O(\alpha^7), \tag{1}$$

where the individual terms $E^{(j)} \equiv (Z\,\alpha)^j\,\mathcal{E}^{(j)}$ are of the order α^j. Here, we assume that $\mathcal{E}^{(i)}$ are real and neglect the radiative decay, which induces imaginary corrections to energies. This effect should be taken into account separately if needed. Furthermore, we will exclude from our consideration the vacuum polarization, which is either negligible or needs to be taken into account separately, depending on the masses of particles 1 and 2. If one of the particles is an electron, then the electron vacuum polarization starts at order α^7 for P-states and thus is not relevant for the present study. If both particles are heavier than the electron, then the electron vacuum polarization starts at order $\alpha\,(Z\,\alpha)^2$ for P-states and needs to be accounted for separately, as was done for muonic atoms in Ref. [6]. The vacuum polarization with heavier particles in the loop (muons, hadrons) starts at order α^7 for P-states and is negligible for the present study.

Regarding expansion in α, the g-factor of a particle a defined as

$$\vec{\mu}_a = \frac{e_a\,g_a}{2\,m_a}\,\vec{s}_a, \tag{2}$$

where $\vec{\mu}$ is the magnetic moment, is obtained from experiments. In consequence, the g_a factors are not expanded in α. As a digression we note that this definition in Eq. (2) differs from the convention sometimes used in the literature. Specifically, the electron g-factor is positive, $g = 2 + O(\alpha)$, and differs by the sign from the definition of Ref. [1]. Returning to Eq. (1), the first term of the expansion in α is just

$$E^{(0)} = m_1 + m_2. \tag{3}$$

The next term, $E^{(2)}$, is the eigenvalue of the nonrelativistic two-body Hamiltonian $H_0 \equiv H^{(2)}$ in the center-of-mass frame,

$$H_0 = \frac{p^2}{2\,\mu} + \frac{e_1\,e_2}{4\,\pi}\,\frac{1}{r}, \tag{4}$$

where $\vec{p} = \vec{p}_1 = -\vec{p}_2$, $\vec{r} = \vec{r}_1 - \vec{r}_2$, and $\mu = m_1\,m_2/(m_1 + m_2)$ is the reduced mass. If we set $e_1 = -e, e_2 = Z\,e$, the nonrelativistic binding energy becomes

$$E^{(2)} \equiv E_0 = -\frac{(Z\,\alpha)^2\,\mu}{2\,n^2}, \tag{5}$$

where n is the principal quantum number of the reference state. The next expansion coefficient, $E^{(4)}$, is the leading relativistic correction. It is given by the expectation value of the Breit Hamiltonian $H^{(4)}$ [7] with the nonrelativistic

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wave function, $E^{(4)} = \langle H^{(4)} \rangle$,

$$H^{(4)} = -\frac{\vec{p}^{\,4}}{8\,m_1^3} - \frac{\vec{p}^{\,4}}{8\,m_2^3} + \frac{e_1\,e_2}{4\,\pi}\left\{\frac{1}{2\,m_1\,m_2}\,p^i\left(\frac{\delta^{ij}}{r} + \frac{r^i\,r^j}{r^3}\right)p^j + \frac{g_1\,g_2}{4\,m_1\,m_2}\,\frac{s_1^i\,s_2^j}{r^3}\left(\delta^{ij} - 3\,\frac{r^i\,r^j}{r^2}\right) - \frac{\vec{r}\times\vec{p}}{2\,r^3}\cdot\left[\frac{g_1}{m_1\,m_2}\,\vec{s}_1 + \frac{g_2}{m_1\,m_2}\,\vec{s}_2 + \frac{(g_2-1)}{m_2^2}\,\vec{s}_2 + \frac{(g_1-1)}{m_1^2}\,\vec{s}_1\right]\right\}, \tag{6}$$

where we assume that the orbital angular-momentum quantum number l of the reference state is positive, $l > 0$, and the spin s of the constituent particles is 0 or 1/2. Let us note that Hamiltonian (6) does not account for any annihilation effects, which are present, e.g., in positronium. It also does not include any strong-interaction effects, which are present for hadronic particles. Such effects, if present, should be evaluated and accounted for separately. The result for the leading relativistic correction $E^{(4)}$ for a state with the principal quantum number n and the orbital angular momentum $l = 1$ is

$$E^{(4)} = \mu^3 (Z\alpha)^4\left\{\frac{1}{8\,n^4}\left(\frac{3}{\mu^2} - \frac{1}{m_1\,m_2}\right) + \frac{1}{6\,n^3}\left[-\frac{2}{\mu^2} + \vec{L}\cdot\vec{s}_1\left(\frac{g_1-1}{m_1^2} + \frac{g_1}{m_1\,m_2}\right) + \vec{L}\cdot\vec{s}_2\left(\frac{g_2-1}{m_2^2} + \frac{g_2}{m_1\,m_2}\right) - \frac{3\,g_1\,g_2}{5\,m_1 m_2} s_1^i s_2^j (L^i L^j)^{(2)}\right]\right\}, \tag{7}$$

where the symmetric traceless tensor $(L^i L^j)^{(2)}$ is defined as

$$(L^i L^j)^{(2)} = \frac{1}{2}(L^i L^j + L^j L^i) - \frac{\delta^{ij}}{3}\vec{L}^2. \tag{8}$$

The QED correction of order α^5 is denoted by $E^{(5)}$ and given by (for states with $l > 0$) [8]

$$E^{(5)} = -\frac{14\,(Z\,\alpha)^2}{3\,m_1\,m_2}\left\langle\frac{1}{4\,\pi}\,\frac{1}{r^3}\right\rangle - \frac{2\,\alpha}{3\,\pi}\left(\frac{1}{m_1} + \frac{Z}{m_2}\right)^2\left\langle\vec{p}\,(H_0 - E_0)\,\ln\left[\frac{2\,(H_0 - E_0)}{\mu(Z\,\alpha)^2}\right]\vec{p}\right\rangle. \tag{9}$$

The matrix element in the second term is related to the so-called Bethe logarithm $\ln[k_0(n, l)]$ by

$$\ln[k_0(n, l)] \equiv \frac{n^3}{2\mu^3 (Z\alpha)^4}\left\langle\phi\middle|\vec{p}\,(H_0 - E_0)\ln\left[\frac{2(H_0 - E_0)}{\mu(Z\alpha)^2}\right]\vec{p}\middle|\phi\right\rangle, \tag{10}$$

which is tabulated for many hydrogenic states in Ref. [9]. The final result for $E^{(5)}$ for states with $l > 0$ is [10]

$$E^{(5)} = -\frac{7}{3\pi}\,\frac{(Z\alpha)^5\mu^3}{m_1 m_2}\,\frac{1}{l(l+1)(2l+1)\,n^3} - \frac{4}{3\pi}\left(\frac{1}{m_1} + \frac{Z}{m_2}\right)^2\frac{\alpha(Z\alpha)^4\mu^3}{n^3}\,\ln[k_0(n, l)]. \tag{11}$$

$E^{(5)}$ is the complete α^5 QED correction, provided that the previous-order correction $E^{(4)}$ is calculated with the physical values of g-factors.

II. NONRELATIVISTIC QED HAMILTONIAN FOR THE α^6 CORRECTION

The correction to energy of order α^6 can be represented as

$$E^{(6)} = \langle H^{(6)} \rangle + \langle H^{(4)}\,\frac{1}{(E_0 - H_0)'}\,H^{(4)} \rangle, \tag{12}$$

where the prime in $1/(E_0 - H_0)'$ means the exclusion of the reference state from the resolvent, and $H^{(4)}$ is the Breit-Pauli Hamiltonian given by Eq. (6). The effective Hamiltonian $H^{(6)}$ can be derived within the framework of nonrelativistic QED (NRQED) [11]. The starting point of the derivation is the NRQED Hamiltonian for an arbitrary-spin ($s = 0, 1/2$) particle, given by [12]

$$\begin{aligned}
H = {} & eA_0 + \frac{\vec{\pi}^{\,2}}{2m} - \frac{e\,g}{2\,m}\,\vec{s}\cdot\vec{B} - \frac{e\,(g-1)}{4\,m^2}\,\vec{s}\cdot(\vec{E}\times\vec{\pi} - \vec{\pi}\times\vec{E}) - \frac{e}{6}\left(r_E^2 + \frac{s\,(s+1)}{m^2}\right)\vec{\nabla}\vec{E} - \frac{e}{120}\,r_{EE}^4\nabla^2\vec{\nabla}\vec{E} \\
& - \frac{\vec{\pi}^{\,4}}{8\,m^3} + \frac{e}{8\,m^3}(2\,\{\vec{\pi}^{\,2}, \vec{s}\cdot\vec{B}\} + (g-2)\,\{\vec{\pi}\cdot\vec{B}, \vec{\pi}\cdot\vec{s}\}) - \frac{e}{12\,m}\left(g\,r_M^2 + \frac{3\,(g-2)}{4\,m^2}\right)\vec{s}\cdot\nabla^2\vec{B} \\
& + \frac{\vec{\pi}^{\,6}}{16\,m^5} + \frac{e\,(g-1/2)}{24\,m^4}\,s(s+1)\{\vec{\pi}^{\,2}, \vec{\nabla}\vec{E}\} + \frac{ie}{32m^4}\left(1 + \frac{s(s+1)}{3}\right)[\vec{\pi}^{\,2}, \vec{\pi}\,\vec{E} + \vec{E}\,\vec{\pi}] \\
& - \frac{e}{12\,m}\left[r_E^2 - \frac{g-2}{2\,m^2}\,s\,(s+1)\right]\{\vec{\pi}\,, \partial_t\vec{E} - \vec{\nabla}\times\vec{B}\} + \frac{e\,(g-1/2)}{16m^4}\,\vec{s}\,\{\vec{\pi}^{\,2}, \vec{E}\times\vec{\pi} - \vec{\pi}\times\vec{E}\} \\
& - \frac{e}{24\,m^2}\left(g\,r_M^2 - r_E^2 + \frac{3\,(g-2)}{4\,m^2}\right)\vec{s}\,(\nabla^2\vec{E}\times\vec{\pi} - \vec{\pi}\times\nabla^2\vec{E}) - \frac{e^2}{2}\left(\alpha_E - \frac{s\,(s+1)}{3\,m^2}\right)\vec{E}^{\,2},
\end{aligned} \tag{13}$$

where $[X, Y] \equiv X\,Y - Y\,X$ denotes the commutator of two operators, and $\{X,\,Y\} \equiv X\,Y + Y\,X$ is the anticommutator, $\vec{\pi} = \vec{p} - e\,\vec{A}$. In comparison to the original work [12] we have redefined the following constants:

$$\alpha_E|_{\rm old} = \alpha_E - \frac{s\,(s+1)}{3\,m^2}, \tag{14}$$

$$r_E^2|_{\rm old} = r_E^2 + \frac{s\,(s+1)}{m^2}, \tag{15}$$

$$r_M^2|_{\rm old} = \frac{g}{2}\left(r_M^2 + \frac{3}{4\,m^2}\right), \tag{16}$$

to bring them in accordance with the standard definitions of the electric dipole polarizability $e^2\,\alpha_E$, the mean square charge radius $r_E^2 \equiv \langle r^2\rangle$, and the mean square magnetic radius r_M^2. Furthermore, $r_{EE}^4 \equiv \langle r^4\rangle$ is the mean fourth power of the charge radius. For the point (scalar or Dirac) particle the parameters are given by

$$r_E^2 = r_{EE}^4 = r_M^2 = \alpha_E = g - 2 = 0, \tag{17}$$

whereas for a Dirac particle with the magnetic moment anomaly κ, they are

$$g = 2\,(1+\kappa),\;\; r_E^2 = \frac{3\,\kappa}{2\,m^2}, \tag{18}$$

$$r_M^2 = r_{EE}^4 = 0,\;\; \alpha_E = -\frac{\kappa\,(1+\kappa)}{4\,m^3}. \tag{19}$$

For extended-size particles, the parameters r_E, r_M, and α_E can be in general arbitrary, but we will assume that r_E and r_M are significantly smaller than the electron Compton wavelength.

III. DERIVATION OF $H^{(6)}$

Using the NRQED Hamiltonian in Eq. (13), one can derive the effective operator $H^{(6)}$ for the bound system of two spinless particles, one spinless and one spin-1/2 particle, and two spin-1/2 particles. The derivation follows Ref. [10], which in turn is based on two former works [11,13] and extends the previous calculations of $H^{(6)}$ to states with $l = 1$, where contact terms contribute. As we will show below, the contact terms have previously been accounted for incorrectly for the positronium *P*-states [13–15].

The typical one-photon exchange contribution between particles a and b is given by

$$\begin{aligned}\langle\phi|\Sigma(E_0)|\phi\rangle = e_a\,e_b \int \frac{d^4k}{(2\,\pi)^4\,i}\,G_{\mu\nu}(k)\,\bigg\{\bigg\langle\phi\bigg|\,j_a^\mu(k)\,e^{i\,\vec{k}\cdot\vec{r}_a}\\ \times\,\frac{1}{E_0 - H_0 - k_0 + i\,\epsilon}\,j_b^\nu(-k)\,e^{-i\,\vec{k}\cdot\vec{r}_b}\,\bigg|\phi\bigg\rangle\\ +\bigg\langle\phi\bigg|\,j_b^\mu(k)\,e^{i\,\vec{k}\cdot\vec{r}_b}\,\frac{1}{E_0 - H_0 - k_0 + i\,\epsilon}\,j_a^\nu(-k)\\ \times\,e^{-i\,\vec{k}\cdot\vec{r}_a}\,\bigg|\phi\bigg\rangle\bigg\},\end{aligned} \tag{20}$$

where $G_{\mu\nu}(k)$ is the photon propagator, which is in Feynman gauge $G^F_{\mu\nu} = g_{\mu\nu}/k^2$, in Coulomb gauge

$$G^C_{\mu\nu}(k) = \begin{cases} -\frac{1}{\vec{k}^2} & \mu=\nu=0,\\ \frac{-1}{k_0^2-\vec{k}^2+i\,\epsilon}\left(\delta_{ij} - \frac{k_ik_j}{\vec{k}^2}\right) & \mu=i,\;\nu=j,\end{cases} \tag{21}$$

and in temporal gauge

$$G^A_{\mu\nu}(k) = \begin{cases} 0 & \mu=\nu=0,\\ \frac{-1}{k_0^2-\vec{k}^2+i\,\epsilon}\left(\delta_{ij} - \frac{k_ik_j}{k_0^2}\right) & \mu=i,\;\nu=j.\end{cases} \tag{22}$$

The state ϕ in Eq. (20) is an eigenstate of H_0, and j_a^μ is the electromagnetic current operator for particle a. The explicit expression for $j^\mu(k)$ is obtained from the NRQED Hamiltonian in Eq. (13) as the coefficient multiplying the polarization vector ϵ^μ of the electromagnetic potential

$$A^\mu(\vec{r},t) \sim \epsilon^\mu_\lambda\,e^{i\,\vec{k}\cdot\vec{r} - i\,k_0\,t}. \tag{23}$$

The first terms of the nonrelativistic expansion of the j^0 component are

$$\begin{aligned} j^0(k) = 1 + \frac{i\,(g-1)}{2\,m}\,\vec{s}\cdot\vec{k}\times\vec{p}\\ - \frac{1}{6}\left(r_E^2 + \frac{s\,(s+1)}{m^2}\right)\vec{k}^2 + \cdots\end{aligned} \tag{24}$$

and those of the $\vec{j}$ component are

$$\vec{j}(k) = \frac{\vec{p}}{m} + \frac{i\,g}{2\,m}\,\vec{s}\times\vec{k} + \cdots. \tag{25}$$

Most of the calculation is performed in the Coulomb gauge in the so-called nonretardation approximation, in which one sets $k_0 = 0$ in the photon propagator $G_{\mu\nu}(k)$ and in $j(k)$. The retardation corrections are considered separately. Applying the nonretardation approximation and symmetrizing $k_0 \leftrightarrow -k_0$, the k_0 integral in Eq. (20) is evaluated as

$$\frac{1}{2}\int\frac{d\,k_0}{2\,\pi\,i}\left[\frac{1}{-\Delta E - k_0 + i\,\epsilon} + \frac{1}{-\Delta E + k_0 + i\,\epsilon}\right] = -\frac{1}{2}, \tag{26}$$

where we have assumed that ΔE is positive, which is the case when ϕ is the ground state. For excited states, the integration contour is deformed in such a way that all poles from the electron propagator lie on the same side. Therefore, the result of the k_0 integration for excited states is the same as for the ground state, yielding

$$\begin{aligned}\langle\phi|\Sigma(E_0)|\phi\rangle = -e^2\int\frac{d^3k}{(2\,\pi)^3}\,G_{\mu\nu}(\vec{k})\\ \times\,\big\langle\phi\big|\,j_a^\mu(\vec{k})\,e^{i\,\vec{k}\cdot(\vec{r}_a-\vec{r}_b)}\,j_b^\nu(-\vec{k})\,\big|\phi\big\rangle.\end{aligned} \tag{27}$$

The $\vec{k}$ integral is the Fourier transform of the photon propagator in the nonretardation approximation

$$\begin{aligned} G_{\mu\nu}(\vec{r}) &= \int\frac{d^3k}{(2\,\pi)^3}\,G_{\mu\nu}(\vec{k})\,e^{i\,\vec{k}\cdot\vec{r}}\\ &= \frac{1}{4\,\pi}\begin{cases} -\frac{1}{r} & \mu=\nu=0,\\ \frac{1}{2\,r}\left(\delta_{ij} + \frac{r_ir_j}{\vec{r}^2}\right) & \mu=i,\;\nu=j.\end{cases}\end{aligned} \tag{28}$$

One easily recognizes that G_{00} is the Coulomb interaction. Next-order terms resulting from j^0 and $\vec{j}$ lead to the Breit Pauli-Hamiltonian, Eq. (6). Below we derive the higher-order terms in the nonrelativistic expansion, namely, the effective

Hamiltonian $H^{(6)}$. It is expressed as a sum of various contributions

$$H^{(6)} = \sum_{i=0,9} \delta H_i. \tag{29}$$

We will follow a similar derivation presented in Refs. [10,11,13] for point particles, and use similar notations, namely, $\vec{r} = \vec{r}_1 - \vec{r}_2$, $e_1 = -e$, $e_2 = Z\,e$, and the static fields $\mathcal{A}^0$, $\vec{\mathcal{A}}$, and $\vec{\mathcal{E}}$ defined as

$$e_1\,\mathcal{A}_1^0 = e_2\,\mathcal{A}_2^0 = -\frac{Z\,\alpha}{r}, \tag{30}$$

$$e_1\mathcal{A}_1^i = -\frac{Z\alpha}{2\,r}\left(\delta^{ij} + \frac{r^i r^j}{r^2}\right)\frac{p_2^j}{m_2} - \frac{Z\,\alpha\,g_2}{2\,m_2}\frac{(\vec{s}_2\times\vec{r})^i}{r^3}, \tag{31}$$

$$e_2\mathcal{A}_2^i = -\frac{Z\alpha}{2\,r}\left(\delta^{ij} + \frac{r^i r^j}{r^2}\right)\frac{p_1^j}{m_1} + \frac{Z\,\alpha\,g_1}{2\,m_1}\frac{(\vec{s}_1\times\vec{r})^i}{r^3}, \tag{32}$$

$$e_1\,\vec{\mathcal{E}}_1 = -Z\,\alpha\,\frac{\vec{r}}{r^3}, \quad e_2\,\vec{\mathcal{E}}_2 = Z\,\alpha\,\frac{\vec{r}}{r^3}. \tag{33}$$

We now examine the individual contributions $\delta E_i \equiv \langle\delta H_i\rangle$. δE_0 is a correction to the kinetic energy,

$$\delta E_0 = \left\langle\frac{p^6}{16\,m_1^5} + \frac{p^6}{16\,m_2^5}\right\rangle. \tag{34}$$

δE_1 is a correction to the Coulomb interaction, where one of the particles interacts by δH,

$$\delta H = -\frac{e}{120}\,r_{EE}^4\,\nabla^2\vec{\nabla}\vec{E} + \frac{e\,(g-1/2)}{24\,m^4}\,s(s+1)\{\vec{\pi}^{\,2},\vec{\nabla}\vec{E}\} + \frac{ie}{32m^4}\left(1+\frac{s(s+1)}{3}\right)[\vec{\pi}^{\,2},\vec{\pi}\,\vec{E}+\vec{E}\,\vec{\pi}]$$
$$+\frac{e\,(g-1/2)}{16m^4}\,\vec{s}\,\{\vec{\pi}^{\,2},\vec{E}\times\vec{\pi}-\vec{\pi}\times\vec{E}\} - \frac{e}{24\,m^2}\left(g\,r_M^2 - r_E^2 + \frac{3\,(g-2)}{4\,m^2}\right)\vec{s}\,(\nabla^2\vec{E}\times\vec{\pi}-\vec{\pi}\times\nabla^2\vec{E}), \tag{35}$$

and the other one by $e\,A^0$. Here, we can use the static Coulomb approximation, obtaining

$$\delta E_1 = \sum_a\left\langle -\frac{Z\,\alpha}{8\,m_a^4}\left(g_a-\frac{1}{2}\right)\vec{L}\cdot\vec{s}_a\left\{p^2,\frac{1}{r^3}\right\} + \frac{1}{32m_a^4}\left(1+\frac{s_a(s_a+1)}{3}\right)\left[p^2,\left[p^2,-\frac{Z\,\alpha}{r}\right]\right]\right.$$
$$\left.+\frac{Z\alpha}{120}\,r_{EEa}^4\,4\pi\,\nabla^2\delta^3(r) + i\,\frac{Z\alpha}{12\,m_a^2}\left(g_a\,r_{Ma}^2 - r_{Ea}^2 + \frac{3\,(g_a-2)}{4\,m_a^2}\right)\vec{s}_a\cdot\vec{p}\times 4\pi\,\delta^3(r)\,\vec{p}\right\rangle, \tag{36}$$

where the second term in Eq. (35) vanishes for the $l = 1$ state. δE_2 is a correction to Coulomb interaction when both vertices are

$$\delta H = -\frac{e\,(g-1)}{4m^2}\,\vec{s}\cdot(\vec{E}\times\vec{\pi}-\vec{\pi}\times\vec{E}) - \frac{e}{6}\left(r_E^2+\frac{s\,(s+1)}{m^2}\right)\vec{\nabla}\vec{E}. \tag{37}$$

It can also be evaluated in the nonretardation approximation, with the result

$$\delta E_2 = \left\langle\frac{Z\alpha}{4\,m_1^2 m_2^2}(g_1-1)(g_2-1)\,(\vec{s}_2\times\vec{p})^i\left(\frac{\delta^{ij}}{r^3} - 3\frac{r^i r^j}{r^5} + \frac{\delta^{ij}}{3}\,4\,\pi\,\delta^3(r)\right)(\vec{s}_1\times\vec{p})^j\right.$$
$$+\frac{Z\alpha}{36}\left(r_{E1}^2+\frac{s_1\,(s_1+1)}{m_1^2}\right)\left(r_{E2}^2+\frac{s_2\,(s_2+1)}{m_2^2}\right)4\pi\,\nabla^2\,\delta^3(r)$$
$$\left.+i\frac{Z\alpha}{12}\left[\left(r_{E1}^2+\frac{s_1\,(s_1+1)}{m_1^2}\right)\frac{(g_2-1)}{m_2^2}\vec{s}_2 + \left(r_{E2}^2+\frac{s_2\,(s_2+1)}{m_2^2}\right)\frac{(g_1-1)}{m_1^2}\vec{s}_1\right]\cdot\vec{p}\times 4\pi\delta^3(r)\,\vec{p}\right\rangle. \tag{38}$$

δE_3 is the relativistic correction to the transverse photon exchange. The first particle is coupled to $\vec{A}$ by the nonrelativistic term

$$\delta H = -\frac{e}{m}\,\vec{p}\cdot\vec{A} - \frac{e\,g}{2\,m}\,\vec{s}\cdot\vec{B}, \tag{39}$$

and the second one by the relativistic correction

$$\delta H = \frac{e}{8\,m^3}[(g-2)\,\{\vec{\pi}\cdot\vec{B},\vec{\pi}\cdot\vec{s}\} + 2\,\{\vec{\pi}^{\,2},\vec{s}\cdot\vec{B}\}] - \frac{e}{12\,m}\left(g\,r_M^2 + \frac{3\,(g-2)}{4\,m^2}\right)\vec{s}\cdot\nabla^2\vec{B} - \frac{\vec{\pi}^{\,4}}{8\,m^3}. \tag{40}$$

It is sufficient to calculate it in the nonretardation approximation, which yields

$$\delta E_3 = \sum_a\left\langle\frac{1}{4\,m_a^3}(\{p^2,\,\vec{s}_a\cdot\vec{\nabla}_a\times e_a\vec{\mathcal{A}}_a\} + \{p^2,\,\vec{p}_a\cdot e_a\vec{\mathcal{A}}_a\}) + \frac{e_a\,(g_a-2)}{8\,m_a^3}\{\vec{p}_a\cdot\vec{\nabla}_a\times\vec{\mathcal{A}}_a,\vec{p}_a\cdot\vec{s}_a\}\right\rangle$$
$$+\left\langle\frac{Z\alpha}{12\,m_1\,m_2}\left(g_1\,r_{M1}^2+\frac{3\,(g_1-2)}{4\,m_1^2}\right)[i\,\vec{s}_1\cdot\vec{p}\times 4\pi\,\delta^3(r)\,\vec{p} + g_2\,\vec{s}_2\times\vec{p}\,4\pi\,\delta^3(r)\vec{s}_1\times\vec{p}] + (1\leftrightarrow 2)\right\rangle. \tag{41}$$

δE_4 comes from the seagull-like coupling

$$\delta H = \frac{e^2}{2\,m}\,\vec{A}^{\,2}. \tag{42}$$

Again, the nonretardation approximation yields

$$\delta E_4 = \sum_a \left\langle \frac{e_a^2}{2\,m_a}\,\vec{\mathcal{A}}_a^2 \right\rangle. \tag{43}$$

δE_5 is a seagull-like term that comes from the coupling

$$\delta H = -\frac{e^2}{2}\left(\alpha_E - \frac{s\,(s+1)}{3\,m^2}\right)\vec{E}^{\,2}, \tag{44}$$

while the second particle is coupled through $e\,A^0$. It can be obtained in the nonretardation approximation as

$$\delta E_5 = -\frac{1}{2}\sum_a \left(\alpha_{Ea} - \frac{s_a(s_a+1)}{3\,m_a^3}\right)\left\langle \frac{Z^2\alpha^2}{r^4}\right\rangle. \tag{45}$$

δE_6 is a seagull-like term that comes from

$$\delta H = -\frac{e\,(g-1)}{4\,m^2}\,\vec{s}\cdot(\vec{E}\times\vec{\pi} - \vec{\pi}\times\vec{E}). \tag{46}$$

Once more the nonretardation approximation can be used, yielding

$$\delta E_6 = \sum_a \frac{e_a^2\,(g_a-1)}{2\,m_a^2}\left\langle \vec{s}_a\cdot\vec{\mathcal{E}}_a\times\vec{\mathcal{A}}_a\right\rangle. \tag{47}$$

δE_7 is a retardation correction to the single transverse exchange

$$\delta E_7 = \delta E_7^A + \delta E_7^B + \delta E_7^C, \tag{48}$$

where

$$\begin{aligned}\delta E_7^A = \frac{Z\alpha}{16\,m_1\,m_2}\bigg\langle &\frac{2Z^2\alpha^2}{r^3} + \frac{iZ\alpha r^i}{r^3}\left[\frac{p^2}{2\,m_2}, \frac{r^i r^j - 3\delta^{ij}\,r^2}{r}\right]p^j \\ &- p^i\left[\frac{r^i r^j - 3\delta^{ij}\,r^2}{r}, \frac{p^2}{2\,m_1}\right]\frac{iZ\alpha r^j}{r^3} \\ &- p^i\left[\frac{p^2}{2\,m_2}, \left[\frac{r^i r^j - 3\delta^{ij}\,r^2}{r}, \frac{p^2}{2\,m_1}\right]\right]p^j\bigg\rangle + (1\leftrightarrow 2),\end{aligned} \tag{49}$$

$$\begin{aligned}\delta E_7^B = \frac{Z\alpha}{8\,m_1\,m_2}\bigg\langle &g_1\left[\left(\vec{s}_1\times\frac{\vec{r}}{r}\right)^i, \frac{p^2}{2\,m_1}\right]\frac{iZ\alpha r^i}{r^3} \\ &- g_2\,\frac{iZ\alpha r^i}{r^3}\left[\frac{p^2}{2\,m_2}, \left(\vec{s}_2\times\frac{\vec{r}}{r}\right)^i\right] \\ &+ g_1\left[\frac{p^2}{2\,m_2}, \left[\left(\vec{s}_1\times\frac{\vec{r}}{r}\right)^i, \frac{p^2}{2\,m_1}\right]\right]p^i \\ &+ g_2\,p^i\left[\frac{p^2}{2\,m_2}, \left[\left(\vec{s}_2\times\frac{\vec{r}}{r}\right)^i, \frac{p^2}{2\,m_1}\right]\right]\bigg\rangle + (1\leftrightarrow 2),\end{aligned} \tag{50}$$

$$\begin{aligned}\delta E_7^C = -\frac{Z\,\alpha\,g_1\,g_2}{16\,m_1^2\,m_2^2}\bigg\langle\bigg[p^2, \bigg[p^2, &\,\vec{s}_1\vec{s}_2\,\frac{2}{3\,r} \\ &+ s_1^i\,s_2^j\,\frac{1}{2\,r}\left(\frac{r^i r^j}{r^2} - \frac{\delta^{ij}}{3}\right)\bigg]\bigg]\bigg\rangle.\end{aligned} \tag{51}$$

δE_8 is a retardation correction in a single transverse photon exchange, where one vertex is nonrelativistic, Eq. (39), and the second one is

$$\delta H = -\frac{e\,(g-1)}{4\,m^2}\,\vec{s}\cdot(\vec{E}\times\vec{p} - \vec{p}\times\vec{E}). \tag{52}$$

The result is

$$\begin{aligned}\delta E_8 = \sum_a\bigg\langle &\frac{e_a^2\,(g_a-1)}{2\,m_a^2}\,\vec{s}_a\cdot\vec{\mathcal{E}}_a\times\vec{\mathcal{A}}_a + \frac{ie_a\,(g_a-1)}{8\,m_a^3} \\ &\times\left[\vec{\mathcal{A}}_a\cdot(\vec{p}_a\times\vec{s}_a) + (\vec{p}_a\times\vec{s}_a)\cdot\vec{\mathcal{A}}_a, p_a^2\right]\bigg\rangle.\end{aligned} \tag{53}$$

The δE_9 contribution arises when one vertex is

$$\delta H = -\frac{e}{12\,m}\left[r_E^2 - \frac{g-2}{2\,m^2}\,s\,(s+1)\right]\{\vec{\pi}, \partial_t\vec{E} - \vec{\nabla}\times\vec{B}\}, \tag{54}$$

and the second vertex is nonrelativistic, Eq. (39). The corresponding current operators are

$$\vec{j}(k) = \frac{\vec{p}}{m} + \frac{g}{2\,m}\,i\,\vec{s}\times\vec{k}, \tag{55}$$

$$\delta\,j^j(k) = \frac{1}{6\,m}\left[r_E^2 - \frac{g-2}{2\,m^2}\,s\,(s+1)\right]p^i\,[(\omega^2 - \vec{k}^2)\delta^{ij} + k^i\,k^j]. \tag{56}$$

For this term we employ the temporal gauge, rather than the Coulomb gauge, and obtain

$$\begin{aligned}\delta E_9 = -e_1 e_2\int\frac{d^3k}{(2\,\pi)^3}&\left\langle\frac{1}{4}\left\{j_1^i(k), \left\{G_A^{ij}\,\delta\,j_2^j(-k), e^{i\,\vec{k}\cdot\vec{r}}\right\}\right\}\right\rangle \\ &+ (1\leftrightarrow 2),\end{aligned} \tag{57}$$

where

$$G_A^{ij}\,\delta\,j^j(k) = -\frac{1}{6\,m}\left[r_E^2 - \frac{g-2}{2\,m^2}\,s\,(s+1)\right]p^i. \tag{58}$$

The result is

$$\begin{aligned}\delta E_9 &= \frac{e_1\,e_2}{6\,m}\left[r_{E2}^2 - \frac{g_2-2}{2\,m_2^2}\,s_2\,(s_2+1)\right]\left\langle\frac{1}{4}\left\{\frac{p_1^i}{m_1}, \left\{\frac{p_2^i}{m_2}, \delta^3(r)\right\}\right\} + \frac{g_1}{4\,m_1}\,(\vec{s}_1\times\vec{\nabla}_1)^i\left\{\frac{p_2^i}{m_2}, \delta^3(r)\right\}\right\rangle + (1\leftrightarrow 2) \\ &= \frac{Z\,\alpha}{12\,m_1\,m_2}\left[r_{E2}^2 - \frac{g_2-2}{2\,m_2^2}\,s_2\,(s_2+1)\right]\left\langle 2\,\pi\,\vec{\nabla}^2\delta^3(r) + i\,g_1\,\vec{s}_1\cdot\vec{p}\times 4\,\pi\,\delta^3(r)\,\vec{p}\right\rangle + (1\leftrightarrow 2).\end{aligned} \tag{59}$$

This concludes our derivation of all effective operators to order α^6 for P-states. Explicit formulas for matrix elements of elementary and contact operators are presented in Appendix A. Matrix elements of other operators can be found in Ref. [10]. We mention here that the original work of Khriplovich [16,17] contained a computational mistake related to a matrix element in δE_2, which was not corrected in subsequent works [14,15]. This will be described in more detail in Sec. VI.

The last part of $E^{(6)}$ to be evaluated is the second-order iteration of the Breit Hamiltonian $H^{(4)}$ in Eq. (12). It has already been derived for arbitrary $l > 0$ in Ref. [10] by the method developed in Ref. [13], and the result is valid also for the case $l = 1$ investigated here. Since the derivation and the final expressions are quite long, we refer the reader to Ref. [10] for the corresponding formulas.

Adding together all contributions, we arrive at our final result for the α^6 correction for nP states. It is written as

$$E^{(6)} = (Z\,\alpha)^6\,\mathcal{E}^{(6)},$$

$$\mathcal{E}^{(6)} = \mathcal{E}_{NS} + \vec{s}_1\cdot\vec{s}_2\,\mathcal{E}_{SS} + \vec{L}\cdot\vec{s}_1\,\mathcal{E}_{L1} + \vec{L}\cdot\vec{s}_2\,\mathcal{E}_{L2} + (L^i\,L^j)^{(2)}\,s_1^i\,s_2^j\,\mathcal{E}_{LL}, \tag{60}$$

where

$$\mathcal{E}_{NS} = \mathcal{E}_{S0} + \tfrac{4}{3}\,s_1\,(s_1+1)\,\mathcal{E}_{S1} + \tfrac{4}{3}\,s_2\,(s_2+1)\,\mathcal{E}_{S2} + \tfrac{16}{9}\,s_1\,(s_1+1)\,s_2\,(s_2+2)\,\mathcal{E}_{S12}, \tag{61}$$

$$\mathcal{E}_{L1} = \mathcal{E}_{LN1} + \tfrac{4}{3}\,s_2(s_2+1)\,\mathcal{E}_{LS1}, \tag{62}$$

$$\mathcal{E}_{L2} = \mathcal{E}_{LN2} + \tfrac{4}{3}\,s_1\,(s_1+1)\,\mathcal{E}_{LS2}, \tag{63}$$

with the individual terms given by

$$\mathcal{E}_{S0} = \mu\left(-\frac{5}{16\,n^6}+\frac{1}{2\,n^5}-\frac{1}{6\,n^4}-\frac{1}{27\,n^3}\right)+\frac{\mu^3}{m_1\,m_2}\left(\frac{3}{16\,n^6}-\frac{13}{30\,n^5}+\frac{2}{5\,n^3}\right)-\frac{\mu^5}{m_1^2\,m_2^2}\,\frac{1}{16\,n^6} + \mu^5\left(\frac{1}{n^3}-\frac{1}{n^5}\right)\left(\frac{2}{27}\,r_{E1}^2\,r_{E2}^2+\frac{r_{E1}^2+r_{E2}^2}{9\,m_1\,m_2}+\frac{r_{EE1}^4+r_{EE2}^4}{45}\right)-\mu^4\,\frac{\alpha_{E1}+\alpha_{E2}}{5}\left(\frac{1}{n^3}-\frac{2}{3\,n^5}\right), \tag{64}$$

$$\mathcal{E}_{S2} = \frac{\mu^3}{m_2^2}\,\frac{g_2^2}{24}\left(\frac{1}{5\,n^5}-\frac{1}{2\,n^4}-\frac{119}{180\,n^3}\right)+\frac{\mu^5}{m_2^4}\left[\frac{g_2}{24}\left(\frac{1}{n^3}-\frac{1}{n^5}\right)+\frac{7}{60\,n^5}-\frac{1}{48\,n^4}-\frac{641}{4320\,n^3}\right] + \frac{\mu^4}{m_2^3}\left[-\frac{g_2^2}{40}\left(\frac{1}{n^3}-\frac{2}{3\,n^5}\right)+\frac{g_2}{24}\left(-\frac{1}{5\,n^5}+\frac{1}{n^4}+\frac{137}{90\,n^3}\right)-\frac{7}{60\,n^5}+\frac{2}{15\,n^3}\right]+\frac{\mu^5}{m_2^2}\,\frac{r_{E1}^2}{18}\left(\frac{1}{n^3}-\frac{1}{n^5}\right), \tag{65}$$

$$\mathcal{E}_{S12} = \frac{\mu^5}{m_1^2\,m_2^2}\left[-\left(\frac{1}{n^4}+\frac{137}{90\,n^3}\right)\frac{g_1^2\,g_2^2}{640}+\frac{1}{24}\left(\frac{1}{n^3}-\frac{1}{n^5}\right)\right], \tag{66}$$

$$\mathcal{E}_{LN2} = \frac{\mu^2}{m_2}\,g_2\left(-\frac{1}{3\,n^5}+\frac{1}{6\,n^4}+\frac{13}{108\,n^3}\right)+\frac{\mu^3}{m_2^2}\left[g_2^2\left(-\frac{1}{40\,n^5}+\frac{1}{48\,n^4}+\frac{227}{4320\,n^3}\right)+g_2\left(\frac{3}{10\,n^5}-\frac{1}{5\,n^3}\right) + \frac{5}{12\,n^5}-\frac{1}{6\,n^4}-\frac{13}{108\,n^3}\right]+\frac{\mu^4}{m_2^3}\left[g_2\left(-\frac{1}{6\,n^5}-\frac{1}{24\,n^4}+\frac{5}{432\,n^3}\right)-\frac{5}{12\,n^5}+\frac{1}{6\,n^3}\right] + \frac{\mu^5}{m_2^4}\left[\frac{1}{4\,n^5}+\frac{1}{48\,n^4}-\frac{41}{864\,n^3}\right]+\frac{1}{9}\left(\frac{1}{n^3}-\frac{1}{n^5}\right)\left[\left(-\frac{\mu^4}{m_2}\,g_2+\frac{\mu^5}{m_2^2}\right)r_{E1}^2+\frac{\mu^5}{m_2^2}\,r_{E2}^2-\frac{\mu^4}{m_2}\,g_2\,r_{M2}^2\right], \tag{67}$$

$$\mathcal{E}_{LS2} = \frac{\mu^4}{m_1^2\,m_2}\,\frac{g_2}{12}\left[\frac{1}{n^5}-\frac{1}{n^3}-g_1\left(\frac{7}{20\,n^5}+\frac{1}{8\,n^4}-\frac{133}{720\,n^3}\right)+g_1^2\left(-\frac{3}{20\,n^5}+\frac{1}{8\,n^4}+\frac{227}{720\,n^3}\right)\right] + \frac{\mu^5}{m_1^2\,m_2^2}\,\frac{1}{12}\left[\frac{1}{n^3}-\frac{1}{n^5}+g_1\,g_2\left(\frac{7}{20\,n^5}+\frac{1}{8\,n^4}-\frac{133}{720\,n^3}\right)+g_1^2\,g_2^2\left(\frac{3}{80\,n^5}+\frac{9}{320\,n^4}-\frac{13}{3200\,n^3}\right)\right], \tag{68}$$

$$\mathcal{E}_{SS} = -\frac{\mu^3}{m_1\,m_2}\,g_1\,g_2\left(\frac{1}{60\,n^5}+\frac{1}{18\,n^4}+\frac{47}{1620\,n^3}\right)+\frac{\mu^4}{m_1\,m_2}\left(\frac{g_1}{m_2}+\frac{g_2}{m_1}\right)\left(\frac{1}{18\,n^5}+\frac{1}{18\,n^4}-\frac{5}{324\,n^3}\right) + \frac{\mu^5}{m_1^2\,m_2^2}\left[-\frac{g_1^2\,g_2^2}{480}\left(\frac{1}{n^4}+\frac{137}{90\,n^3}\right)+\frac{1}{30\,n^5}-\frac{1}{18\,n^4}-\frac{191}{1620\,n^3}\right]+\frac{2}{27}\left(\frac{1}{n^3}-\frac{1}{n^5}\right)\frac{\mu^5}{m_1\,m_2}\,g_1\,g_2\,(r_{M1}^2+r_{M2}^2), \tag{69}$$

$$\mathcal{E}_{LL} = \frac{\mu^3}{m_1\,m_2}\,\frac{g_1\,g_2}{4}\left(\frac{51}{50\,n^5} - \frac{7}{12\,n^4} - \frac{3697}{5400\,n^3}\right) + \frac{\mu^4}{m_1\,m_2}\left[\left(\frac{g_1}{m_1} + \frac{g_2}{m_2}\right) g_1\,g_2\left(\frac{9}{200\,n^5} - \frac{3}{80\,n^4} - \frac{227}{2400\,n^3}\right)\right.$$
$$\left. + \left(\frac{g_1}{m_2} + \frac{g_2}{m_1}\right)\left(-\frac{19}{150\,n^5} + \frac{1}{12\,n^4} + \frac{1171}{5400\,n^3}\right)\right] + \frac{\mu^5}{m_1^2\,m_2^2}\left[\frac{g_1^2\,g_2^2}{200}\left(-\frac{3}{n^5} - \frac{7}{8\,n^4} + \frac{1291}{720\,n^3}\right)\right.$$
$$\left. + g_1\,g_2\left(-\frac{6}{25\,n^5} - \frac{3}{40\,n^4} + \frac{37}{1200\,n^3}\right) - \frac{g_1+g_2}{10}\left(\frac{1}{n^3} - \frac{1}{n^5}\right) + \frac{2}{25\,n^5} - \frac{1}{12\,n^4} - \frac{1063}{5400\,n^3}\right]$$
$$+ \frac{\mu^5}{m_1\,m_2}\,\frac{g_1\,g_2}{9}\left(\frac{1}{n^3} - \frac{1}{n^5}\right)\left(r_{M1}^2 + r_{M2}^2\right). \tag{70}$$

We remind the reader that $E^{(6)}$ is the complete α^6 QED correction, provided that the lower-order correction $E^{(4)}$ is calculated with the physical values of g-factors.

We now turn to the comparison of the obtained formulas for the $l = 1$ states with the general $l > 0$ result of Ref. [10] derived with the omission of contact terms. The contact terms vanish in the $l > 1$ case but are present for $l = 1$ (even for the point particles). We will consider separately the cases of two spinless particles, of one spinless and one spin-1/2 particle, and of two spin-1/2 particles.

IV. SPIN $s_1 = s_2 = 0$

For a system consisting of two spinless particles, $s_1 = s_2 = 0$, $\mathcal{E}^{(6)} = \mathcal{E}_{S0}$. This result differs from the general result $\mathcal{E}_G^{(6)}$ from Ref. [10] by the finite-size terms only, as it should,

$$\mathcal{E}^{(6)} - \mathcal{E}_G^{(6)}\big|_{l=1} = \frac{\mu^5}{9}\left(\frac{1}{n^3} - \frac{1}{n^5}\right)\left(\frac{2}{3}\,r_{E1}^2\,r_{E2}^2 + \frac{r_{E1}^2 + r_{E2}^2}{m_1\,m_2} + \frac{r_{EE1}^4 + r_{EE2}^4}{5}\right). \tag{71}$$

In the infinite-mass limit of one of the particles (and only in this limit), $\mathcal{E}^{(6)}$ corresponds to a solution of the Klein-Gordon equation. For an arbitrary mass ratio there is no fundamental equation and energy levels can be obtained only from the QED theory.

An example of a bound system of two scalar particles is the pionic helium atom investigated by Masaki Hori [18,19]. However, in this case the short-range interactions are dominated by strong forces, and the above formula thus has limited applicability.

V. SPIN $s_1 = 0, s_2 = 1/2$

For a system consisting of particles with $s_1 = 0$ and $s_2 = 1/2$, the binding energy at the order α^6 is

$$\mathcal{E}^{(6)} = \mathcal{E}_{S0} + \mathcal{E}_{S2} + \vec{L}\cdot\vec{s}_2\,\mathcal{E}_{LN2}. \tag{72}$$

The difference of $\mathcal{E}^{(6)}$ and the general result $\mathcal{E}_G$ from Ref. [10] is

$$\mathcal{E}^{(6)} - \mathcal{E}_G^{(6)}\big|_{l=1} = \left[\frac{r_{E1}^2 + \tilde{r}_{E2}^2}{m_1\,m_2} + \frac{2}{3}\,r_{E1}^2\left(r_{E2}^2 + \frac{3}{4\,m_2^2}\right) + \frac{r_{EE1}^4 + r_{EE2}^4}{5} + \vec{L}\cdot\vec{s}_2\left(-\frac{g_2\left(\tilde{r}_{M2}^2 + r_{E1}^2\right)}{m_1\,m_2} + \frac{r_{E2}^2 - g_2\,\tilde{r}_{M2}^2 - (g_2-1)\,r_{E1}^2}{m_2^2}\right)\right] \times \frac{\mu^5}{9}\left(\frac{1}{n^3} - \frac{1}{n^5}\right), \tag{73}$$

where

$$g\,\tilde{r}_M^2 = g\,r_M^2 + \frac{3\,(g-2)}{4\,m^2}, \tag{74}$$
$$\tilde{r}_E^2 = r_E^2 - \frac{3\,(g-2)}{8\,m^2}. \tag{75}$$

With the rotational angular momentum $l = 1$ coupled to the spin $s_2 = 1/2$, the total angular momentum J can be either $J = 1/2$ or $3/2$. The corresponding energies are

$$\mathcal{E}^{(6)}|_{J=1/2} = \mathcal{E}_{S0} + \mathcal{E}_{S2} - \mathcal{E}_{LN2}, \tag{76}$$
$$\mathcal{E}^{(6)}|_{J=3/2} = \mathcal{E}_{S0} + \mathcal{E}_{S2} + \tfrac{1}{2}\mathcal{E}_{LN2}. \tag{77}$$

The explicit formulas for $\mathcal{E}^{(6)}$ are quite long. However, their expansion for a small mass ratio m_2/m_1 is quite compact. Specifically, assuming that particle 2 is point-like ($\kappa_2 = r_{E2}^2 = r_{M2}^2 = r_{EE2}^4 = 0$) and neglecting the polarizabilities ($\alpha_{E1} = \alpha_{E2} = 0$), we obtain $\mathcal{E}^{(6)} = \mathcal{E}^{(6,0)} + \mathcal{E}^{(6,1)} + \cdots$,

$$\mathcal{E}^{(6,0)}|_{J=1/2} = m_2\left[\left(-\frac{5}{16\,n^6} + \frac{3}{4\,n^5} - \frac{3}{8\,n^4} - \frac{1}{8\,n^3}\right) + \frac{1}{6}\left(\frac{1}{n^3} - \frac{1}{n^5}\right) m_2^2\,r_{E1}^2 + \frac{1}{45}\left(\frac{1}{n^3} - \frac{1}{n^5}\right) m_2^4\,r_{EE1}^4\right], \tag{78}$$

$$\mathcal{E}^{(6,1)}|_{J=1/2} = \frac{m_2^2}{m_1}\left[\left(\frac{1}{2\,n^6} - \frac{19}{15\,n^5} + \frac{3}{8\,n^4} + \frac{21}{40\,n^3}\right) - \frac{1}{2}\left(\frac{1}{n^3} - \frac{1}{n^5}\right) m_2^2\,r_{E1}^2 - \frac{1}{9}\left(\frac{1}{n^3} - \frac{1}{n^5}\right) m_2^4\,r_{EE1}^4\right], \tag{79}$$

$$\mathcal{E}^{(6,0)}|_{J=3/2} = m_2 \left[\left(-\frac{5}{16\,n^6} + \frac{3}{8\,n^5} - \frac{3}{32\,n^4} - \frac{1}{64\,n^3}\right) + \frac{1}{45}\left(\frac{1}{n^3} - \frac{1}{n^5}\right) m_2^4\, r_{EE1}^4\right], \tag{80}$$

$$\mathcal{E}^{(6,1)}\big|_{J=3/2} = \frac{m_2^2}{m_1}\left[\left(\frac{1}{2\,n^6} - \frac{23}{30\,n^5} + \frac{3}{32\,n^4} + \frac{133}{320\,n^3}\right) - \frac{1}{9}\left(\frac{1}{n^3} - \frac{1}{n^5}\right) m_2^4\, r_{EE1}^4\right]. \tag{81}$$

In the point-nucleus limit, these formulas are in agreement with the literature results [1]. Furthermore, the finite-size corrections in the nonrecoil limit agree with those derived in Ref. [20]. The finite-size recoil corrections given by Eqs. (79) and (81) have not been previously calculated. We have verified them by comparing with numerical calculations performed to all orders in $Z\alpha$ in Sec. VIII.

VI. SPIN $s_1 = s_2 = 1/2$

The most complicated case considered here is when both particles have spin $s = 1/2$. The binding energy $\mathcal{E}^{(6)}$ can then be expressed as

$$\mathcal{E}^{(6)} = \mathcal{E}_{S0} + \mathcal{E}_{S1} + \mathcal{E}_{S2} + \mathcal{E}_{S12} + \vec{s}_1\cdot\vec{s}_2\,\mathcal{E}_{SS} + \vec{L}\cdot\vec{s}_1\,(\mathcal{E}_{LN1} + \mathcal{E}_{LS1}) + \vec{L}\cdot\vec{s}_2\,(\mathcal{E}_{LN2} + \mathcal{E}_{LS2}) + (L^i L^j)^{(2)}\, s_1^i\, s_2^j\, \mathcal{E}_{LL}. \tag{82}$$

It differs from the general result $\mathcal{E}_G$ from Ref. [10] by

$$\begin{aligned}
\mathcal{E}^{(6)} - \mathcal{E}_G^{(6)}\big|_{l=1} = \frac{\mu^5}{9}\left(\frac{1}{n^3} - \frac{1}{n^5}\right)\bigg\{ &\frac{\tilde r_{E1}^2 + \tilde r_{E2}^2}{m_1\, m_2} + \frac{2}{3}\left(r_{E1}^2 + \frac{3}{4\,m_1^2}\right)\left(r_{E2}^2 + \frac{3}{4\,m_2^2}\right) + \frac{r_{EE1}^4 + r_{EE2}^4}{5}\\
&+ \vec{L}\cdot\vec{s}_1\left[-\frac{g_1\,(\tilde r_{M1}^2 + \tilde r_{E2}^2)}{m_1\, m_2} - \frac{g_1\,\tilde r_{M1}^2}{m_1^2} + \frac{r_{E1}^2}{m_1^2} - \frac{g_1 - 1}{m_1^2}\left(r_{E2}^2 + \frac{3}{4\,m_2^2}\right)\right]\\
&+ \vec{L}\cdot\vec{s}_2\left[-\frac{g_2\,(\tilde r_{M2}^2 + \tilde r_{E1}^2)}{m_1\, m_2} - \frac{g_2\,\tilde r_{M2}^2}{m_2^2} + \frac{r_{E2}^2}{m_2^2} - \frac{g_2 - 1}{m_2^2}\left(r_{E1}^2 + \frac{3}{4\,m_1^2}\right)\right]\\
&+ \vec{s}_1\cdot\vec{s}_2\left[\frac{2}{3}\,\frac{g_1\, g_2}{m_1\, m_2}(\tilde r_{M1}^2 + \tilde r_{M2}^2) - \frac{1}{4\,m_1\, m_2}\left(g_2\,\frac{g_1 - 2}{m_1^2} + g_1\,\frac{g_2 - 2}{m_2^2}\right) + \frac{(g_1 - 1)\,(g_2 - 1)}{2\,m_1^2\, m_2^2}\right]\\
&+ (L^i L^j)^{(2)}\, s_1^i\, s_2^j\left[\frac{g_1\, g_2}{m_1\, m_2}\,(\tilde r_{M1}^2 + \tilde r_{M2}^2) + \frac{3}{10\,m_1\, m_2}\left(g_2\,\frac{g_1 - 2}{m_1^2} + g_1\,\frac{g_2 - 2}{m_2^2}\right) + \frac{3\,(g_1 - 1)\,(g_2 - 1)}{m_1^2\, m_2^2}\right]\bigg\}.
\end{aligned} \tag{83}$$

The above difference does not vanish in the point-particle limit, which indicates a disagreement not only with Ref. [10] but also with previous calculations [13–15] since Ref. [10] was claimed to agree with them in the limit $m_1 = m_2$.

We now examine this discrepancy in detail. For the positronium atom, the difference (83) becomes

$$\begin{aligned}
\delta E_{\rm pos} &= \mathcal{E}^{(6)} - \mathcal{E}_G^{(6)}\big|_{l=1, m_1=m_2}\\
&= \frac{m\,(Z\alpha)^6}{32}\left(\frac{1}{n^3} - \frac{1}{n^5}\right)\left(\frac{1}{24} - \frac{\vec{L}\cdot(\vec{s}_1 + \vec{s}_2)}{12}\right.\\
&\quad\left. + \frac{\vec{s}_1\cdot\vec{s}_2}{18} + \frac{(L^i L^j)^{(2)}\, s_1^i s_2^j}{3}\right).
\end{aligned} \tag{84}$$

Evaluating explicitly the spin-angular dependence in the above formula, we obtain

$$\delta E_{\rm pos}(s = 0,\, j = 1) = 0, \tag{85}$$

$$\delta E_{\rm pos}(s = 1,\, j = 0) = \frac{m\,(Z\alpha)^6}{64}\left(\frac{1}{n^3} - \frac{1}{n^5}\right), \tag{86}$$

$$\delta E_{\rm pos}(s = 1,\, j = 1) = 0, \tag{87}$$

$$\delta E_{\rm pos}(s = 1,\, j = 2) = 0. \tag{88}$$

We thus find an additional α^6 correction for the orthopositronium $j = 0$ state, given by Eq. (86).

On closer inspection, we relate this discrepancy to the $\delta E_2 = \langle \delta H_2 \rangle$ contribution. Zatorski calculates it for point particles [13], Eq. (94), separately for the $l = 1$ case [13], Eq. (99) and for the $l > 1$ case [13], Eq. (103), closely following the original calculation of Khriplovich [16,17]. Later he writes that "...the correction δE_2 for $l = 1$ still can be obtained from Eq. (103)," which we find to be incorrect. The difference between Eqs. (103) and (99) of Ref. [13] is exactly equal to Eq. (86) in the above. Moreover, our calculation of δE_2 is in agreement with Ref. [13], Eq. (99) in the point particle limit. This means that the original approach of Khriplovich [16,17] is valid for $l > 1$ but not for $l = 1$. The subsequent works [14,15] followed the original Khriplovich calculations and thus reproduced the incorrect result for the $l = 1$ levels, although they agreed between themselves. Furthermore, Zatorski in Ref. [13], Eq. (204) presented the result for the positronium $l = 1$ levels employing Ref. [13], Eq. (103) instead of Ref. [13], Eq. (99) and claimed agreement with the previous result of Ref. [15].

We thus conclude that the previous result for the positronium P-levels repeatedly reported in the literature [13–15] was incorrect. The corrected formula for the positronium P-levels is presented in Appendix B. The additional correction found in this work shifts the previous theoretical predictions of the $j = 0$ level of positronium, but the corresponding numerical value is too small to affect the comparison with the (much less accurate) experimental result [21].

Returning to Eq. (82), we present formulas for its expansion in the small mass ratio m_2/m_1, for the case of the point-like second particle ($\kappa_2 = r_{E2}^2 = r_{M2}^2 = r_{EE2}^4 = 0$) and negligible polarizabilities ($\alpha_{E1} = \alpha_{E2} = 0$). The results are

$$\mathcal{E}^{(6,0)} = m_2 \left\{ \left(-\frac{5}{16\,n^6} + \frac{1}{2\,n^5} - \frac{3}{16\,n^4} - \frac{5}{96\,n^3} \right) + \vec{L}\cdot\vec{s}_2 \left(-\frac{1}{4\,n^5} + \frac{3}{16\,n^4} + \frac{7}{96\,n^3} \right) + \frac{1}{9}\left(\frac{1}{n^3} - \frac{1}{n^5}\right) \left[\left(\frac{1}{2} - \vec{L}\cdot\vec{s}_2\right) m_2^2\, r_{E1}^2 + \frac{1}{5}\, m_2^4\, r_{EE1}^4 \right] \right\}, \tag{89}$$

$$\begin{aligned}\mathcal{E}^{(6,1)} = \frac{m_2^2}{m_1} \Biggl\{ & \left(\frac{1}{2\,n^6} - \frac{14}{15\,n^5} + \frac{3}{16\,n^4} + \frac{217}{480\,n^3} \right) + \vec{L}\cdot\vec{s}_2 \left(\frac{1}{3\,n^5} - \frac{3}{16\,n^4} - \frac{7}{96\,n^3} \right) \\ & + g_1\, \vec{L}\cdot\vec{s}_1 \left(-\frac{43}{120\,n^5} + \frac{3}{16\,n^4} + \frac{83}{480\,n^3} \right) + g_1\, \vec{s}_1\cdot\vec{s}_2 \left(\frac{1}{45\,n^5} - \frac{1}{18\,n^4} - \frac{119}{1620\,n^3} \right) \\ & + g_1\, (L^i L^j)^{(2)}\, s_1^i\, s_2^j \left(\frac{169}{300\,n^5} - \frac{43}{120\,n^4} - \frac{5441}{10800\,n^3} \right) + \frac{1}{9}\left(\frac{1}{n^3} - \frac{1}{n^5}\right) \Biggl[-m_2^4\, r_{EE1}^4 \\ & - 3\left(\frac{1}{2} - \vec{L}\cdot\vec{s}_2\right) m_2^2\, r_{E1}^2 + \left(\frac{4}{3}\,\vec{s}_1\cdot\vec{s}_2 - \vec{L}\cdot\vec{s}_1 + 2\,(L^i L^j)^{(2)}\, s_1^i\, s_2^j \right) m_2^2\, g_1\, r_{M1}^2 \Biggr] \Biggr\}. \end{aligned} \tag{90}$$

The above expression for $\mathcal{E}^{(6,0)}$ agrees with that for the $s_1 = 0, s_2 = 1/2$ case, as it should. Similarly, $\mathcal{E}^{(6,1)}$ agrees with the $s_1 = 0, s_2 = 1/2$ case up to the terms with $\vec{s}_1$. The $\vec{s}_1$-dependent terms are responsible for the hyperfine structure at the α^6 order and for mixing of the $P_{1/2,F=1}$ and $P_{3/2,F=1}$ states.

VII. 2P FINE STRUCTURE IN LIGHT MUONIC ATOMS

Accurate theoretical predictions of the fine and hyperfine structure of the $2P$ levels in muonic atoms are required for the determination of the nuclear charge radii from experimental $2P$-$2S$ transition energies. QED calculations of the $2P$ fine structure of μHe ions have been performed in Refs. [22,23], neglecting higher-order terms in the mass ratio, namely, $(Z\alpha)^6\, m_\mu\, (m_\mu/m_N)^{(2+)}$, where the subscripts μ and N refer to the muon and the nucleus, respectively. In the present work we obtain the result for the α^6 contribution with full dependence on the mass ratio m_μ/m_N.

The binding energy of a muonic atom can be decomposed in terms of basic angular-momentum operators, similarly to Eq. (60),

$$E = E_{NS} + \vec{L}\cdot\vec{s}_\mu\, E_{L\mu} + \vec{L}\cdot\vec{s}_N\, E_{LN} + (L^i L^j)^{(2)}\, s_N^i\, s_\mu^j\, E_{LL} + \vec{s}_N\cdot\vec{s}_\mu\, E_{SS}. \tag{91}$$

Here, the spin-independent term E_{NS} corresponds to the energy centroid, the second term is responsible for the fine splitting, $E_{\rm fs} \equiv 3/2\, E_{L\mu}$, whereas the remaining terms induce the hyperfine splitting and mixing between the fine and hyperfine structure.

We are now interested in the fine structure of the $2P$ state. The leading fine structure of order $(Z\alpha)^4$ is obtained from Eq. (7), with the result

$$E_{\rm fs}^{(4)} = \frac{\mu^3 (Z\alpha)^4}{32} \left(\frac{g_\mu - 1}{m_\mu^2} + \frac{g_\mu}{m_{\rm N}\, m_\mu} \right). \tag{92}$$

For the α^6 correction, we set $g_\mu = 2$ because the magnetic-moment anomaly is only a part of the α^7 correction. Similarly, we neglect QED corrections to r_E^2 and r_M^2 of the muon. We obtain for the $s_N = 0$ nucleus

$$\begin{aligned} E_{\rm fs}^{(6)} &= \frac{3}{2}\, E_{L\mu}(n=2, g_\mu = 2, s_N = 0) \\ &= \mu\, \frac{(Z\alpha)^6}{64} \left[\frac{5}{4} + \frac{1}{4}\, \frac{\mu}{m_N} - \frac{19}{18}\left(\frac{\mu}{m_N}\right)^2 - \frac{3}{4}\left(\frac{\mu}{m_N}\right)^3 + \frac{11}{36}\left(\frac{\mu}{m_N}\right)^4 - \mu^2\, r_E^2 \left(1 - \frac{\mu^2}{m_N^2}\right) \right], \end{aligned} \tag{93}$$

whereas for $s_N = 1/2$

$$\begin{aligned} E_{\rm fs}^{(6)} &= \frac{3}{2}\, E_{L\mu}(n=2, g_\mu = 2, s_N = 1/2) \\ &= \mu\, \frac{(Z\alpha)^6}{64} \left[\frac{5}{4} + \frac{1}{4}\, \frac{\mu}{m_N} + \left(-\frac{19}{18} + \frac{2729}{3600}\, g_N^2 \right) \left(\frac{\mu}{m_N}\right)^2 + \left(-\frac{3}{4} + \frac{5}{72}\, g_N - \frac{188}{225}\, g_N^2 \right) \left(\frac{\mu}{m_N}\right)^3 \right. \\ &\quad \left. + \left(\frac{11}{36} - \frac{5}{72}\, g_N + \frac{31}{400}\, g_N^2 \right) \left(\frac{\mu}{m_N}\right)^4 - \mu^2 \left(r_E^2 + \frac{3}{4\, m_N^2} \right) \left(1 - \frac{\mu^2}{m_N^2}\right) \right]. \end{aligned} \tag{94}$$

TABLE I. $2P$ fine structure of μHe ions, in meV. The root-mean-square nuclear-charge radii are [3,6] $r_E(h) = 1.970$ fm and $r_E(\alpha) = 1.679$ fm. Our uncertainty is due to higher order in α terms, mainly due to the two-loop electron vacuum polarization. From the previous results in Refs. [22,24] we have subtracted BP(tot) = 0.1947 meV due to a different definition of the fine structure of μ^3He used in these works.

Contribution	$\mu^3\text{He}^+$	$\mu^4\text{He}^+$
$E^{(4)}_{\text{fs}}$	144.510 95	145.898 24
$E^{(4)}_{\text{fs,vp}}$	0.269 81	0.275 65
$E^{(6)}_{\text{fs}}$	0.004 05	0.007 64
E_{fs}	144.785(3)	146.182(3)
Refs. [22,23]	144.785(5)	146.181(5)
Exp. [3,24]	144.763(114)	146.047(96)

It is worth mentioning that the spin-0 case can be obtained from the spin-1/2 one by setting $g_N = 0$ and redefining the charge radius. We also note that the first two terms in powers of μ/m_N are universal and do not depend on the nuclear spin.

In addition to $E^{(4)}_{\text{fs}}$ and $E^{(6)}_{\text{fs}}$, one needs to account for the one-loop electron vacuum polarization correction to the leading fine structure, which can be calculated as described in Ref. [25]. Our numerical results for the $2P$ fine structure of μHe^+ are listed in Table I. They are in agreement with the previous calculation of Karshenboim *et al.* [22,23] and with available experimental results [3,24]. The observed agreement supports the determination of the nuclear charge radii reported in these works. This confirmation is important in view of a significant discrepancy in the charge radii difference $r_E^2(h) - r_E^2(\alpha)$ between the electronic- and muonic-spectroscopy determinations [3,6,26].

VIII. NUCLEAR RECOIL IN LIGHT MUONIC ATOMS

In this section we examine the nuclear recoil correction for muonic atoms, as obtained within two different approaches, namely, the leading-order $Z\alpha$ expansion result given by Eqs. (79) and (81) and the all-order (in $Z\alpha$) approach. The comparison of results of the two different methods will, first, validate the formulas derived in the present work and, second, give us an idea about the higher-order (in $Z\alpha$) effects.

The general expression for the nuclear recoil correction in electronic and muonic atoms valid to all orders in $Z\alpha$ was derived in Refs. [27–29]. For a muonic atom, it reads

$$E_{\text{rec}} = \frac{m_\mu^2}{m_N}\,\frac{i}{2\pi}\int_{-\infty}^{\infty} d\omega \sum_n \frac{1}{\varepsilon_a + \omega - \varepsilon_n(1-i0)} \times \langle a|\vec{p} - \vec{D}(\omega)|n\rangle\langle n|\vec{p} - \vec{D}(\omega)|a\rangle, \tag{95}$$

where $\vec{p}$ is the momentum operator, $D^j(\omega) = -4\pi Z\alpha\, \alpha^i\, D_C^{ij}(\omega,\vec{r})$, α^i are the Dirac matrices, D_C^{ij} is the transverse part of the photon propagator in the Coulomb gauge, and the summation over n is performed over the complete Dirac spectrum of a bound muon. The photon propagator D_C^{ij} describing the interaction between a point-like and an extended-size particle was derived in Ref. [30].

To separate out the contribution of order α^6 and higher from E_{rec}, we subtract the contribution of previous orders. Specifically, we introduce the higher-order remainder function $E^{(6+)}_{\text{rec}}$ as follows:

$$E^{(6+)}_{\text{rec}} = E_{\text{rec}} - \frac{m_\mu^2}{m_N}\left[\frac{(Z\alpha)^2}{2n^2} + \frac{(Z\alpha)^4}{2n^3}\left(\frac{1}{j+1/2} - \frac{1}{n}\right) + \frac{(Z\alpha)^5}{\pi n^3}\,D_{50}\right], \tag{96}$$

where D_{50} is defined by Eq. (11),

$$D_{50}(2p) = -\tfrac{8}{3}\,\ln[k_0(2p)] - \tfrac{7}{18} = -0.308\,844\,332\ldots. \tag{97}$$

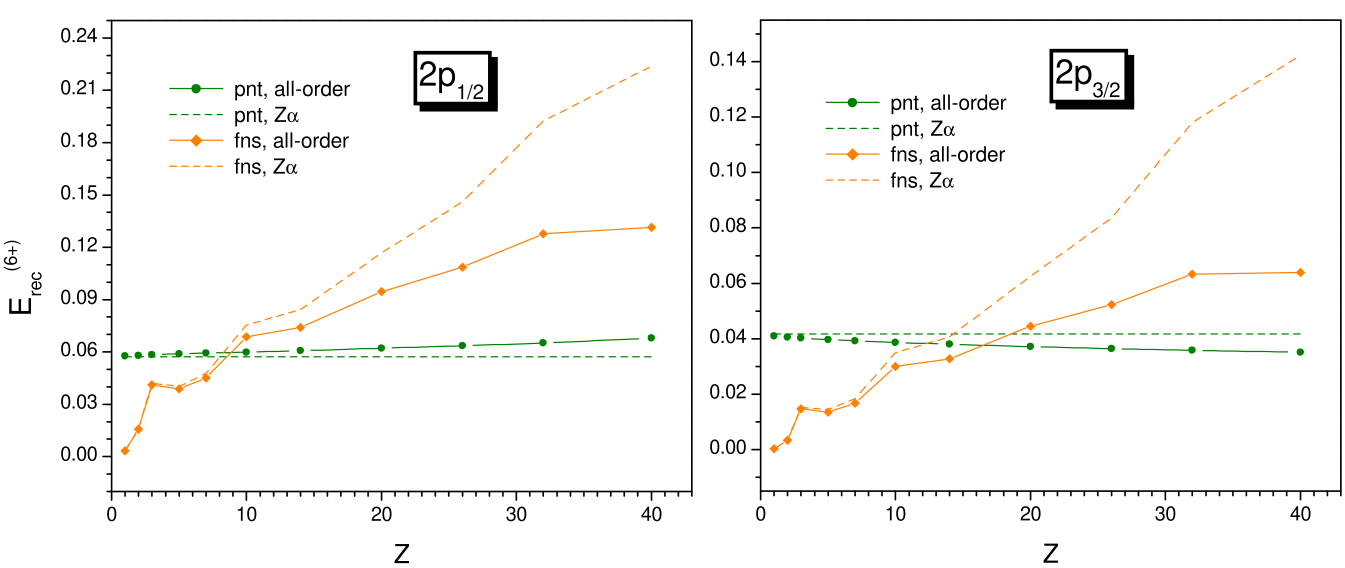

FIG. 1. Nuclear-recoil point-nucleus and fns corrections $E^{(6+)}_{\text{rec}}$ for the $2p_{1/2}$ and $2p_{3/2}$ states of muonic atoms, as a function of the nuclear charge number Z. Units are $m_\mu^2/m_N\,(Z\alpha)^6$. The nonsmoothness of the fns plots is due to the irregular dependence of the nuclear charge radius on Z.

TABLE II. Nuclear-recoil point-nucleus and fns corrections $E_{\rm rec}^{(6+)}$ for the $2p_{1/2}$ and $2p_{3/2}$ states of muonic atoms. Units are $m_\mu^2/m_N\,(Z\alpha)^6$.

		point				fns			
		$2p_{1/2}$		$2p_{3/2}$		$2p_{1/2}$		$2p_{3/2}$	
Z	r_E [fm]	All-order	$Z\alpha$-exp.	All-order	$Z\alpha$-exp.	All-order	$Z\alpha$-exp.	All-order	$Z\alpha$-exp.
1	0.8409	0.057 66	0.057 29	0.040 98	0.041 67	−0.010 46	−0.010 57	−0.000 94	−0.001 07
2	1.6755	0.058 01	0.057 29	0.040 60	0.041 67	−0.053 27	−0.054 60	−0.015 70	−0.016 87
3	2.4440	0.058 31	0.057 29	0.040 28	0.041 67	−0.149 86	−0.156 65	−0.070 78	−0.076 37
5	2.4060	0.058 82	0.057 29	0.039 71	0.041 67	−0.139 89	−0.149 53	−0.063 72	−0.071 73
7	2.5582	0.059 28	0.057 29	0.039 25	0.041 67	−0.163 72	−0.179 63	−0.078 37	−0.091 68
10	3.005	0.059 92	0.057 29	0.038 66	0.041 67	−0.255 04	−0.296 06	−0.139 81	−0.174 66
14	3.1224	0.060 75	0.057 29	0.037 99	0.041 67	−0.272 41	−0.33449	−0.150 07	−0.203 46
20	3.4776	0.062 05	0.057 29	0.037 15	0.041 67	−0.345 84	−0.475 60	−0.199 83	−0.313 07
26	3.7377	0.063 50	0.057 29	0.036 43	0.041 67	−0.390 10	−0.605 53	−0.228 68	−0.417 78
32	4.0742	0.065 19	0.057 29	0.035 80	0.041 67	−0.447 58	−0.812 87	−0.268 46	−0.589 79
40	4.2694	0.067 95	0.057 29	0.035 05	0.041 67	−0.440 82	−0.956 17	−0.259 70	−0.711 21

We perform our numerical calculations of $E_{\rm rec}$ by the approach described in detail in Ref. [31], for the exponential model of the nuclear charge distribution. The total correction is conveniently separated into the point-nucleus (point) and the finite-nuclear-size (fns) parts. The results are presented in Table II and Fig. 1. The numerical all-order results are labeled as "all-order," whereas the leading-order contributions obtained with Eqs. (79) and (81) are labeled as "$Z\alpha$-exp." We observe that the numerical all-order results rapidly converge to the lowest-order analytical prediction as Z is decreased. The higher-order in $Z\alpha$ corrections are quite small for the point-nucleus contribution but become prominent for the fns correction already for medium-Z ions; e.g., for $Z = 40$, the lowest-order fns formula overestimates the corresponding all-order result by a factor of about two. It is also interesting that the fns part of $E_{\rm rec}$ rapidly grows with the nuclear charge and dominates over the point-nucleus contribution for $Z > 10$ for the $2p_{1/2}$ state and $Z > 20$ for the $2p_{3/2}$ state.

IX. SUMMARY

We have derived the complete QED correction of order α^6 to the binding energies of the nP states of two-body systems consisting of the spin-0 or 1/2 extended-size particles of arbitrary masses and magnetic moments. The derivation has been verified by an all-order in $Z\alpha$ numerical calculation of the first-order in m/M recoil contribution. We have corrected the literature result for the positronium $l = 1$ energies [13–15] and verified previous calculations of the $2P$ fine splitting in light muonic atoms [22,23].

The obtained formulas for the $l = 1$ states extend the previous $l > 1$ results of Ref. [10] and can be applied to a wide class of two-body systems of immediate experimental interest, such as hydrogen, hydrogen-like ions, muonic hydrogen, muonic helium ion, positronium, muonium, etc. In the future, even more exotic two-body atomic systems may become accessible for experimental studies, such as protonium and other hydrogen-like hadronic atoms [32]. Comparisons of theoretical predictions of these systems in highly rotational states with accurate spectroscopic measurements would serve as tests of the yet unexplored region of long-range interactions between hadronic particles.

The current theoretical predictions of energies of the $l > 0$ levels of two-body systems can be improved further by a calculation of the α^7 correction, which is presently known in the nonrecoil limit only [33], and by inclusion of the electron vacuum polarization in a nonperturbative manner as was done for muonic atoms [25].

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APPENDIX A: MATRIX ELEMENTS OF VARIOUS OPERATORS FOR *P*-STATES

Here, we list results for matrix elements of various operators needed for our evaluation of $E^{(6)}$ for nP-states,

$$\left\langle\frac{1}{r}\right\rangle = \frac{\mu\,Z\alpha}{n^2}, \tag{A1}$$

$$\left\langle\frac{1}{r^2}\right\rangle = \frac{2\,(\mu\,Z\alpha)^2}{3\,n^3}, \tag{A2}$$

$$\left\langle\frac{1}{r^3}\right\rangle = \frac{(\mu\,Z\alpha)^3}{3\,n^3}, \tag{A3}$$

$$\left\langle\frac{1}{r^4}\right\rangle = 2\,(\mu\,Z\alpha)^4\left(\frac{1}{5\,n^3}-\frac{2}{15\,n^5}\right), \tag{A4}$$

$$\langle\,\vec p\,4\pi\,\delta^3(r)\,\vec p\,\rangle = \frac{4\,(\mu\,Z\alpha)^5}{3}\left(\frac{1}{n^3}-\frac{1}{n^5}\right), \tag{A5}$$

$$\langle\vec p\times 4\pi\,\delta^3(r)\,\vec p\rangle = i\,\frac{4\,(\mu\,Z\alpha)^5}{3}\left(\frac{1}{n^3}-\frac{1}{n^5}\right)\vec L, \tag{A6}$$

$$\langle (p^i 4\pi\,\delta^3(r) p^j)^{(2)}\rangle = -\,\frac{4\,(\mu\,Z\alpha)^5}{3}\left(\frac{1}{n^3}-\frac{1}{n^5}\right)(L^iL^j)^{(2)}. \tag{A7}$$

APPENDIX B: POSITRONIUM P-LEVELS AT THE α^6 ORDER

The complete α^6 correction to the energy levels of the nP-states of positronium is given by

$$E^{(6)}_{\rm pos}(n^1P_1) = m\,\alpha^6\bigg(-\frac{69}{512\,n^6}+\frac{23}{120\,n^5}-\frac{1}{12\,n^4}+\frac{163}{4320\,n^3}\bigg), \tag{B1}$$

$$E^{(6)}_{\rm pos}(n^3P_0) = m\,\alpha^6\bigg(-\frac{69}{512\,n^6}+\frac{461}{960\,n^5}-\frac{1}{3\,n^4}-\frac{1531}{8640\,n^3}-\frac{a_1^2+6\,a_2}{24\,\pi^2\,n^3}\bigg), \tag{B2}$$

$$E^{(6)}_{\rm pos}(n^3P_1) = m\,\alpha^6\bigg(-\frac{69}{512\,n^6}+\frac{77}{320\,n^5}-\frac{25}{192\,n^4}+\frac{553}{17\,280\,n^3}+\frac{a_1^2-2\,a_2}{48\,\pi^2\,n^3}\bigg), \tag{B3}$$

$$E^{(6)}_{\rm pos}(n^3P_2) = m\,\alpha^6\bigg(-\frac{69}{512\,n^6}+\frac{559}{4800\,n^5}-\frac{169}{4800\,n^4}+\frac{17\,977}{432\,000\,n^3}+\frac{-a_1^2+18\,a_2}{240\,\pi^2\,n^3}\bigg), \tag{B4}$$

where a_1 and a_2 are the expansion coefficients of the electron magnetic-moment anomaly a,

$$a = \frac{\alpha}{\pi}\,a_1 + \Big(\frac{\alpha}{\pi}\Big)^2 a_2 + \cdots, \tag{B5}$$

$$a_1 = \tfrac{1}{2}, \tag{B6}$$

$$a_2 = \frac{3}{4}\,\zeta(3) - \frac{\pi^2}{2}\,\ln 2 + \frac{\pi^2}{12} + \frac{197}{144}. \tag{B7}$$

The presented formulas agree with Ref. [13], Eq. (204) for all states except the n^3P_0 one. Note that in this section we switched to the literature definition of $E^{(6)}_{\rm pos}$ and included contributions from the expansion of g-factors in α, originating from $E^{(4)}$ in Eq. (7).

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