# Relativistic Reduced-Mass and Recoil Corrections to Vacuum Polarization in Muonic Hydrogen, Muonic Deuterium and Muonic Helium Ions 

U. D. Jentschura<br>Department of Physics, Missouri University of Science and Technology, Rolla, Missouri, MO65409, USA


#### Abstract

The reduced-mass dependence of relativistic and radiative effects in simple muonic bound systems is investigated. The spin-dependent nuclear recoil correction of order $(Z \alpha)^{4} \mu^{3} / m_{N}^{2}$ is evaluated for muonic hydrogen and deuterium, and muonic helium ions ( $\mu$ is the reduced mass and $m_{N}$ is the nuclear mass). Relativistic corrections to vacuum polarization of order $\alpha(Z \alpha)^{4} \mu$ are calculated, with a full account of the reduced-mass dependence. The results shift theoretical predictions. The radiative-recoil correction to vacuum polarization of order $\alpha(Z \alpha)^{5} \ln ^{2}(Z \alpha) \mu^{2} / m_{N}$ is obtained in leading logarithmic approximation. The results emphasize the need for a unified treatment of relativistic corrections to vacuum polarization in muonic hydrogen, muonic deuterium and muonic helium ions, where the mass ratio of the orbiting particle to the nuclear mass is larger than the fine-structure constant.


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## I. INTRODUCTION

In muonic hydrogen and muonic deuterium, the mass ratio $\xi_{N}=m_{\mu} / m_{N}$ of the orbiting particle (muon mass $m_{\mu}$ ) to the mass of the atomic nucleus $m_{N}$ is not really small against unity. It evaluates to

$$
\begin{align*}
& \xi_{p}=\frac{m_{\mu}}{m_{p}}=0.112609 \ldots \approx \frac{1}{9}  \tag{1a}\\
& \xi_{d}=\frac{m_{\mu}}{m_{d}}=0.0563327 \ldots \approx \frac{1}{18} \tag{1b}
\end{align*}
$$

where the latest recommended values of the masses have been used [1]. For muonic helium ions, we have

$$
\begin{align*}
\xi_{\mathrm{He}^{3}} & =\frac{m_{\mu}}{m_{\mathrm{He}^{3}}}=0.0376223 \ldots \approx \frac{1}{26}  \tag{1c}\\
\xi_{\mathrm{He}^{4}} & =\frac{m_{\mu}}{m_{\mathrm{He}^{4}}}=0.0283465 \ldots \approx \frac{1}{35} \tag{1d}
\end{align*}
$$

In all cases, $\xi_{N}$ is larger than the fine-structure constant $\alpha \approx 1 / 137.036$ that governs the relativistic and quantum electrodynamic (QED) effects. Consequently, the reduced-mass dependence of all quantum electrodynamic (QED) effects that influence the spectrum must be taken into account exactly, i.e., to all orders. In calculations, one must first take into account $\xi_{N}$ (if possible) to all orders, before advancing to the next order in the $Z \alpha$ expansion; otherwise the higher-order effects in $Z \alpha$ will be shadowed by the unknown reduced-mass dependence of lower-order terms in the $Z \alpha$-expansion.

Hence, particular emphasis has been laid in Ref. [2] on the correct treatment of the reduced-mass dependence of all relativistic and QED corrections. The statement made in the text preceding Eq. (17) in Ref. [2], which says "the external field approximation does not give an accurate result," can hardly be overemphasized. Here, the external field approximation refers to the Dirac equation, which is appropriate for heavy muonic atoms where the parameter $Z \alpha$ (with $Z$ denoting the nuclear charge number) is much larger than the mass ratio $m_{\mu} / m_{N}$, where $m_{N}$ is the mass
of the heavy nucleus. Even a tiny conceivable error in the handling of, say, the reduced-mass dependence of the oneloop vacuum polarization (VP) shift in muonic hydrogen could drastically influence the comparison of theory and experiment: the current discrepancy [3] of theory and experiment for the muonic hydrogen Lamb shift amounts to roughly 0.3 meV , which is about one part per thousand of the leading vacuum-polarization contribution and thus smaller than a conceivable additional reduced-mass correction to the leading VP effect of relative order $\xi_{N}^{3}$.

In comparison to previous studies on heavy muonic atoms and ions (excellent theoretical overviews are provided in Refs. [4, [5]), the magnitude of the mass ratio is the main characteristic property of muonic hydrogen and deuterium. In this article, we thus revisit the precise treatment of the vacuum-polarization contribution to the Lamb shift in muonic hydrogen $(\mu \mathrm{H})$ and muonic deuterium $(\mu \mathrm{D})$, as well as muonic helium ions $\left(\mu \mathrm{He}^{3}\right.$ and $\mu \mathrm{He}^{4}$ ), with full account of the two-body structure of the bound system. Starting from the nonrelativistic Hamiltonian (Sec. III), we proceed to discuss the nuclear-spin dependent terms in the Breit Hamiltonian (Sec. III), before proceeding to the radiatively corrected Breit Hamiltonian (Sec. IV) and the radiative-recoil correction (Sec. V). Conclusions are drawn in Sec. VI.

## II. NONRELATIVISTIC HAMILTONIAN

The nonrelativistic $\mu \mathrm{H}$ Hamiltonian is separable, and the nonrelativistic (Schrödinger) Hamiltonian in the center-of-mass system, where the muon and the nuclear particle carry opposite momenta $\vec{p}$ and $-\vec{p}$, respectively, reads (in natural units, $\hbar=c=\epsilon_{0}=1$ ),

$$
\begin{equation*}
H=\frac{\vec{p}^{2}}{2 m_{\mu}}+\frac{\vec{p}^{2}}{2 m_{N}}-\frac{Z \alpha}{r}=\frac{\vec{p}^{2}}{2 \mu}-\frac{Z \alpha}{r}, \quad \mu=\frac{m_{\mu}}{1+\xi_{N}} \tag{2}
\end{equation*}
$$

This equation can be solved exactly in terms of Schrödinger eigenstates. The nonrelativistic spinor wave
functions for the $2 S_{1 / 2}$ and $2 P_{1 / 2}$ states are exact eigenstates of $H$ and read, explicitly,

$$
\begin{align*}
\psi_{2 S}(\vec{r}) & =\frac{(Z \alpha \mu)^{3 / 2}}{2 \sqrt{2}}(2-Z \alpha \mu r) \mathrm{e}^{-\frac{1}{2} Z \alpha \mu r} \chi_{-1}^{M}(\hat{r}),  \tag{3}\\
\psi_{2 P_{1 / 2}}(\vec{r}) & =\frac{(Z \alpha \mu)^{5 / 2} r}{2 \sqrt{6}} \mathrm{e}^{-\frac{1}{2} Z \alpha \mu r} \chi_{+1}^{M}(\hat{r}), \tag{4}
\end{align*}
$$

where $M= \pm \frac{1}{2}$ is the magnetic projection, $\chi_{\varkappa}^{M}(\hat{r})$ is the standard two-component spin-angular function [6], and $\varkappa=(-1)^{j+\ell+1 / 2}$ is the Dirac angular quantum number. The reduced-mass dependence of the wave functions in Eq. (3) is exact.

The one-loop vacuum-polarization potential $V_{\mathrm{vp}}$ can be expressed in terms of the action of a linear operator $K$ on a screened Coulomb potential $v_{\mathrm{vp}}$ as follows,

$$
\begin{equation*}
V_{\mathrm{vp}}(r)=K\left[v_{\mathrm{vp}}\left(m_{e} \rho ; r\right)\right], \quad v_{\mathrm{vp}}(\lambda ; r)=-\frac{Z \alpha}{r} \mathrm{e}^{-\lambda r} \tag{5}
\end{equation*}
$$

with

$$
\begin{equation*}
K[f(\rho)]=\frac{2 \alpha}{3 \pi} \int_{2}^{\infty} \mathrm{d} \rho \frac{2+\rho^{2}}{\rho^{3}} \sqrt{1-\frac{4}{\rho^{2}}} f(\rho) \tag{6}
\end{equation*}
$$

where $m_{e}$ is the electron mass. In the following, we often use the identification $\lambda=m_{e} \rho$ and define the ratio

$$
\begin{equation*}
\beta_{N}=\frac{m_{e}}{(Z \alpha \mu)} \tag{7}
\end{equation*}
$$

which evaluates to $\beta_{p}=0.7373836 \ldots$ for $\mu \mathrm{H}$ and $\beta_{d}=$ $0.7000861 \ldots$ for $\mu \mathrm{D}$ (proton and deuteron nuclei, respectively). For muonic helium ions, the values are $\beta_{\mathrm{He}^{3}}=$ $0.3438429 \ldots$ and $\beta_{\mathrm{He}^{4}}=0.3407691 \ldots$ (We here refrain from assigning a subscript to the reduced mass $\mu$, even though it of course depends on the nucleus $N$, because the symbol $\mu_{N}$ is reserved, canonically, for the nuclear magnetic moment.) We then use the exact nonrelativistic unperturbed wave functions defined in Eq. (3) and calculate the leading VP energy shifts as

$$
\begin{equation*}
\left\langle 2 S_{1 / 2}\right| V_{\mathrm{vp}}\left|2 S_{1 / 2}\right\rangle=-(Z \alpha)^{2} \mu K\left[\frac{2 \beta_{N}^{2} \rho^{2}+1}{4\left(\beta_{N} \rho+1\right)^{4}}\right] \tag{8a}
\end{equation*}
$$

and

$$
\begin{equation*}
\left\langle 2 P_{1 / 2}\right| V_{\mathrm{vp}}\left|2 P_{1 / 2}\right\rangle=-(Z \alpha)^{2} \mu K\left[\frac{1}{4\left(1+\beta_{N} \rho\right)^{4}}\right] . \tag{8b}
\end{equation*}
$$

A numerical evaluation of these compact expressions is found to be in agreement with the literature (see Refs. [2, 3, [7, [8]) and confirms that the reduced-mass dependence of the leading VP effect is correctly described by Schrödinger wave functions scaled with the reduced mass of the system. It is even possible [9, 10] to carry
out the integration over the spectral parameter $\rho$ analytically, with the result

$$
\begin{align*}
& \left\langle 2 P_{1 / 2}\right| V_{\mathrm{vp}}\left|2 P_{1 / 2}\right\rangle-\left\langle 2 S_{1 / 2}\right| V_{\mathrm{vp}}\left|2 S_{1 / 2}\right\rangle \\
& =\frac{\alpha}{\pi}(Z \alpha)^{2} \mu\left[\frac{8 \pi \beta_{N}^{3}}{3}+\frac{1-26 \beta_{N}^{2}+352 \beta_{N}^{4}-768 \beta_{N}^{6}}{18\left(1-4 \beta_{N}^{2}\right)^{2}}\right. \\
& \left.\quad+\frac{4 \beta_{N}^{4}\left(15-80 \beta_{N}^{2}+128 \beta_{N}^{4}\right)}{3\left(1-4 \beta_{N}^{2}\right)^{5 / 2}} \ln \left(\frac{1-\sqrt{1-4 \beta_{N}^{2}}}{2 \beta_{N}}\right)\right] \tag{9}
\end{align*}
$$

for the Lamb shift difference of the leading VP energy correction. For reference, the $2 P_{1 / 2}-2 S_{1 / 2}$ difference of the leading nonrelativistic vacuum polarization effect is 205.0073 meV for $\mu \mathrm{H}, 227.6346 \mathrm{meV}$ for $\mu \mathrm{D}$, 1641.885 meV for $\mu \mathrm{He}^{3}$, and 1665.772 meV for $\mu \mathrm{He}^{4}$. The latter value differs by 0.010 meV from the value of 1665.782 meV given in Eq. (10) of Ref. [11]; the difference probably is due to updated physical constants used in our calculation (see also Ref. [1]).

## III. BREIT HAMILTONIAN AND BARKER-GLOVER TERMS

The Breit Equation and the corresponding Hamiltonian follow from the Bethe-Salpeter equation in the limit on an instantaneous interaction kernel [12] and describe the bound states of general two-body systems of arbitrary mass ratio $\xi_{N}$, including higher-order relativistic corrections 13]. For the $2 P_{1 / 2}-2 S_{1 / 2}$ Lamb shift in muonic bound systems, the relevant terms in the Breit Hamiltonian read ( $\delta_{I}=1$ for half-integer and $\delta_{I}=0$ for integer nuclear spin, see [14])

$$
\begin{align*}
\delta H & =\sum_{j=1}^{4} \delta H_{j}, \quad \delta H_{1}=-\frac{\vec{p}^{4}}{8 m_{\mu}^{3}}-\frac{\vec{p}^{4}}{8 m_{N}^{3}}, \\
\delta H_{2} & =\left(\frac{1}{m_{\mu}^{2}}+\frac{\delta_{I}}{m_{N}^{2}}\right) \frac{\pi Z \alpha \delta^{3}(r)}{2}, \\
\delta H_{3} & =-\frac{Z \alpha}{2 m_{\mu} m_{N} r}\left(\vec{p}^{2}+\frac{1}{r^{2}} r^{i} r^{j} p^{i} p^{j}\right), \\
\delta H_{4} & =\frac{Z \alpha}{r^{3}}\left(\frac{1}{4 m_{\mu}^{2}}+\frac{1}{2 m_{\mu} m_{N}}\right) \vec{\sigma} \cdot \vec{L} . \tag{10}
\end{align*}
$$

where we use the summation convention for the superscripts $i$ and $j$ which denote the Cartesian components of the position and momentum operators. Using the relations

$$
\begin{equation*}
\vec{\nabla}^{2}\left(\frac{1}{r}\right)=-4 \pi \delta^{3}(r) \tag{11}
\end{equation*}
$$

and

$$
\begin{equation*}
\nabla^{i} \nabla^{j}\left(\frac{x^{i} x^{j}}{r^{3}}\right)=+4 \pi \delta^{3}(r) \tag{12}
\end{equation*}
$$

one may transform $\delta H_{3}$ to a more symmetric form,

$$
\begin{equation*}
\delta H_{3}=-\frac{Z \alpha}{2 m_{\mu} m_{N}} p^{i}\left(\frac{1}{r}+\frac{r^{i} r^{j}}{r^{3}}\right) p^{j} . \tag{13}
\end{equation*}
$$

After some algebra, the expectation values of the eigenstates given in Eq. (3) of the Breit Hamiltonian read

$$
\begin{align*}
\left\langle 2 S_{1 / 2}\right| \delta H\left|2 S_{1 / 2}\right\rangle= & -(Z \alpha)^{4} \mu \frac{5+\xi_{N}\left(11+13 \xi_{N}\right)}{128\left(1+\xi_{N}\right)^{2}} \\
& +\delta_{I} \frac{(Z \alpha)^{4} \mu \xi_{N}^{2}}{16\left(1+\xi_{N}\right)^{2}}  \tag{14a}\\
\left\langle 2 P_{1 / 2}\right| \delta H\left|2 P_{1 / 2}\right\rangle= & -\left(Z \alpha^{4}\right) \mu \frac{15+\xi_{N}\left(33+7 \xi_{N}\right)}{384\left(1+\xi_{N}\right)^{2}}, \tag{14b}
\end{align*}
$$

and the $2 P_{1 / 2}-2 S_{1 / 2}$ difference ( $2 P_{1 / 2}$ is energetically higher) amounts to

$$
\begin{align*}
L\left(2 P_{1 / 2}-2 S_{1 / 2}\right) & =\frac{(Z \alpha)^{4} \mu \xi_{N}^{2}}{48\left(1+\xi_{N}\right)^{2}}\left(4-3 \delta_{I}\right) \\
& = \begin{cases}\frac{(Z \alpha)^{4} \mu^{3}}{48 m_{N}^{2}} & \left(\delta_{I}=1\right) \\
\frac{(Z \alpha)^{4} \mu^{3}}{12 m_{N}^{2}} & \left(\delta_{I}=0\right)\end{cases} \tag{15}
\end{align*}
$$

The Barker-Glover [15] correction $L$ given in Eq. (15) evaluates to 0.05747 meV for $\mu \mathrm{H}$ and to 0.12654 meV for $\mu \mathrm{He}^{3}$, in full agreement with the literature [Eq. (46) of Ref. [2]]. Because the zitterbewegung term is absent for the spin-1 deuteron nucleus [14] and for the spin-zero alpha particle, the shift evaluates to $L=0.06722 \mathrm{meV}$ for $\mu \mathrm{D}$ and to $L=0.29518 \mathrm{meV}$ for $\mu \mathrm{He}^{4}$ [cf. Eq. (61) of Ref. [11] and Eq. (10) of Ref. [16]]. It constitutes a nuclear spin-dependent recoil correction to the Lamb shift, which is essential for the correct description of the muonic isotope shift. Equation (15) is exact to all orders in $\xi_{N}$.

## IV. RADIATIVELY CORRECTED BREIT HAMILTONIAN

The massive Breit interaction uses a strictly static timelike photon propagator component

$$
\begin{equation*}
G_{00}(\vec{q})=-\frac{1}{\vec{q}^{2}+\lambda^{2}} \tag{16}
\end{equation*}
$$

and spatial components

$$
\begin{equation*}
G_{i j}(\vec{q})=-\frac{1}{\vec{q}^{2}+\lambda^{2}}\left[\delta^{i j}-\frac{q^{i} q^{j}}{\vec{q}^{2}+\lambda^{2}}\right] \tag{17}
\end{equation*}
$$

The spatial components are no longer transverse. One then follows the standard derivation of the Breit interaction given in Chap. 83 of Ref. [18] but has to avoid pitfalls. The derivation necessitates the evaluation of Fourier

TABLE I. Detailed breakdown of the first-order and secondorder individual contributions $\delta E_{i}^{(1)}$ and $\delta E_{j}^{(2)}$ to the relativistic Breit correction $\delta E_{\mathrm{vp}}$ of vacuum polarization for $\mu \mathrm{H}$, $\mu \mathrm{D}$, and muonic helium ions. All units are meV.

|  | $\mu \mathrm{H}$ | $\mu \mathrm{D}$ | $\mu \mathrm{He}^{3}$ | $\mu \mathrm{He}^{4}$ |
| :---: | :---: | :---: | :---: | :---: |
| $2 P_{1 / 2}[\mathrm{meV}]$ |  |  |  |  |
| $\overline{\delta E_{1}^{(1)}}$ | -0.000558 | -0.000679 | -0.020331 | $-0.020970$ |
| $\delta E_{2}^{(1)}$ | 0.000064 | 0.000038 | 0.000467 | 0.000360 |
| $\delta E_{3}^{(1)}$ | -0.000290 | $-0.000181$ | $-0.004587$ | -0.003584 |
| $\delta E_{4}^{(1)}$ | -0.002026 | $-0.002303$ | -0.085970 | $-0.087587$ |
| $\delta E^{(1)}$ | $-0.002811$ | $-0.003125$ | -0.110421 | $-0.111781$ |
| $\delta E_{1}^{(2)}$ | -0.001124 | -0.001545 | -0.099980 | $-0.105132$ |
| $\delta E_{2}^{(2)}$ | 0.0 | 0.0 | 0.0 | 0.0 |
| $\delta E_{3}^{(2)}$ | -0.000269 | $-0.000177$ | -0.008427 | -0.006624 |
| $\delta E_{4}^{(2)}$ | $-0.001283$ | $-0.001521$ | -0.093497 | $-0.095762$ |
| $\delta E^{(2)}$ | -0.002676 | $-0.003243$ | -0.201904 | -0.207518 |
| $\delta E_{\mathrm{vp}}$ | $-0.005486$ | -0.006368 | -0.312324 | -0.319300 |
| $2 S_{1 / 2}[\mathrm{meV}]$ |  |  |  |  |
| $\overline{\delta E_{1}^{(1)}}$ | 0.029112 | 0.034636 | 0.846700 | 0.872150 |
| $\delta E_{2}^{(1)}$ | -0.001928 | -0.001142 | -0.014512 | -0.011243 |
| $\delta E_{3}^{(1)}$ | $-0.002280$ | $-0.001416$ | -0.032734 | -0.025535 |
| $\delta E_{4}^{(1)}$ | 0.0 | 0.0 | 0.0 | 0.0 |
| $\delta E^{(1)}$ | 0.024904 | 0.032078 | 0.799454 | 0.835372 |
| $\delta E_{1}^{(2)}$ | -0.084996 | -0.108282 | -2.875794 | -2.995690 |
| $\delta E_{2}^{(2)}$ | 0.044911 | 0.053594 | 1.361115 | 1.402803 |
| $\delta E_{3}^{(2)}$ | -0.009064 | $-0.005539$ | -0.106444 | -0.082889 |
| $\delta E_{4}^{(2)}$ | 0.0 | 0.0 | 0.0 | 0.0 |
| $\delta E^{(2)}$ | -0.049149 | $-0.060227$ | -1.621122 | $-1.675776$ |
| $\delta E_{\mathrm{vp}}$ | -0.024245 | -0.028149 | -0.821668 | -0.840404 |
| $2 P_{1 / 2}-2 S_{1 / 2}[\mathrm{meV}]$ and comparison to other work |  |  |  |  |
| $\Delta E_{\text {vp }}$ (this work) | 0.018759 | 0.021781 | 0.509344 | 0.521104 |
| (Ref. [17]) | 0.0169 |  |  |  |
| (Ref. [11]) |  |  |  | -0.202 |
| $\left(\right.$ Ref. [16]) ${ }^{a}$ | 0.0169 | 0.0214 | 0.495 | 0.508 |

${ }^{a}$ A conceptually different approach is used in Ref. [16].
transforms, the most interesting of which is related to the interaction [cf. Eq. (83.13) of [18] and Sec. 2 of Ref. [19]],

$$
\begin{align*}
U(\vec{p}, \vec{q}, \lambda)= & -\frac{4 \pi Z \alpha}{m_{\mu} m_{N}}\left[\frac{\vec{p}^{2}}{\vec{q}^{2}+\lambda^{2}}-\frac{(\vec{p} \cdot \vec{q})^{2}}{\left(\vec{q}^{2}+\lambda^{2}\right)^{2}}\right. \\
& \left.+\frac{\lambda^{2} \vec{q}^{2}}{4\left(\vec{q}^{2}+\lambda^{2}\right)^{2}}-\frac{\lambda^{2} \vec{q} \cdot \vec{p}}{\left(\vec{q}^{2}+\lambda^{2}\right)^{2}}\right] \tag{18}
\end{align*}
$$

For $\lambda=0$, the Fourier transform of this expression with respect to $\vec{q}$ gives the term $\delta H_{3}$ in Eq. (10). For a massive photon, we find

$$
\begin{equation*}
\int \frac{\mathrm{d}^{3} q}{(2 \pi)^{3}} U(\vec{p}, \vec{q}, \lambda) \mathrm{e}^{\mathrm{i} \vec{q} \cdot \vec{r}}=\delta v_{2}(r)+\delta v_{3}(r) \tag{19}
\end{equation*}
$$

where $\delta v_{2}(r)$ and $\delta v_{3}(r)$ contribute to the Breit potential $\delta v_{\mathrm{vp}}$ for massive photon exchange,

$$
\begin{equation*}
\delta v_{\mathrm{vp}}=K\left[\delta v_{1}+\delta v_{2}+\delta v_{3}+\delta v_{4}\right] \tag{20}
\end{equation*}
$$

where $\delta v_{1}(r)$ depends on the nuclear spin,

$$
\begin{equation*}
\delta v_{1}=\frac{Z \alpha}{8}\left(\frac{1}{m_{\mu}^{2}}+\frac{\delta_{I}}{m_{N}^{2}}\right)\left(4 \pi \delta^{3}(r)-\frac{\lambda^{2}}{r} \mathrm{e}^{-\lambda r}\right) \tag{21}
\end{equation*}
$$

and the momentum operators act on the ket state in

$$
\begin{align*}
& \delta v_{2}=-\frac{Z \alpha \lambda^{2} \mathrm{e}^{-\lambda r}}{4 m_{\mu} m_{N} r}\left(1-\frac{\lambda r}{2}+2 \mathrm{i} \vec{r} \cdot \vec{p}\right)  \tag{22a}\\
& \delta v_{3}=-\frac{Z \alpha \mathrm{e}^{-\lambda r}}{2 m_{\mu} m_{N} r}\left(\vec{p}^{2}+\frac{1+\lambda r}{r^{2}} r^{i} r^{j} p^{i} p^{j}\right) \tag{22b}
\end{align*}
$$

whereas the spin-orbit coupling is modified to

$$
\begin{equation*}
\delta v_{4}=Z \alpha\left(\frac{1}{4 m_{\mu}^{2}}+\frac{1}{2 m_{\mu} m_{N}}\right) \frac{\mathrm{e}^{-\lambda r}(1+\lambda r)}{r^{3}} \vec{\sigma} \cdot \vec{L} \tag{23}
\end{equation*}
$$

In the terms $\delta v_{2}$ and $\delta v_{3}$, all the momentum operators act on the "incoming" wave function (Dirac ket state), and the Hamiltonian may be used for the evaluation of diagonal matrix elements. For off-diagonal elements, it is helpful to symmetrize $\delta v_{2}$ and $\delta v_{3}$ with respect to outgoing and incoming momenta, effectively replacing terms of the form $f(\vec{r}) \mathrm{i} \vec{r} \cdot \vec{p}$ by the commutator $\mathrm{i}[f(\vec{r}) \vec{r}, \vec{p}]$ and terms of the form $f^{i j}(\vec{r}) p^{i} p^{j}$ by the anticommutator $\frac{1}{2}\left\{f^{i j}(\vec{r}), p^{i} p^{j}\right\}$. In a second step, using the relation $\frac{1}{2}\left\{A^{2}, B\right\}=A B A+\frac{1}{2}[A,[A, B]]$, one obtains an even more symmetric form, with

$$
\begin{align*}
\delta w_{1} & =\delta v_{1}, \quad \delta w_{4}=\delta v_{4}  \tag{24a}\\
\delta w_{2} & =-\frac{Z \alpha \lambda^{2} \mathrm{e}^{-\lambda r}}{4 m_{\mu} m_{N} r}\left(1-\frac{\lambda r}{2}\right)  \tag{24b}\\
\delta w_{3} & =-\frac{Z \alpha \mathrm{e}^{-\lambda r}}{4 m_{\mu} m_{N}} p^{i}\left(\frac{\delta^{i j}}{r}+\frac{1+\lambda r}{r^{3}} r^{i} r^{j}\right) p^{j}  \tag{24c}\\
\delta v_{\mathrm{vp}} & =K\left[\delta w_{1}+\delta w_{2}+\delta w_{3}+\delta w_{4}\right] \tag{24d}
\end{align*}
$$

The terms $\delta w_{2}$ and $\delta w_{3}$ are used in Eq. (21) of Ref. [2]. The $\alpha(Z \alpha)^{4} \mu$ relativistic reduced-mass correction to vacuum polarization then is the sum of four first-order perturbations $\delta E_{i}^{(1)}$ and four second-order terms $\delta E_{j}^{(2)}$,

$$
\begin{align*}
& \delta E_{\mathrm{vp}}=\delta E^{(1)}+\delta E^{(2)}=\sum_{i=1}^{4} \delta E_{i}^{(1)}+\sum_{j=1}^{4} \delta E_{j}^{(2)}  \tag{25a}\\
& \delta E_{i}^{(1)}=K\left[\left\langle n \ell_{j}\right| \delta w_{i}\left|n \ell_{j}\right\rangle\right]  \tag{25b}\\
& \delta E_{j}^{(2)}=2 K\left[\left\langle n \ell_{j}\right| \delta H_{j}\left|\delta \psi_{n \ell_{j}}\right\rangle\right] \tag{25c}
\end{align*}
$$

where $\left|\delta \psi_{n \ell_{j}}\right\rangle$ is the wave function correction due to VP,

$$
\begin{equation*}
\left|\delta \psi_{n \ell_{j}}\right\rangle=\left(\frac{1}{E_{n \ell}-H}\right)^{\prime} v_{\mathrm{vp}}\left|n \ell_{j}\right\rangle \tag{26}
\end{equation*}
$$

Using a generalization of techniques outlined in Ref. 20], the perturbation $\delta \psi_{n \ell_{j}}$ can be evaluated analytically. The detailed expressions for the reduced Green functions (indicated by a prime) of the $2 S_{1 / 2}$ and $2 P_{1 / 2}$ states have been given in Eqs. (23) and (24) of Ref. [2]. All individual contributions are listed in Table in order to facilitate a numerical comparison with independent calculations. For $\mu \mathrm{H}$, we obtain a result of $\Delta E_{\mathrm{vp}}=\delta E_{\mathrm{vp}}\left(2 P_{1 / 2}\right)-$ $\delta E_{\mathrm{vp}}\left(2 S_{1 / 2}\right)=0.018759 \mathrm{meV}$. This result is not in perfect agreement with published values [2, 16, 17]. For comparison, the result indicated in Eq. (25) of Ref. [2] reads 0.059 meV ; and in Eq. (25) of Ref. [17] a result of 0.0169 meV has been indicated. In Table 1 on page 8 of Ref. [16], a numerically equivalent result of 0.0169 meV is given. (We note that Ref. [16] contains many unnumbered tables; the referenced table is numbered). The matrix elements of the relativistic recoil operator given in Eq. (7) of Ref. [16] are evaluated using unperturbed wave functions. All values given in Table $\square$ are nonperturbative in the mass ratio and take the wave function correction into account. A precise comparison of individual contributions to the approach of Ref. 16] is not possible at present. As evident from Table there are quite significant differences with published values for $\mu \mathrm{He}^{4}$ : e.g., the entries in Eqs. (26)-(29) and Eq. (41) of Ref. [11] add up to a correction of -0.202 meV for the $2 P_{1 / 2}-2 S_{1 / 2}$ Lamb shift in $\mu \mathrm{He}^{4}$, whereas we obtain +0.521 meV .

A very important question concerns the verifiability of the results. In self-energy calculations [21], a crosscheck of the calculation consists in the cancellation of an overlapping parameter that separates different momentum and energy regions of the physical process. For VP effects in muonic systems, no such checks are immediately available. Here, we note that the entries for the first-order matrix elements in Table $\square$ for $\mu \mathrm{He}^{4}$ are in full agreement with the results given in Eqs. (26)-(29) of Ref. [11]. For the matrix elements needed for $\delta E^{(1)}$, the limit as $\lambda \rightarrow 0$ of the matrix elements $\left\langle n \ell_{j}\right| \delta w_{i}\left|n \ell_{j}\right\rangle$ can be verified independently, and the calculation can otherwise be performed analytically, with ease. For the matrix elements needed in the evaluation of the secondorder effects $\delta E^{(2)}$, we can verify the first few terms in the asymptotic limit as $\lambda \rightarrow 0$, using the relation

$$
\begin{align*}
& 2\left\langle n \ell_{j}\right| \delta H\left(\frac{1}{E-H}\right)^{\prime} v_{\mathrm{vp}}\left|n \ell_{j}\right\rangle  \tag{27}\\
& =2\left\langle n \ell_{j}\right| \delta H\left(\frac{1}{E-H}\right)^{\prime}(Z \alpha) \frac{\partial}{\partial(Z \alpha)}\left|n \ell_{j}\right\rangle \\
& \quad-\left\langle n \ell_{j}\right| \delta H\left(\frac{1}{E-H}\right)^{\prime} Z \alpha r\left|n \ell_{j}\right\rangle \lambda^{2}+\mathcal{O}\left(\lambda^{3}\right)
\end{align*}
$$

In deriving this relation, the Hellmann-Feynman theorem is useful for the zeroth-order term in $\lambda$. The wave function perturbation in the term of order $\lambda^{2}$ can be evaluated analytically.


FIG. 1. Feynman diagrams for the radiative-recoil correction in two-body muonic bound systems. The three given diagrams correspond to the vacuum-polarization insertion in the seagull and two-photon exchange and lead to the leading double logarithm given in Eq. (29).

## V. RECOIL CORRECTIONS TO VACUUM POLARIZATION

Beyond the radiative modifications of the static Breit Hamiltonian, the recoil correction to vacuum polarization can be obtained by the insertion of vacuum polarization loops into the Salpeter recoil correction 22 24]. The recoil correction is the sum of four terms [24]; two of these (low- and middle-energy part) describe the frequencydependent part of the Breit interaction, beyond the static Breit Hamiltonian given in Eq. (10), and two further terms (seagull and high-energy part) correspond to twophoton exchange.

The seagull term corresponding to Fig. 1 (left), with a vacuum polarization insertion in the exchange photon, leads to the integral

$$
\begin{aligned}
& \delta E_{S}=-\frac{e^{4}}{2 m_{\mu} m_{N}} K\left[\int \frac{\mathrm{~d}^{3} k_{1}}{(2 \pi)^{3}} \frac{\mathrm{~d}^{3} k_{2}}{(2 \pi)^{3}} \frac{1}{\omega_{1} k_{2}} \frac{1}{\omega_{1}+k_{2}}\right. \\
& \left.\left(\delta^{i j}-\frac{k_{1}^{i} k_{1}^{j}}{\omega_{1}^{2}}\right)\left(\delta^{i j}-\frac{k_{2}^{i} k_{2}^{j}}{k_{2}^{2}}\right)\right]\left\langle n \ell_{j}\right| \mathrm{e}^{\mathrm{i}\left(\vec{k}_{1}+\vec{k}_{2}\right) \cdot \vec{r}}\left|n \ell_{j}\right\rangle
\end{aligned}
$$

where $\omega_{1}=\sqrt{\vec{k}_{1}^{2}+\lambda^{2}}$ is the frequency of the massive photon in the vacuum-polarization loop. An ultraviolet cutoff $\Lambda$ is introduced via multiplication of the integrand by a multiplicative regularization factor $\frac{\Lambda^{2}}{\vec{k}_{1}^{2}+\Lambda^{2}} \frac{\Lambda^{2}}{\vec{k}_{2}^{2}+\Lambda^{2}}$. The auxiliary parameter $\Lambda$ cancels when the high-energy part from two-photon exchange [see Figs. 11 middle, and Fig. [1] right] is added to the result (see also Ref. [24]). From the integral (28), we extract a leading double logarithmic correction,

$$
\begin{equation*}
\delta E_{S}=-\frac{4 \alpha(Z \alpha)^{5} \mu^{3} \delta_{\ell 0}}{3 \pi^{2} m_{\mu} m_{N} n^{3}} \ln ^{2}\left(4 Z \alpha \beta_{N}^{2}\right) \tag{29}
\end{equation*}
$$

which is nonvanishing only for $S$ states $(\ell=0)$. This correction evaluates to 0.0003 meV for the $2 P_{1 / 2}-2 S_{1 / 2}$ Lamb shift in $\mu \mathrm{H}, 0.0002 \mathrm{meV}$ for $\mu \mathrm{D}, 0.0072 \mathrm{meV}$ for $\mu \mathrm{He}^{3}$, and 0.0056 meV for $\mu \mathrm{He}^{4}$. Because subleading logarithmic terms, and nonlogarithmic terms are missing, the theoretical uncertainty of the results in Eq. (29) should be taken as $100 \%$ of the leading logarithmic correction calculated here.

## VI. CONCLUSIONS

Our theoretical investigations are motivated by the necessity to shed light on the recently observed discrepancy of theory and experiment in $\mu \mathrm{H}$ (see Ref. [3]. By an explicit evaluation of the matrix elements of the two-body Breit Hamiltonian, we obtain the nuclear-spin dependent recoil contributions to the Lamb shift in $\mu \mathrm{H}$ and $\mu \mathrm{D}$ given in Eq. (15), and confirm that the results are exact in the mass ratio, so that the existence of further recoil corrections [15] can be ruled out at order $(Z \alpha)^{4}$. The calculation of the relativistic reduced-mass corrections to vacuum polarization using the massive Breit Hamiltonian is shown to involve a nontrivial nuclear-spin dependent term [see Eq. (21)]. Our detailed numerical investigation (see Table 【I) slightly decreases the observed experimental-theoretical discrepancy [3] (in contrast to a recent investigation [25], where the authors obtain an increase of the discrepancy, based on a treatment which is perturbative in the mass ratio).

A detailed breakdown of the relativistic corrections to vacuum polarization, including the reduced-mass corrections is given in Table for muonic hydrogen, muonic deuterium and muonic helium ions. For muonic hydrogen, the sum of the entries in rows 3 and 19 of the theory in the supplemental material of Ref. [3], minus the entry in row 1 of the same supplemental material, amounts to $(205.0282-0.0041-205.0074) \mathrm{meV}=0.0167 \mathrm{meV}$; this is close to the result indicated in Table 1 of Ref. [16], which is 0.0169 meV . In Refs. [3, 7, 16], the second entry in the mentioned combination $(-0.0041 \mathrm{meV})$ has been referred to as a "recoil correction to vacuum polarization", whereas we here refer to the effect as a relativistic correction to vacuum polarization with a proper account of the reduced-mass dependence. Our approach is nonperturbative in the mass ratio $\xi_{N}$ and isolates the terms of order $\alpha(Z \alpha)^{4}$, while treating the two-body aspects of the problem to all orders.

Our calculations lead to significant shifts of theoretical predictions for $\mu \mathrm{He}^{4}$ with respect to published values (experiments are planned for the near future). Specifically, for $\mu \mathrm{He}^{4}$, our nuclear-spin dependent Barker-Glover type correction $L$ of 0.295 meV differs from the value of 0.074 meV given in Refs. 11, 16] by +0.221 meV . For $\mu \mathrm{He}^{4}$, our result for the relativistic correction to vacuum polarization, with a full account of the reduced-mass dependence, reads as 0.521 meV for the $2 P-2 S$ difference, to be compared with a value of -0.202 meV given in Ref. 11]. This leads to a total upward shift of theoretical predictions for the $2 P_{1 / 2}-2 S_{1 / 2}$ Lamb shift in $\mu \mathrm{He}^{4}$ by $[0.521-(-0.202)+0.221-0.010] \mathrm{meV}=+0.934 \mathrm{meV}$ relative to Ref. [11] (where we add the small correction of the reference value of the leading VP correction) and by $(+0.221+0.013) \mathrm{meV}=0.234 \mathrm{meV}$ relative to Ref. [16] (where we add the difference in the relativistic correction to vacuum polarization from Table (1).

The radiative-recoil correction obtained in Eq. (29) is numerically small; however, this two-loop bound-state
correction has traditionally been one of the most elusive effects in bound-state quantum electrodynamics for two-body systems. Its calculation in leading logarithmic approximation helps to determine the overall uncertainty of theoretical predictions with regard to the conceptually involved higher-order recoil corrections to VP, given by
the two-body nature of the bound system.

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