Nonrelativistic contributions of order $\alpha^5 m_\mu c^2$ to the Lamb shift in muonic **hydrogen and deuterium, and in the muonic helium ion**

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Contributions to the energy levels in light muonic atoms and, in particular, to the Lamb shift fall into a few well-distinguished classes. The related diagrams are calculated using different approaches. In particular, there is a specific type of nonrelativistic (NR) contribution. Here, we consider such corrections to the Lamb shift of order $\alpha^5 m_\mu$. These contributions are due to free vacuum-polarization loops as well as to various effects of light-by-light scattering. The closed loop in the related diagrams is an electronic one, which allows an NR consideration of the muon. Both types of contributions have been known for some time, however, the results obtained to date are only partial results. We complete a calculation of the $\alpha^5 m_\mu$ contributions for muonic hydrogen. The results are also adjusted for muonic deuterium atom and helium ion.

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The recent progress of the Paul Scherrer Institut (PSI) experiment by Pohl *et al.* concerning the Lamb shift in muonic hydrogen [\[1\]](#page-3-0) has attracted interest in the theory of the Lamb shift in light muonic atoms. Their study can provide us with information on certain nuclear structure effects with accuracy that is not available in any other experiment.

To obtain such data, one has to be able to separate quantum electrodynamics (QED) effects from the nuclear structure effects, and, for this purpose, an adequate QED theory providing high accuracy is required. Contributions to the energy levels in light muonic atoms and, in particular, to the Lamb shift fall into a few different well-distinguished classes. A specific theory stands behind each of them. There are corrections, the evaluation of which is identical for hydrogen and muonic hydrogen, and corrections that are specific for muonic atoms. The latter involve a certain part of QED, recoil effects, and effects of the finite nuclear size. An important class of such specific contributions, which, in fact, also include the dominant term for the Lamb shift, is due to nonrelativistic (NR) physics.

Note that atomic momenta in light muonic atoms $\sim Z \alpha m_{\mu} \simeq 1.5 Z m_e$ are compatible with the electron mass, while the atomic energy $\sim (Z\alpha)^2 m_\mu \simeq 0.01 Z^2 m_e$ is much smaller than the electron mass. (The relativistic units in which $\hbar = c = 1$ are applied throughout the paper.) Such an environment produces an important sector of corrections, which deal with an NR bound muon, while the QED effects are present only through the closed electron loops. Meanwhile, the Compton wavelength of electron $\lambda r_e = 1/m_e$ determines the radius of the effective interaction induced by this type

of diagram. The loops may be for either free-loop vacuumpolarization (VP) effects, related to the Uehling and Källen-Sabry potentials and higher-order diagrams, or light-by-light (LbL) scattering contributions.

The VP leading term is of order $\alpha(Z\alpha)^2 m_\mu$, and it has been known for some time, while the second-order VP contribution [of order $\alpha^2 (Z\alpha)^2 m_\mu$] was relatively recently calculated with appropriate accuracy for muonic hydrogen in Ref. [\[2\]](#page-3-0). The accuracy of current and planned experiments requires a complete theory for the NR contributions to the Lamb shift of order $\alpha^5 m_\mu$. The LbL contributions are depicted in Fig. [1,](#page-1-0) while the VP diagrams are presented in Fig. [2.](#page-1-0) Both types of contributions have been known for some time; however, the results obtained up to now were only partial results. In particular, in the case of muonic hydrogen, the contribution in Fig. [1\(c\)](#page-1-0) has not yet been calculated, while there are also some questions [\[3\]](#page-3-0) about the applicability of the so-called scattering approximation applied in Ref. [\[4\]](#page-3-0) to evaluate the contribution in Fig. [1\(b\).](#page-1-0)

Certain LbL contributions have specific names. The first one in Fig. [1](#page-1-0) is a so-called Wichmann-Kroll contribution, and it was calculated for muonic hydrogen with sufficient accuracy in Ref. [\[5\]](#page-3-0). It was also reproduced in Ref. [\[4\]](#page-3-0); we also confirm this contribution. For muonic deuterium and muonic helium-4 ion, the results have been obtained in Refs. [\[6,7\]](#page-3-0), and we confirm the deuterium result [\[6\]](#page-3-0) and obtain a result for a muonic helium ion,

$$
\Delta E_{1a}^{\text{He}} = -0.0198(4) \text{ meV}, \qquad (1)
$$

which is consistent with −0*.*02 meV from Ref. [\[7\]](#page-3-0), but is more accurate, and strongly disagrees with +0*.*135 meV from Ref. [\[8\]](#page-3-0).

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FIG. 1. Characteristic diagrams for three basic contributions of LbL scattering effects to the Lamb shift in muonic hydrogen of order $\alpha^5 m_\mu$. Here, N stands for a nucleus, which may be a proton, a deuteron, etc. The horizontal double line is for the muon propagator in the Coulomb field.

In our calculation, we used approximations for the Wichmann-Kroll potential in the form

$$
V_{\text{WK}}(r) = \frac{\alpha (Z\alpha)^2}{\pi} \frac{Z\alpha}{r} \times 0.361\,662\,331
$$

$$
\times \exp \left[0.372\,8079x - \sqrt{4.416\,798x^2 + 11.399\,11x + 2.906\,096} \right],
$$

as discussed in Ref. [\[3\]](#page-3-0) (see also Ref. [\[9\]](#page-3-0)) and

$$
V_{\text{WK}}(r) = \frac{(Z\alpha)^3 10^{-4}}{r} \begin{cases} \frac{1.528 - 0.489x}{1.374x^3 + 1.41x^2 + 2.672x + 1}, & x \le 1, \\ \frac{0.207x^2 + 0.367x - 0.413}{x^6}, & x > 1, \end{cases}
$$

as considered in Refs. [\[2,10\]](#page-3-0). Here, $x = m_e r$. The results are consistent. Indeed, if higher accuracy is required, one can apply an exact expression $[11]$ for $V_{\text{WK}}(r)$ as a two-dimensional integral.

The second term [Fig. $1(b)$] is called the virtual-Delbrückscattering contribution. It has been calculated for muonic hydrogen in Ref. [\[4\]](#page-3-0). The calculation was based on Refs. [\[10,12\]](#page-3-0), where, at first, a scattering approximation was applied, and, subsequently, a number of further approximations was made. Note that the scattering approximation suggests that the external muon legs in the diagram in Fig. 1(b) are on-shell (i.e., $p^2 = m_\mu^2$), and the muon propagator there is substituted

FIG. 2. Characteristic diagrams for free-electron-VP contributions to the Lamb shift in muonic hydrogen of order $\alpha^5 m_\mu$.

for a free one (i.e., the kinematics is exactly the same if one calculates a related Born scattering amplitude). Since atomic momenta $Z \alpha m_{\mu}$ in light muonic atoms are compatible with the electron mass m_e , the validity of such an approximation is questionable (see, e.g., the discussion in Ref. [\[3\]](#page-3-0)).

We, however, have proved that the scattering approximation is applicable within the uncertainty of order $(Z\alpha)^2 m_\mu / m_e$ (in fractional units), which is at the level of about 1% in muonic hydrogen and deuterium and of about 4% in muonic helium. That is also correct for other simplifying approximations, which were made in the calculations for this contribution in light muonic atoms [\[4,6,7,10,12\]](#page-3-0). A general idea of our evaluation is presented in the Appendix, while the details of our evaluation are to be published elsewhere [\[13\]](#page-3-0).

Eventually, we conclude that the uncertainty of the method applied in Refs. $[4,6,7]$ is substantially smaller than the uncertainty of the related numerical evaluations for the Lambshift correction in muonic hydrogen [\[4\]](#page-3-0), muonic deuterium [\[6\]](#page-3-0), and muonic helium-4 ion [\[7\]](#page-3-0).

The contribution in Fig. $1(c)$ has no specific name. Since all other LbL contributions have one (Wichmann-Kroll term and virtual-Delbrück-scattering contribution), sometimes it is referred to as an light-by-light contribution, which can be somewhat confusing.

This contribution has remained uncalculated for some time. By studying the applicability of the scattering approximation for the diagram in Fig. $1(b)$, we have also managed to prove [\[13\]](#page-3-0) that this remaining contribution can be expressed in terms of the well-known Wichmann-Kroll term,

$$
\Delta E_{1c} = \frac{1}{Z^2} \Delta E_{1a}.
$$
 (2)

The uncertainty of this identity is of order $(Z\alpha)^2 m_\mu/m_e$ (in fractional units), which is at the level of about 1% in muonic hydrogen and deuterium and of about 4% in muonic helium.

By combining our results concerning the uncertainty of various approximations with the numerical results of other authors, we obtain the complete result for all LbL contributions of Fig. 1. The result is listed in the summary table (Table I). With Eq. (2) proved and a possibility to obtain a result for the Wichmann-Kroll (ΔE_{1a}) term with high accuracy for any light muonic atom, the uncertainty in the

TABLE I. The NR QED contributions to the Lamb shift $\Delta E(2s -)$ 2*p*) in light muonic atoms: hydrogen (H), deuterium (D), helium-4 ion (He), which include VP contributions of the first $\left[\alpha(Z\alpha)^2 m_\mu\right]$, the second $\left[\alpha^2(Z\alpha)^2 m_\mu\right]$, and the third $\left[\alpha^3(Z\alpha)^2 m_\mu\right]$ (Fig. 2) order as well as a complete LbL contribution. The latter is a sum of contributions of order $\alpha(Z\alpha)^4 m_\mu$ [Fig. 1(a)], $\alpha^2(Z\alpha)^3 m_\mu$ [Fig. 1(b)], and $\alpha^3(Z\alpha)^2 m_\mu$ [Fig. 1(c)]. Results marked with a \star were obtained in this work.

Term	(meV)	$\Delta E^{\rm H}(2p-2s) \ \Delta E^{\rm D}(2p-2s) \ \Delta E^{\rm He}(2p-2s)$ (meV)	(meV)
First-order VP	205.00736	227.634.67	1665.7729
Second-order VP	1.65885	1.83804	13.2769
Third-order VP	0.00752	$0.00842(7)^*$	$0.074(3)^{*}$
LbL (Fig. 1)		-0.000 71(15)* -0.000 73(16)*	$-0.005(10)^{*}$
NR total		206.673 02(15) 229.480 40(17)	1679.119(10)

calculation of the complete LbL contribution now comes from the virtual-Delbrück-scattering term, which should determine the eventual uncertainty of the NR $\alpha^5 m_\mu$ term for muonic hydrogen, deuterium, and helium ion.

Another major NR contribution of order $\alpha^5 m_\mu$ is due to VP contributions. The VP terms of this order were studied for muonic hydrogen in Ref. [\[14\]](#page-3-0). The diagrams are depicted in Fig. [2,](#page-1-0) which includes contributions of the first [Fig. $2(a)$ – $2(d)$], the second [Fig. $2(e)$ and $2(d)$], and the third [Fig. $2(f)$] order of NR perturbation theory (NRPT).

The most complicated terms are indeed related to the first line of Fig. [2;](#page-1-0) however, these diagrams were crosschecked due to their contributions to the anomalous magnetic moment of a muon [\[15,16\]](#page-3-0), and we can rely on them.

The contributions of the second line of Fig. [2](#page-1-0) are specific for muonic atoms and do not correlate directly with any calculation for the muon $g - 2$. Those, as well as part of the diagrams in the first line, have been recalculated completely independent from the results in Ref. [\[14\]](#page-3-0).

We confirm the second-order terms of NRPT, while our result [\[17\]](#page-3-0) for the third-order term (the last diagram in Fig. [2\)](#page-1-0) disagrees with the one originally published in Ref. [\[14\]](#page-3-0). After a correction [\[18\]](#page-3-0), their result agrees with ours. In our calculations, we used techniques developed while investigating second-order VP contributions to the hyperfine structure of muonic hydrogen [\[19\]](#page-3-0).

The diagrams in Fig. [2](#page-1-0) were also discussed in various papers in the context of the Lamb shift in muonic deuterium $[6]$ and muonic helium-4 ion [\[8\]](#page-3-0). For this purpose, a part of the contributions was recalculated there.

Here, we reevaluate all the VP contributions, and the results are listed in Table [I.](#page-1-0) When we compare these with the results of the paper previously mentioned, we have to acknowledge that our results are not in complete agreement with theirs.

In Ref. $[6]$, only contributions of Figs. $2(a)$ and $2(b)$ were directly calculated for muonic deuterium, and their results agree with ours. However, those results were not applied there, but instead, the muonic hydrogen result was rescaled. That was achieved by assuming that the result for muonic hydrogen, presented in Ref. [\[14\]](#page-3-0) in the form of

$$
\Delta E(2p - 2s) = C_3 \left(\frac{\alpha}{\pi}\right)^3 (Z\alpha)^2 m_r, \tag{3}
$$

where m_r is the muon reduced mass, can be directly applied for the result of muonic deuterium. That has not been claimed in Ref. [\[14\]](#page-3-0) and is indeed incorrect, and the value of the coefficient [\[17,18\]](#page-3-0),

$$
C_3 = 0.118\,680(12),\tag{4}
$$

is valid only for muonic hydrogen [cf. with $C_3 =$ 0*.*120 045(12) from Ref. [\[14\]](#page-3-0), which needs a correction [\[17\]](#page-3-0) as explained previously]. The related values for other light muonic atoms obtained here,

$$
C_3 = \begin{cases} 0.1262(11) & \text{for } \mu\text{D}, \\ 0.270(17) & \text{for } \mu\text{He}^+, \end{cases}
$$
 (5)

obviously differ from Eq. (4).

The muonic helium-4 paper [\[8\]](#page-3-0) lacks a complete result, and only a part of the diagrams of Fig. [2](#page-1-0) were recalculated. Our results are not in fair agreement, and, in particular, we strongly disagree with the contribution of Fig. $2(e)$ for muonic helium. In the Wichmann-Kroll contribution [Fig. $1(a)$], we also strongly disagree with the result in Ref. [\[8\]](#page-3-0), while we agree with the result in Ref. [\[7\]](#page-3-0), for which we obtain higher accuracy [see Eq. (1)].

Finally, in Table [I,](#page-1-0) we summarize a complete theory of NR QED contributions to the Lamb shift in muonic hydrogen, deuterium, and helium ions up to the order $\alpha^5 m_\mu$ (see Ref. [\[3\]](#page-3-0) for references to the calculation of the low-order corrections).

Note added. Recently, we have calculated the LbL contribution within a static-muon approximation (see the Appendix). The preliminary results for ΔE_{1b} , which are 0.001 15(1) meV for μ H, 0.001 24(1) meV for μ D, and 0.0114(4) meV for μ He⁺, are somewhat below the former results [\[4,6,7\]](#page-3-0), but still are in fair agreement with them. These more accurate results will be reported in detail in a future publication [\[13\]](#page-3-0).

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APPENDIX: ON APPROXIMATIONS FOR THE LbL CONTRIBUTION

We have proven a type of theorem [\[13\]](#page-3-0) that the diagrams in Fig. [1](#page-1-0) can be calculated in light muonic atoms (for simplicity, we consider further muonic hydrogen) within the static-muon approximation, in which the complete muon-line factor shrinks to

$$
\mathcal{F}(\mathbf{q}) = \int \frac{d^3 p}{(2\pi)^3} \Psi^*(\mathbf{p}) \Psi(\mathbf{p} + \mathbf{q}),
$$

where q is the total momentum transfer to the muon line, Ψ is the wave function, and the error is of the order of $(Z\alpha)^2 m_\mu/m_e$.

The scattering approximation [\[4,6\]](#page-3-0) agrees with the staticmuon approximation within the same uncertainty.

The proof of the theorem will be presented elsewhere [\[13\]](#page-3-0), and, here, we will explain its main idea. The proton and the muon are both NR particles. Their descriptions are very similar.

FIG. 3. Reduction of diagrams with free or bound fermion propagators to static-fermion diagrams [i.e., to the static-proton approximation (which is more commonly refered to as the externalfield approximation)] (left) and to the static-muon approximation (right).

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Let us first compare the related diagrams with free NR fermion propagators (cf. Fig. [3\)](#page-2-0). The expressions for the muon and proton lines are identical. Apparently, one can approximate the proton line within the external-field approach or, which is similar, by a static proton. To transform the complete NR expressions to the static-proton case, we have to neglect the proton kinetic energy in the proton propagators. Once that is done, after a chain of identities, we should arrive at the external-field approximation.

A reason to neglect the energy is the fact that a characteristic energy, related to a particle of the mass *M*, is $E_M \sim \gamma^2/M$, where $\gamma = Z \alpha m_{\mu}$ is a characteristic atomic momentum. One can prove that we can expand using small parameters E_M/m_e and E_M/γ . However, in muonic hydrogen, they are of the same order since $\gamma \sim m_e$. The parameter E_M/m_e (and the related error) differs indeed for a muon and a proton, but it is small for both.

Thus, as long as the muon propagator is a free one, there is no difference in proving that we can apply the staticmuon approximation and the static-proton approximation (see Fig. [3\)](#page-2-0).

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Meanwhile, in reality, the situation for a muon and a proton is somewhat different. The muon characteristic momentum is of the same order as the electron mass $\gamma \sim m_e$, and we should treat it as a bound one.

The NR Coulomb Green function of a muon includes

$$
G_C(E, \mathbf{p}, \mathbf{p}') = i \sum_{\lambda} \frac{|\lambda(\mathbf{p})\rangle \langle \lambda(\mathbf{p}')|}{E - E_{\lambda} + i0},
$$

a summation over all intermediate states *λ* of a continuous and discrete spectrum, involving energy of the intermediates. The characteristic energy of an intermediate state is indeed of an order of magnitude of the atomic bound energy $E_\lambda \sim \gamma^2/m_\mu$, and we can neglect it, as we already did in the case of the free propagators. After that, the sum over intermediates shrinks to the unity operator, and the Coulomb propagator becomes equal to a free one with the kinetic-energy term $p^2/2m_\mu$ neglected

$$
i\sum_{\lambda}\frac{|\lambda\rangle\langle\lambda|}{E-E_{\lambda}+i0}\rightarrow i\sum_{\lambda}\frac{|\lambda\rangle\langle\lambda|}{E+i0}=\frac{i}{E+i0}.
$$

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