

Two-loop vacuum polarization in a Coulomb field

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The leading-order two-loop vacuum-polarization potential, linear in the Coulomb field of a nucleus, was first derived in the seminal 1955 work of Källén and Sabry [*Dan. Mat. Fys. Medd.* **29**, 1 (1955)]. The higher-order two-loop vacuum-polarization corrections, however, have remained unknown until now. In this work, we compute Coulomb corrections to the Källén-Sabry potential, specifically those involving three, five, and seven Coulomb interactions inside the vacuum-polarization loop. The potentials are evaluated in momentum space and subsequently used to calculate one-electron energy shifts. Our results reduce the theoretical uncertainty of the two-loop vacuum-polarization contribution to transition energies, which is required for next-generation tests of bound-state QED in heavy one- and few-electron ions as well as for the determination of nuclear charge radii.

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I. INTRODUCTION

Theoretical and experimental investigations of the Lamb shift in atomic systems provide stringent tests of bound-state quantum electrodynamics (QED) theory, including the regime where the electron-nucleus coupling parameter $Z\alpha$ is not small (where Z is the nuclear charge number and α is the fine-structure constant) [1]. QED effects of first order in α have been extensively calculated and verified by numerous experiments [2]. In contrast, calculations of two-loop QED effects, of order α^2 , have not been fully completed yet. In hydrogenlike atoms, the two-loop effects typically determine the theoretical uncertainty of energy levels and thus represent a central challenge in advancing our understanding of these systems [3]. Similarly, in few-electron highly charged ions, two-loop QED corrections contribute significantly to the theoretical uncertainties, thereby limiting comparisons with available experimental data [4,5] and possible determinations of nuclear charge radii [6].

The two-loop QED effects have been extensively investigated during the last few decades, both using methods based on the $Z\alpha$ expansion [7–10] and also using the all-order (in $Z\alpha$) approach [11,12]. In particular, the two-loop self-energy correction has been evaluated nonperturbatively in $Z\alpha$ [13,14], along with most two-loop diagrams with vacuum-polarization loops [15]. The largest uncertainty of the two-loop QED contribution for hydrogenlike atoms comes [3] from two uncalculated effects: (1) Coulomb corrections to the two-loop vacuum polarization and (2) the electron self-energy with a light-by-light-scattering insertion into the photon line. The goal of the present investigation is to compute the first of the two missing effects, which is an important step towards

completing the long-standing project of calculating the full set of one-electron two-loop QED diagrams.

The vacuum-polarization (VP) potential can be conveniently represented [16] in the form of a double expansion in α and $Z\alpha$,

$$V_{\text{VP}}(\mathbf{r}) = \sum_{i,j} V_{ij}(\mathbf{r}) \equiv \sum_{\substack{i=1,2,\dots \\ j=1,3,\dots}} \alpha^i (Z\alpha)^j \tilde{V}_{ij}(\mathbf{r}). \quad (1)$$

According to the Furry theorem, the expansion terms with even powers of $Z\alpha$ vanish, so the summation over j includes only odd j 's.

At the one-loop ($i = 1$) level, the VP potential has been extensively studied in the literature. The first term of the expansion, $V_{11}(\mathbf{r})$, is the well-known Uehling potential [17]. The next-order term, $V_{13}(\mathbf{r})$, was derived by Wichmann and Kroll [18], with its explicit coordinate-space form obtained in Ref. [16]. The Coulomb corrections of order $(Z\alpha)^3$ and higher to the one-loop VP are commonly referred to as the Wichmann-Kroll potential, which has been calculated to all orders in $Z\alpha$ numerically [19–21]. For the point nuclear model, accurate approximate formulas for the Wichmann-Kroll potential are available in the literature [22,23].

The two-loop ($i = 2$) VP potential has been studied to a significantly lesser extent. Only the leading $Z\alpha$ -expansion term, V_{21} , commonly referred to as the Källén-Sabry potential, is presently known [24]. Explicit formulas for this potential can be found in Refs. [16,25]. Some partial results for higher-order VP energy shifts were reported in Ref. [26]. In the present investigation we compute the Coulomb corrections to the Källén-Sabry potential of orders $(Z\alpha)^3$, $(Z\alpha)^5$, and $(Z\alpha)^7$, namely, potentials V_{23} , V_{25} , and V_{27} .

It is important to note that the $Z\alpha$ expansion of the VP potential in Eq. (1) remains useful not only when the parameter $Z\alpha$ is small but even as it approaches unity, as is the case for heavy ions. For example, in the case of the $1s$ state of uranium ($Z = 92$), V_{11} induces an energy shift of -94 eV, V_{13} contributes 4.6 eV, and V_{15} contributes 0.57 eV, with the net effect of the remaining one-loop VP tail amounting to merely

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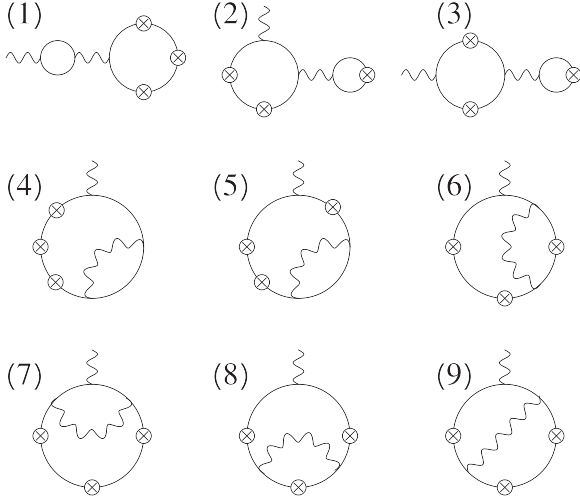


FIG. 1. Feynman diagrams contributing to V_{23} . Solid lines denote free-electron propagators, wavy lines denote the photon propagators, and the circled crosses denote the Coulomb interactions with the nucleus.

0.17 eV. This is in contrast to the $Z\alpha$ expansion of *energy shifts*, which converge poorly in the high- Z regime. For example, for the $1s$ state of uranium, the leading $Z\alpha$ -expansion term gives -64 eV, significantly deviating from the full result of -89 eV. With this in mind, we will adopt the $Z\alpha$ expansion of the potential in Eq. (1) for our calculations of the two-loop VP potential. This approach should remain applicable for most atoms of practical interest, with the exception of superheavy elements.

An additional advantage of using the expansion of Eq. (1) is that the potentials $\tilde{V}_{ij}$ do not depend on Z or, indeed, on any other parameter. As a result, the potentials $\tilde{V}_{23}$, $\tilde{V}_{25}$, and $\tilde{V}_{27}$, once they are computed and stored on a grid, can be employed for evaluating energy shifts in arbitrary atoms, including muonic, antiprotonic, and other exotic atoms.

This paper is organized as follows. In Sec. II we describe the method to calculate the VP potentials in momentum space. Section III describes the calculations of the corresponding energy shifts. Section IV presents the numerical results obtained for the VP potential and the corresponding energy shifts and discusses the experimental consequences of the obtained results.

Relativistic units ($\hbar = c = m = 1$) are used throughout this paper, where m is the electron mass. We use boldface ($\mathbf{p}$) for three-vectors and italic style (p) for four-vectors. Four-vectors have the form $p = (p_0, \mathbf{p})$. We also use the notation $\not{p} = p_\mu \gamma^\mu$; the tensor $g_{\mu\nu}$ corresponds to the signature $(+, -, -, -)$, and the Dirac matrices fulfill the condition $\gamma_\mu \gamma_\nu + \gamma_\nu \gamma_\mu = 2g_{\mu\nu}$. The Coulomb potential is $V_C(r) = -Z\alpha/r$ in coordinate space.

II. CALCULATION OF POTENTIALS

We calculate here the potentials V_{23} , V_{25} , and V_{27} . The calculation is performed in momentum space, with the Fourier

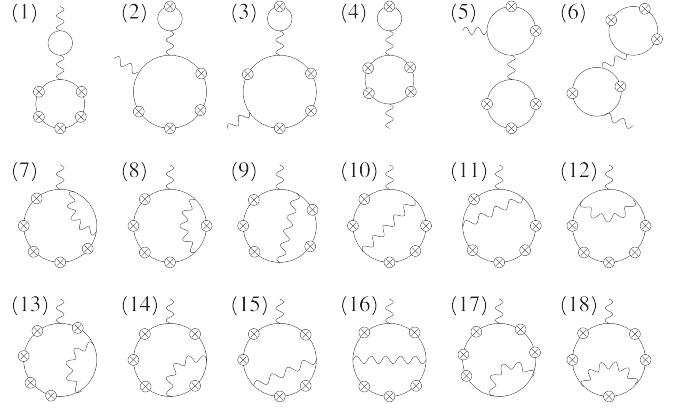


FIG. 2. Feynman diagrams contributing to V_{25} .

transform of the potential defined by

$$V(\mathbf{p}) = \int e^{-i\mathbf{p}\cdot\mathbf{r}} V(\mathbf{r}) d^3\mathbf{r}.$$

The Feynman diagrams contributing to V_{23} , V_{25} , and V_{27} are shown in Figs. 1–3, respectively. The set of Feynman diagrams for V_{ij} is obtained by taking all possible graphs that satisfy the following conditions: (1) They are connected, (2) they have one external photon line, j Coulomb-potential insertions, and no other external lines, (3) they have i independent loops, and (4) they do not have electron loops with an odd number of vertices (Furry's theorem).

In our approach, graphs 2–9 in Fig. 1, 2–18 in Fig. 2, and 2–30 in Fig. 3 will be treated as genuine two-loop diagrams, while graph 1 in Figs. 1–3 is expressed as a product of two one-loop diagrams in momentum space and evaluated separately.

We employ methods of free QED in our calculation. To this end, we first *unfold* each Feynman diagram. Unfolding means

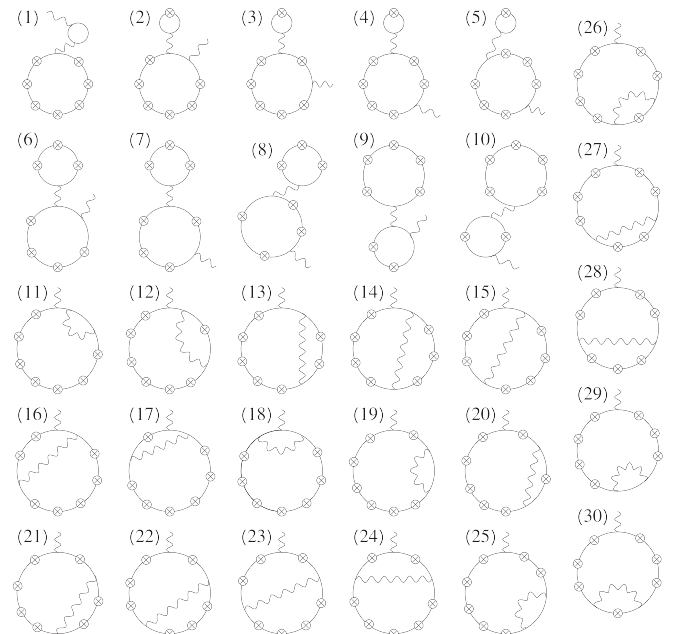


FIG. 3. Feynman diagrams contributing to V_{27} .

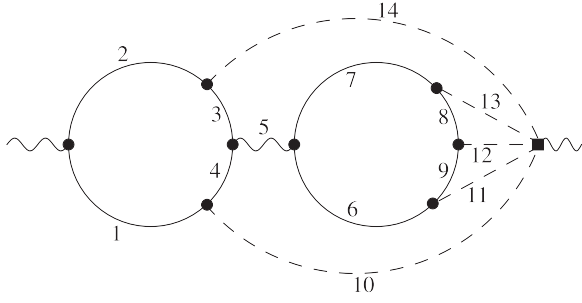


FIG. 4. The unfolded Feynman diagram corresponding to graph 6 in Fig. 2.

replacing each Coulomb-potential insertion with a Coulomb-propagator line extending to an artificially added vertex; see Fig. 4 for an example. In Fig. 4, the additional vertex is shown as a black square, and the dashed lines represent the Coulomb propagators. The new vertex has a fictitious external line that carries away the excess momentum, so that momentum conservation holds for all vertices. The additional vertex contributes no multiplier and carries no tensor index. In the Feynman gauge, the photon, electron, and Coulomb propagators are (up to prefactors)

$$\frac{i(\not{q} + m)}{q^2 - m^2 + i0}, \quad \frac{-ig_{\mu\nu}}{q^2 + i0}, \quad \frac{-\delta(q_0)\delta_{\mu 0}}{q^2}, \quad (2)$$

respectively. The unfolded diagrams for V_{23} , V_{25} , and V_{27} have four, six, and eight loops, respectively. The large number of loops makes the computation of these Feynman diagrams demanding and time-consuming.

In this work, we do not employ dimensional regularization or any other schemes based on expansions around singular points, which are commonly used in the literature. Instead, we remove all divergences by performing point-by-point subtractions in the Feynman parametric space by modifying integrands with suitably chosen counterterms that make the integrals finite. Point-by-point subtraction methods are relatively rarely used in quantum field calculations because of the complicated structure of divergences in Feynman diagrams. However, they become advantageous in numerical computations of diagrams with many loops. These methods were developed for calculations of the free-electron anomalous magnetic moment [27–32]; developments for other problems also exist [33].

Our method is based on a variant of the Bogoliubov-Parasiuk-Hepp-Zimmermann (BPHZ) renormalization method [34–36]. Applications of BPHZ to the two-loop QED effects in a Coulomb field were previously studied in Ref. [37]. An advantage of our approach is that it directly reduces the problem to numerically computable integrals. Our general approach is based on a direct application of Zimmermann’s forest formula [36,38]. This formula implements renormalization “in place” by adding counterterms to each Feynman amplitude. According to Zimmermann’s forest formula, the renormalized Feynman amplitude is defined as follows:

(1) A summation over forests F of ultraviolet (UV) divergent subdiagrams is performed; a forest is a set of sub-

diagrams, where each pair of subdiagrams is either nested or nonintersecting.

(2) In each term, we replace the Feynman amplitude of each subdiagram $G' \in F$ with a momentum-space polynomial whose degree corresponds to the UV degree of divergence of G' , obtained by applying suitable projections. The transformation is organized so that it is first applied to smaller subgraphs (with respect to inclusion) and then carried over to larger subgraphs, ultimately yielding the final amplitude. In the original formulations of the forest formula [36,38], Taylor expansions around zero momenta were used; here, however, we employ slightly different projectors for certain types of subgraphs.

(3) The coefficient of the term is $(-1)^{|F|}$.

With N_l and N_γ denoting the numbers of external electron and photon (or Coulomb) lines of a subdiagram, the UV-divergent subdiagrams in QED are *electron self-energy* ($N_l = 2$, $N_\gamma = 0$), *vertexlike* ($N_l = 2$, $N_\gamma = 1$), *photon self-energy* ($N_l = 0$, $N_\gamma = 2$), and *photon-photon scattering* ($N_l = 0$, $N_\gamma = 4$). All such subdiagrams of the original Feynman diagram must be included in the forest formula. However, additional subdiagrams must also be included in the forest formula for the unfolded diagram, namely, those with exactly two photon external lines (one fictitious) and no other external lines (except those connected to a fictitious vertex). These subdiagrams correspond to lower-order potential insertions and are also UV divergent. For example, in Fig. 4 the following subdiagrams must be included: $\{1, 2, 3, 4\}$, $\{6, 7, 8, 9\}$, $\{6, 7, 8, 9, 11, 12, 13\}$, and $\{1, 2, \dots, 14\}$, where subgraphs are encoded by sets of internal graph lines. The full diagram is always included. In Zimmermann’s forest formula, we take the value at zero momenta for these special subdiagrams, as well as for photon-photon scattering subgraphs. All subtraction contributions vanish identically due to gauge invariance once all Feynman diagrams are summed.

The subtraction projectors for the electron self-energy and vertexlike subdiagrams in Zimmermann’s forest formula are usually chosen to correspond to QED on-mass-shell renormalization conditions. The drawback of this choice is that these conditions generate infrared (IR) divergences.¹ We avoid IR divergences by using the projector U , defined as

$$(U\Gamma)_\mu(p, q) = a(m_0^2)\gamma_\mu,$$

$$(U\Sigma)(p) = u(m^2) + v(m^2)m + v((m_0^2)^2)(\not{p} - m),$$

where $\Gamma_\mu(p, q)$ is a vertexlike Feynman amplitude; $p - \frac{q}{2}$ and $p + \frac{q}{2}$ are the incoming and outgoing electron momenta, respectively; q is the photon momentum,

$$\begin{aligned} \Gamma_\mu(p, 0) &= a(p^2)\gamma_\mu + b(p^2)p_\mu + c(p^2)\not{p}p_\mu \\ &\quad + d(p^2)(\not{p}\gamma_\mu - \gamma_\mu\not{p}); \end{aligned}$$

$\Sigma(p)$ is an electron self-energy Feynman amplitude,

$$\Sigma(p) = u(p^2) + v(p^2)\not{p};$$

¹See, e.g., the explicit one-loop expression for the renormalization constant (119.7a) in [39].

and $(m_0)^2$ is a free parameter. In our calculations, we set

$$(m_0)^2 = -5m^2$$

to minimize numerical cancellations inside integrals (this choice is motivated by our numerical experience). Similar projectors were introduced previously for the free electron g -factor calculations: first in Ref. [40], with $(m_0)^2 = m^2$, and later in the current form in Ref. [41]. The projector U preserves the Ward identity, extracts the mass part completely at the physical point m^2 , and does not generate IR divergences. It introduces an electron wave-function renormalization factor relative to standard QED on-mass-shell renormalization, but this factor does not appear in our case, as our Feynman diagrams have no external electron lines.²

Our method yields a single Feynman-parametric integral

$$\int_{z \geq 0} F(\mathbf{p}, z_1, \dots, z_n) \delta(z_1 + \dots + z_n - 1) d^n z \quad (3)$$

for each Feynman diagram. Here, z_j corresponds to the j th internal line of the *unfolded* diagram, and $\mathbf{p}$ is the external momentum. These integrals are finite and can be computed separately for each diagram and then summed. Our procedure for obtaining the functions F involves the Schwinger parametrization as an intermediate step as follows:

(1) Introduce the Schwinger parametrization for the propagators in Eq. (2), obtaining

$$(q + m) e^{iz_j(q^2 - m^2 + i\varepsilon)}, \quad ig_{\mu\nu} e^{iz_j(q^2 + i\varepsilon)}, \\ i\delta(q_0) \delta_{\mu 0} e^{iz_j(q^2 + i\varepsilon)},$$

where $z_1, \dots, z_n \geq 0$ are the Schwinger parameters, $\varepsilon > 0$ is an infrared regulator, and j labels the diagram line.

(2) Perform the loop-momentum integrations. We assume the forest formula described above is applied, but the *whole diagram is excluded from it*. The momentum integral diverges, but in this step we ignore the divergence and use the standard formulas for multidimensional Gaussian integrals with polynomial factors. We obtain

$$F^{\text{Schw}}(\mathbf{p}, z_1, \dots, z_n, \varepsilon) \\ = \frac{1}{D_0(z)^{1/2} D_1(z)^{3/2}} \left[\sum_{l=0}^{s/2} R_l(\mathbf{p}^2, z) \right] e^{iA(z)\mathbf{p}^2 + iB(z) - \varepsilon \sum_{j=1}^n z_j} \\ + \text{counterterms},$$

where D_0 and D_1 are the first Symanzik polynomials (see, for example, Ref. [45]) of the original and unfolded diagrams, respectively; R_l is a polynomial in $\mathbf{p}^2$ (constant for $l = s/2$) and rational and homogeneous, of degree $-l$, in z ; the symbol s denotes the number of electron lines in the diagram; A and B

are rational, homogeneous functions of degree 1 and real; and counterterms have the same form, but with different D_j , R_j , and A (see, for example, [43,46,47]).

(3) Switch to Feynman parameters by

$$F(\mathbf{p}, z) = \frac{1}{\mathbf{p}^2} \lim_{\varepsilon \rightarrow +0} \int_0^{+\infty} \lambda^{n-1} \\ \times [F^{\text{Schw}}(\mathbf{p}, \lambda z, \varepsilon) - F^{\text{Schw}}(\mathbf{0}, \lambda z, \varepsilon)] d\lambda, \quad (4)$$

where the denominator $\mathbf{p}^2$ originates from the propagator of the external photon (which must be included in the potential as an internal photon propagator), while the subtraction of the $\mathbf{p} = \mathbf{0}$ term implements the remaining subtraction of the whole diagram in Zimmermann's forest formula.

The integration over λ and the limit can be performed analytically, yielding

$$F(\mathbf{p}, z) = \frac{1}{D_0(z)^{1/2} D_1(z)^{3/2}} \\ \times \left\{ \frac{W_0(z)}{\mathbf{p}^2} \log \left(1 + \frac{A(z)}{B(z)} \mathbf{p}^2 \right) \right. \\ \left. + \sum_{l=1}^{s/2} \left[\frac{W_l(z)}{\mathbf{p}^2} \left(\frac{1}{[A(z)\mathbf{p}^2 + B(z)]^l} - \frac{1}{B(z)^l} \right) \right] \right. \\ \left. + \sum_{l=1}^{s/2} \frac{Y_l(\mathbf{p}^2, z)}{[A(z)\mathbf{p}^2 + B(z)]^l} \right\} + \text{counterterms},$$

where $W_l(z)$ are rational in z and $Y_l(\mathbf{p}^2, z)$ are polynomial in $\mathbf{p}^2$ and rational in z . Each $W_l(z)$ is easily extractable from the constant term of $R_{\frac{s}{2}-l}(\mathbf{p}^2, z)$ in $\mathbf{p}^2$, while each $Y_l(\mathbf{p}^2, z)$ comes from the remaining terms. The log term³ arises from the logarithmic overall UV divergence of the full diagram; the separate subtraction ensures that these log terms are finite.

The value $F(\mathbf{0}, z)$ can easily be obtained by taking the limit $\mathbf{p} \rightarrow \mathbf{0}$. However, the corresponding integral (3) may diverge at $\mathbf{p} = \mathbf{0}$. The total value of $V_{ij}(\mathbf{p} = \mathbf{0})$ is finite, but in our calculation we cannot guarantee explicitly finite individual integrals at $\mathbf{p} = \mathbf{0}$. As a consequence, we are able to perform computations for small nonzero values of $|\mathbf{p}|$, but not at $\mathbf{p} = \mathbf{0}$. However, extrapolation to $\mathbf{p} = \mathbf{0}$ suffices for all practical purposes.

We evaluate the integrals (3) numerically using the Monte Carlo method. It is well-known that the convergence rate of Monte Carlo integration depends critically on the choice of the probability density function (PDF). Adaptive algorithms that fit the PDF to the integrand exist in the literature, but they can adjust only a relatively small number of parameters. For the complicated structure of typical integrands in Feynman-parameter integrations, such adaptive algorithms become inefficient at high dimensionality. In the present work, we employ a nonadaptive algorithm based on a theoretical analysis of the integrand's behavior in Feynman-parametric space. This algorithm provides a unique PDF for each Feynman diagram. The problem of constructing this PDF is closely related

²In our case it can be checked immediately by collecting the corresponding differences in all Feynman diagrams, taking into account the one-loop Ward identity. The general-case statement is an important component of the QED renormalizability proof. See, for example, [42]. A clear explanation is also given in [43]. See also an application example of changing the subtraction point in Sec. 19.9 of [44].

³Since $W_0(z)$ can be multiplied by an arbitrary constant, there is no need to specify the base of log.

TABLE I. The values of $\tilde{V}_{23}(\mathbf{p})$ for different $|\mathbf{p}|$.

$ \mathbf{p} $	$\tilde{V}_{23}(\mathbf{p})$	$ \mathbf{p} $	$\tilde{V}_{23}(\mathbf{p})$	$ \mathbf{p} $	$\tilde{V}_{23}(\mathbf{p})$	$ \mathbf{p} $	$\tilde{V}_{23}(\mathbf{p})$
0.001	0.062303(73)	0.003	0.062197(69)	0.005	0.062214(68)	0.01	0.062164(67)
0.03	0.062011(66)	0.05	0.062171(66)	0.1	0.061785(64)	0.15	0.061358(63)
0.16	0.061254(63)	0.17	0.061148(63)	0.18	0.061115(63)	0.19	0.060879(62)
0.2	0.060828(62)	0.22	0.060551(61)	0.24	0.060286(61)	0.26	0.059995(61)
0.28	0.059852(61)	0.3	0.059321(60)	0.32	0.059028(59)	0.34	0.058693(59)
0.36	0.058397(58)	0.38	0.057974(58)	0.4	0.057655(57)	0.42	0.057203(57)
0.44	0.056844(56)	0.46	0.056455(54)	0.48	0.056028(54)	0.5	0.055616(53)
0.55	0.054473(52)	0.6	0.053423(52)	0.65	0.052335(50)	0.7	0.051293(48)
0.75	0.049992(46)	0.8	0.048804(45)	0.85	0.047781(44)	0.9	0.046518(43)
0.95	0.045357(42)	1	0.044156(40)	1.1	0.041927(37)	1.2	0.039814(34)
1.3	0.037642(32)	1.4	0.035669(30)	1.5	0.033819(28)	1.6	0.032027(27)
1.7	0.030337(27)	1.8	0.028775(25)	1.9	0.027324(22)	2	0.025955(22)
2.1	0.024688(21)	2.2	0.023483(20)	2.3	0.022408(18)	2.4	0.021361(17)
2.5	0.020364(16)	2.6	0.019493(15)	2.7	0.018654(15)	2.8	0.017837(14)
2.9	0.017099(14)	3	0.016403(13)	3.5	0.013579(11)	4	0.0114472(89)
4.5	0.0098321(77)	5	0.0085598(65)	5.5	0.0075518(60)	6	0.0067090(51)
6.5	0.0060201(47)	7	0.0054442(42)	7.5	0.0049455(38)	8	0.0045219(34)
9	0.0038329(29)	10	0.0032963(25)	11	0.0028723(22)	12	0.0025336(19)
13	0.0022512(17)	14	0.0020171(15)	15	0.0018173(14)	16	0.0016467(13)
18	0.0013783(10)	20	$1.17228(88) \times 10^{-3}$	22	$1.00985(76) \times 10^{-3}$	24	$8.8080(66) \times 10^{-4}$
26	$7.7702(59) \times 10^{-4}$	28	$6.9022(52) \times 10^{-4}$	30	$6.1699(47) \times 10^{-4}$	32	$5.5609(42) \times 10^{-4}$
36	$4.5895(35) \times 10^{-4}$	40	$3.8649(30) \times 10^{-4}$	44	$3.3052(25) \times 10^{-4}$	48	$2.8593(22) \times 10^{-4}$
52	$2.5017(19) \times 10^{-4}$	56	$2.2067(17) \times 10^{-4}$	60	$1.9661(15) \times 10^{-4}$	64	$1.7654(14) \times 10^{-4}$
72	$1.4452(11) \times 10^{-4}$	80	$1.20605(93) \times 10^{-4}$	88	$1.02467(79) \times 10^{-4}$	96	$8.8140(68) \times 10^{-5}$
104	$7.6793(59) \times 10^{-5}$	112	$6.7465(52) \times 10^{-5}$	120	$5.9828(46) \times 10^{-5}$	128	$5.3474(41) \times 10^{-5}$
144	$4.3557(34) \times 10^{-5}$	160	$3.6165(28) \times 10^{-5}$	176	$3.0591(24) \times 10^{-5}$	192	$2.6203(20) \times 10^{-5}$
208	$2.2756(18) \times 10^{-5}$	224	$1.9979(16) \times 10^{-5}$	240	$1.7617(14) \times 10^{-5}$	256	$1.5720(12) \times 10^{-5}$
288	$1.2768(10) \times 10^{-5}$	320	$1.05402(82) \times 10^{-5}$	352	$8.8978(70) \times 10^{-6}$	384	$7.6032(60) \times 10^{-6}$
416	$6.5813(52) \times 10^{-6}$	448	$5.7475(45) \times 10^{-6}$	480	$5.0872(40) \times 10^{-6}$	512	$4.5276(35) \times 10^{-6}$
1000	$1.3361(10) \times 10^{-6}$	2000	$3.7243(29) \times 10^{-7}$	5000	$6.7753(54) \times 10^{-8}$	10000	$1.8487(15) \times 10^{-8}$
100000	$2.3623(19) \times 10^{-10}$						

to constructing a good upper bound on the integrand absolute value and to proving the finiteness of renormalized Feynman amplitudes. We borrow several ideas from these analyses.

To construct the PDF, we partition the integration domain into so-called Hepp sectors [35]:

$$z_{j_1} \geq z_{j_2} \geq \dots \geq z_{j_n}.$$

Each ordering of the Feynman parameters defines one Hepp sector. For example, for V_{27} we have $n = 18$, yielding $18! = 6\,402\,373\,705\,728\,000$ sectors per diagram.

Our PDFs take the form

$$C \times \frac{\prod_{i=2}^n (z_{j_i}/z_{j_{i-1}})^{\text{Deg}(\{j_i, j_{i+1}, \dots, j_M\})}}{z_1 \times z_2 \times \dots \times z_n} + \text{stability terms},$$

where $\text{Deg}(s)$ are positive numbers defined on all nonempty proper subsets of the set of all internal lines of the diagram. For example, for V_{27} we have $2^{18} - 2 = 262\,142$ such numbers per diagram. Functions of a similar form were first used in Ref. [48]. The necessity of stability terms and their general construction were discussed in Ref. [49], along with other stabilization techniques. Efficient random-sample generation with such PDFs was described in Ref. [50]; a similar algorithm was also implemented in `feyntrop` [51,52]. The procedure for obtaining $\text{Deg}(s)$ and stabilization terms, as well as further details, will be presented elsewhere.

The most resource-intensive part of the computation is the Monte Carlo integration itself. We employed NVidia P100 graphics processing units (GPUs; accompanied by one Intel Xeon E5-2698 CPU core per GPU). Since all divergences are canceled numerically under the integral sign, the subtractions may lead to large roundoff errors. To control these, we used the interval arithmetic: At each arithmetic operation, we generate an interval $[x_1, x_2]$ that is guaranteed to contain the exact result x . We employed five types of interval arithmetic that differ in speed and interval widths. We begin with a fast version of double-precision interval arithmetic, which distributes arithmetic operations into blocks and estimates the interval width in each block without computing intervals for single operations [49].⁴ We then switch to the conventional interval arithmetic with double precision. If the achieved precision is insufficient, the same sample is recomputed with a higher-precision arithmetic. Arbitrary-precision arithmetics with mantissas of 128, 256, and 384 bits were used. High-precision arithmetic is especially crucial for small values of $|\mathbf{p}|$. The computations were performed on the MPIK

⁴Note that NVidia GPUs allow specifying rounding policies in arithmetic operations and also provide a precision-preserving realization of $\log(1+x)$.

TABLE II. The values of $\tilde{V}_{25}(\mathbf{p})$ for different $|\mathbf{p}|$.

$ \mathbf{p} $	$\tilde{V}_{25}(\mathbf{p})$	$ \mathbf{p} $	$\tilde{V}_{25}(\mathbf{p})$	$ \mathbf{p} $	$\tilde{V}_{25}(\mathbf{p})$	$ \mathbf{p} $	$\tilde{V}_{25}(\mathbf{p})$
0.001	0.014832(67)	0.003	0.014779(66)	0.005	0.014825(66)	0.01	0.014859(67)
0.03	0.015011(67)	0.05	0.014838(66)	0.1	0.014815(66)	0.15	0.014764(66)
0.16	0.014836(66)	0.17	0.014713(65)	0.18	0.014739(65)	0.19	0.014735(65)
0.2	0.014766(64)	0.22	0.014605(64)	0.24	0.014693(64)	0.26	0.014628(64)
0.28	0.014656(64)	0.3	0.014582(64)	0.32	0.014589(64)	0.34	0.014557(64)
0.36	0.014388(63)	0.38	0.014435(63)	0.4	0.014515(63)	0.42	0.014308(62)
0.44	0.014204(61)	0.46	0.014232(62)	0.48	0.014094(61)	0.5	0.014074(61)
0.55	0.013827(60)	0.6	0.013734(60)	0.65	0.013670(59)	0.7	0.013371(57)
0.75	0.013176(56)	0.8	0.013021(56)	0.85	0.012758(54)	0.9	0.012657(54)
0.95	0.012420(53)	1	0.012235(52)	1.1	0.011815(50)	1.2	0.011402(48)
1.3	0.010959(46)	1.4	0.010643(45)	1.5	0.010117(42)	1.6	0.009692(41)
1.7	0.009350(39)	1.8	0.009028(37)	1.9	0.008634(36)	2	0.008362(34)
2.1	0.007971(33)	2.2	0.007741(32)	2.3	0.007468(30)	2.4	0.007182(29)
2.5	0.006917(28)	2.6	0.006681(27)	2.7	0.006475(26)	2.8	0.006293(25)
2.9	0.006058(24)	3	0.005907(23)	3.5	0.005059(20)	4	0.004406(17)
4.5	0.003849(15)	5	0.003451(13)	5.5	0.003088(12)	6	0.002776(10)
6.5	0.0025248(94)	7	0.0023178(87)	7.5	0.0021048(78)	8	0.0019559(73)
9	0.0016760(61)	10	0.0014618(53)	11	0.0012837(47)	12	0.0011450(42)
13	0.0010231(38)	14	0.0009142(33)	15	0.0008299(30)	16	0.0007583(27)
18	0.0006360(23)	20	0.0005433(20)	22	0.0004716(17)	24	0.0004152(15)
26	0.0003655(13)	28	0.0003237(12)	30	0.0002919(11)	32	$2.6274(95) \times 10^{-4}$
36	$2.1976(80) \times 10^{-4}$	40	$1.8432(67) \times 10^{-4}$	44	$1.5679(57) \times 10^{-4}$	48	$1.3651(50) \times 10^{-4}$
52	$1.2011(44) \times 10^{-4}$	56	$1.0711(39) \times 10^{-4}$	60	$9.468(34) \times 10^{-5}$	64	$8.541(31) \times 10^{-5}$
72	$6.975(25) \times 10^{-5}$	80	$5.821(21) \times 10^{-5}$	88	$4.988(18) \times 10^{-5}$	96	$4.278(16) \times 10^{-5}$
104	$3.764(14) \times 10^{-5}$	112	$3.290(12) \times 10^{-5}$	120	$2.909(11) \times 10^{-5}$	128	$2.612(10) \times 10^{-5}$
144	$2.1286(78) \times 10^{-5}$	160	$1.7672(65) \times 10^{-5}$	176	$1.5059(55) \times 10^{-5}$	192	$1.2793(47) \times 10^{-5}$
208	$1.1140(41) \times 10^{-5}$	224	$9.834(36) \times 10^{-6}$	240	$8.645(31) \times 10^{-6}$	256	$7.675(28) \times 10^{-6}$
288	$6.258(23) \times 10^{-6}$	320	$5.161(19) \times 10^{-6}$	352	$4.373(16) \times 10^{-6}$	384	$3.759(14) \times 10^{-6}$
416	$3.233(12) \times 10^{-6}$	448	$2.852(11) \times 10^{-6}$	480	$2.5110(93) \times 10^{-6}$	512	$2.2388(83) \times 10^{-6}$
1000	$6.649(25) \times 10^{-7}$	2000	$1.8530(69) \times 10^{-7}$	5000	$3.389(13) \times 10^{-8}$	10000	$9.278(35) \times 10^{-9}$
100000	$1.1819(44) \times 10^{-10}$						

Heidelberg computing cluster and required 15 GPU-days for both V_{23} and V_{25} and 42 GPU-days for V_{27} . The corresponding numbers of Monte Carlo samples were 9×10^{12} , 2.3×10^{12} , and 6.1×10^{11} , respectively. The compiled integrand code sizes were 30 MB for V_{23} , 450 MB for V_{25} , and 11 GB for V_{27} .

III. CALCULATION OF ENERGY SHIFTS

Once numerical values of the VP potentials are available, the corresponding corrections to energy levels can be computed as expectation values of the potentials with the Dirac wave function of the reference state. Since the potentials are obtained in the momentum representation in this work, it is natural to evaluate the expectation values also in momentum space,

$$\langle V_{ij} \rangle = \int \frac{d^3 \mathbf{p}_1}{(2\pi)^3} \int \frac{d^3 \mathbf{p}_2}{(2\pi)^3} \psi_a^\dagger(\mathbf{p}_1) V_{ij}(\mathbf{p}_1 - \mathbf{p}_2) \psi_a(\mathbf{p}_2). \quad (5)$$

Integration over most angular variables is easily performed analytically (see, e.g., Sec. 2C of Ref. [53]), leaving a three-dimensional integral to be carried out numerically:

$$\langle V_{ij} \rangle = \frac{1}{32\pi^5} \int_0^\infty dp_1 dp_2 \int_{-1}^1 d\xi (p_1 p_2)^2 V_{ij}(q) \times [g_a(p_1) g_a(p_2) P_{l_a}(\xi) + f_a(p_1) f_a(p_2) P_{\bar{l}_a}(\xi)], \quad (6)$$

where $p_1 = |\mathbf{p}_1|$, $p_2 = |\mathbf{p}_2|$, $q = |\mathbf{p}_1 - \mathbf{p}_2|$, $\xi = \mathbf{p}_1 \cdot \mathbf{p}_2 / (p_1 p_2)$, P_l is the Legendre polynomial, $l_a = |\kappa_a + 1/2| - 1/2$, $\bar{l}_a = |\kappa_a - 1/2| - 1/2$, and $g_a(p)$ and $f_a(p)$ are the upper and lower radial components of the Dirac wave function, respectively, defined as in Ref. [53].

To perform the numerical integrations, it is convenient to make the change in variables [54] $(p_1, p_2, \xi) \rightarrow (x, y, q)$, where $x = p_1 + p_2$ and $y = |p_1 - p_2|$, with the result

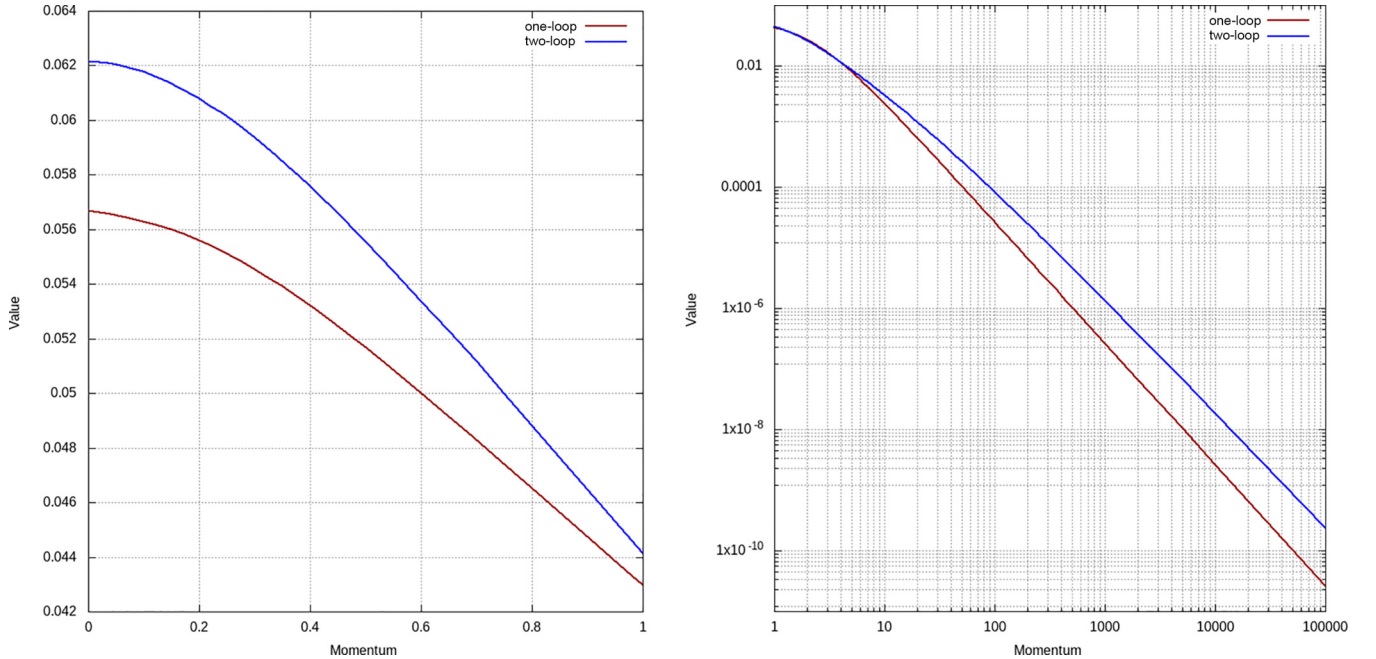
$$\langle V_{ij} \rangle = \frac{1}{32\pi^5} \int_0^\infty dx \int_0^x dy \int_y^x dq p_1 p_2 q V_{ij}(q) \times [g_a(p_1) g_a(p_2) P_{l_a}(\xi) + f_a(p_1) f_a(p_2) P_{\bar{l}_a}(\xi)]. \quad (7)$$

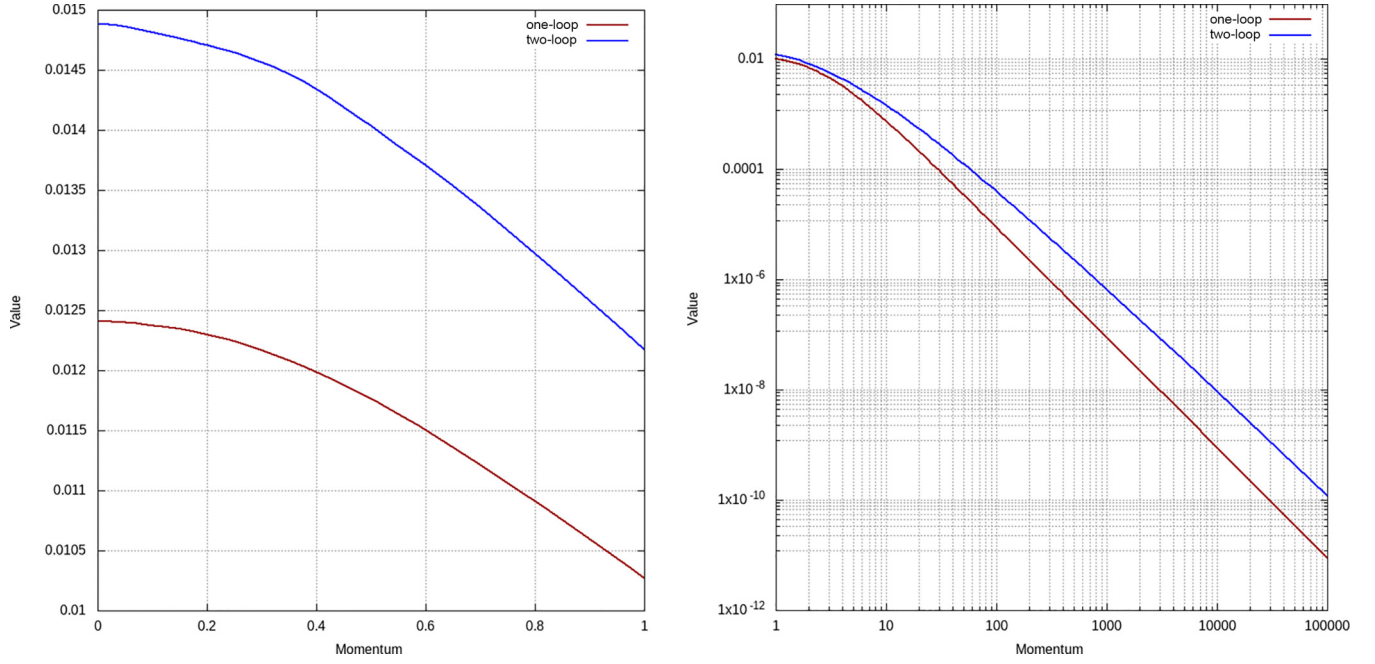
IV. RESULTS

Our numerical results obtained for the potentials $\tilde{V}_{23}(\mathbf{p})$, $\tilde{V}_{25}(\mathbf{p})$, and $\tilde{V}_{27}(\mathbf{p})$ are presented in Tables I–III, respectively. The specified uncertainties originate from Monte Carlo integrations and represent 1σ deviations. The uncertainties for different $\mathbf{p}$'s are statistically independent. For small $\mathbf{p}$ our results for the potential $\tilde{V}_{23}(\mathbf{p})$ are in good agreement with the analytical result by Krachkov and Lee [55], $\tilde{V}_{23}(\mathbf{0}) = 0.062\,214\dots$ As a cross-check of our method and numerical procedure, we also calculated the one-loop potentials $\tilde{V}_{13}(\mathbf{p})$, $\tilde{V}_{15}(\mathbf{p})$, and $\tilde{V}_{17}(\mathbf{p})$ and the two-loop potential $\tilde{V}_{21}(\mathbf{p})$, with

TABLE III. The values of $\tilde{V}_{27}(\mathbf{p})$ for different $|\mathbf{p}|$.

$ \mathbf{p} $	$\tilde{V}_{27}(\mathbf{p})$	$ \mathbf{p} $	$\tilde{V}_{27}(\mathbf{p})$	$ \mathbf{p} $	$\tilde{V}_{27}(\mathbf{p})$	$ \mathbf{p} $	$\tilde{V}_{27}(\mathbf{p})$
0.001	0.00824(14)	0.003	0.00850(14)	0.005	0.00814(15)	0.01	0.00844(14)
0.03	0.00841(14)	0.05	0.00866(15)	0.1	0.00829(14)	0.15	0.00814(14)
0.16	0.00825(14)	0.17	0.00838(14)	0.18	0.00850(14)	0.19	0.00829(14)
0.2	0.00829(14)	0.22	0.00850(14)	0.24	0.00815(14)	0.26	0.00829(14)
0.28	0.00809(14)	0.3	0.00834(14)	0.32	0.00820(13)	0.34	0.00803(14)
0.36	0.00821(14)	0.38	0.00809(13)	0.4	0.00813(14)	0.42	0.00804(14)
0.44	0.00801(14)	0.46	0.00808(13)	0.48	0.00800(13)	0.5	0.00789(13)
0.55	0.00776(13)	0.6	0.00764(13)	0.65	0.00785(13)	0.7	0.00786(13)
0.75	0.00753(13)	0.8	0.00766(12)	0.85	0.00746(12)	0.9	0.00725(12)
0.95	0.00705(12)	1	0.00708(12)	1.1	0.00716(11)	1.2	0.00672(11)
1.3	0.00654(11)	1.4	0.00626(10)	1.5	0.00608(10)	1.6	0.005817(94)
1.7	0.005681(92)	1.8	0.005497(89)	1.9	0.005420(85)	2	0.005154(82)
2.1	0.004938(78)	2.2	0.004875(76)	2.3	0.004726(75)	2.4	0.004564(71)
2.5	0.004348(68)	2.6	0.004215(68)	2.7	0.004190(68)	2.8	0.003984(64)
2.9	0.003957(63)	3	0.003736(59)	3.5	0.003347(52)	4	0.002932(45)
4.5	0.002692(42)	5	0.002322(35)	5.5	0.002033(31)	6	0.001873(28)
6.5	0.001700(24)	7	0.001556(23)	7.5	0.001466(22)	8	0.001328(19)
9	0.001165(17)	10	0.001011(15)	11	0.000877(13)	12	0.000791(12)
13	0.000722(10)	14	0.0006303(91)	15	0.0005762(85)	16	0.0005149(73)
18	0.0004433(64)	20	0.0003773(52)	22	0.0003286(49)	24	0.0002928(41)
26	0.0002540(38)	28	0.0002278(33)	30	0.0002082(29)	32	0.0001805(27)
36	0.0001510(21)	40	0.0001281(19)	44	0.0001079(16)	48	0.0000945(14)
52	0.0000833(12)	56	0.0000729(11)	60	$6.405(91) \times 10^{-5}$	64	$6.026(86) \times 10^{-5}$
72	$4.758(71) \times 10^{-5}$	80	$4.023(59) \times 10^{-5}$	88	$3.485(49) \times 10^{-5}$	96	$2.987(43) \times 10^{-5}$
104	$2.533(36) \times 10^{-5}$	112	$2.300(33) \times 10^{-5}$	120	$2.042(29) \times 10^{-5}$	128	$1.820(26) \times 10^{-5}$
144	$1.468(21) \times 10^{-5}$	160	$1.212(18) \times 10^{-5}$	176	$1.032(15) \times 10^{-5}$	192	$8.90(13) \times 10^{-6}$
208	$7.90(12) \times 10^{-6}$	224	$6.91(10) \times 10^{-6}$	240	$5.948(91) \times 10^{-6}$	256	$5.390(78) \times 10^{-6}$
288	$4.351(65) \times 10^{-6}$	320	$3.575(53) \times 10^{-6}$	352	$2.955(43) \times 10^{-6}$	384	$2.592(38) \times 10^{-6}$
416	$2.305(35) \times 10^{-6}$	448	$1.990(29) \times 10^{-6}$	480	$1.763(26) \times 10^{-6}$	512	$1.565(23) \times 10^{-6}$
1000	$4.596(70) \times 10^{-7}$	2000	$1.261(19) \times 10^{-7}$	5000	$2.348(36) \times 10^{-8}$	10 000	$6.271(94) \times 10^{-9}$
100 000	$8.10(12) \times 10^{-11}$						

FIG. 5. The values of $\tilde{V}_{13}(p)$ (one-loop potential) and $\tilde{V}_{23}(p)$ (two-loop potential). The numerical data have been smoothed to enhance visual clarity.

FIG. 6. The values of $\tilde{V}_{15}(p)$ (one-loop potential) and $\tilde{V}_{25}(p)$ (two-loop potential).

numerical values presented in the Supplemental Material [56]. They were shown to be in excellent agreement with a numerical Fourier transform of the corresponding coordinate-space potentials; see Ref. [15] for details.

Figures 5–7 present plots of the two-loop potentials $\tilde{V}_{23}(\mathbf{p})$, $\tilde{V}_{25}(\mathbf{p})$, and $\tilde{V}_{27}(\mathbf{p})$ in comparison with their one-loop counterparts, $\tilde{V}_{13}(\mathbf{p})$, $\tilde{V}_{15}(\mathbf{p})$, and $\tilde{V}_{17}(\mathbf{p})$. Note that the one- and two-loop prefactors were pulled out in the definition of $\tilde{V}_{ij}$, so the normalized one- and two-loop potentials are expected to be of the same order of magnitude. We observe that the normalized two-loop potentials behave similarly to their

one-loop counterparts for small momenta, approaching constant values as $\mathbf{p} \rightarrow \mathbf{0}$. However, they behave differently at large momenta, with two-loop potentials decreasing more slowly than their one-loop analogs.

We now examine the energy shifts induced by the two-loop VP potentials in hydrogenlike ions. It is convenient to represent them in terms of the dimensionless function $G(Z\alpha)$, pulling out their leading α , $Z\alpha$, and n dependence,

$$\delta E = \left(\frac{\alpha}{\pi}\right)^2 \frac{(Z\alpha)^6}{n^3} G(Z\alpha), \quad (8)$$

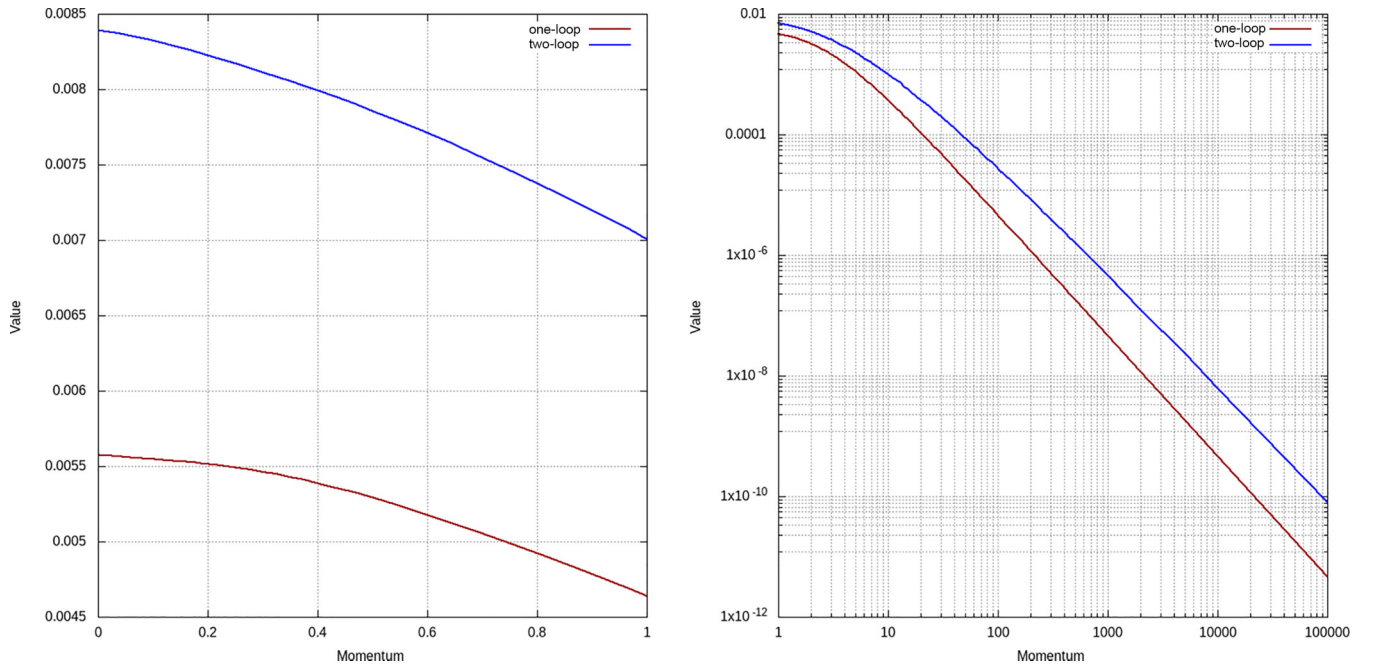
FIG. 7. The values of $\tilde{V}_{17}(p)$ (one-loop potential) and $\tilde{V}_{27}(p)$ (two-loop potential).

TABLE IV. Energy shifts induced by the two-loop vacuum-polarization potentials V_{23} , V_{25} , and V_{27} for the $1s$ state of hydrogenlike ions in terms of the function $G(Z\alpha)$ defined by Eq. (8). Expectation values of the potentials are evaluated for the point nuclear model; FNS denotes estimates of the finite-nuclear-size correction.

Z	$\langle V_{23} \rangle_{\text{pnt}}$	$\langle V_{25} \rangle_{\text{pnt}}$	$\langle V_{27} \rangle_{\text{pnt}}$	FNS	Total
1	0.1915(7)				0.1915(7)
2	0.1881(5)				0.1881(5)
3	0.1849(3)				0.1849(3)
5	0.1789(2)	0.0001			0.1789(2)
7	0.1734(1)	0.0001			0.1735(1)
10	0.1660(1)	0.0002			0.1662(1)
15	0.1557	0.0005			0.1562
20	0.1473	0.0008			0.1481
25	0.1405	0.0013			0.1417
30	0.1349	0.0018	0.0001	-0.0001	0.1366
35	0.1304	0.0024	0.0001	-0.0001(1)	0.1328(1)
40	0.1269	0.0031	0.0002	-0.0002(1)	0.1300(1)
45	0.1243	0.0039	0.0003	-0.0002(1)	0.1283(1)
50	0.1226(1)	0.0049	0.0004	-0.0003(2)	0.1275(2)
55	0.1216(1)	0.0059	0.0006	-0.0005(2)	0.1277(3)
60	0.1215(1)	0.0072	0.0008	-0.0007(3)	0.1289(4)
65	0.1223(1)	0.0087	0.0012	-0.0010(5)	0.1311(6)
70	0.1240(1)	0.0104	0.0017	-0.0015(7)	0.1346(9)
75	0.1267(1)	0.0125	0.0023(1)	-0.002(1)	0.139(1)
80	0.1308(1)	0.0149	0.0032(1)	-0.003(2)	0.146(2)
83	0.1339(1)	0.0167	0.0039(1)	-0.004(2)	0.151(3)
90	0.1439(2)	0.0217	0.0060(2)	-0.007(4)	0.165(5)
92	0.1476(2)	0.0235(1)	0.0068(2)	-0.009(4)	0.169(6)
100	0.1677(3)	0.0328(1)	0.0114(3)	-0.017(9)	0.195(12)

where n is the principal quantum number of the reference state.

Table IV presents our numerical results for individual two-loop VP contributions for the $1s$ state of hydrogenlike ions. The columns labeled $\langle V_{23} \rangle_{\text{pnt}}$, $\langle V_{25} \rangle_{\text{pnt}}$, and $\langle V_{27} \rangle_{\text{pnt}}$ represent expectation values of the potentials V_{23} , V_{25} , and V_{27} evaluated with the point-nucleus Dirac wave functions. The column labeled FNS shows our estimations of the finite-nuclear-size (FNS) correction, $\langle V_{23} + V_{25} + V_{27} \rangle_{\text{FNS}}$. It was obtained by multiplying the point-nucleus result $\langle V_{23} + V_{25} + V_{27} \rangle_{\text{pnt}}$ by the relative FNS correction for the V_{21} expectation value [15], $\langle V_{21} \rangle_{\text{FNS}} / \langle V_{21} \rangle_{\text{pnt}}$, with an uncertainty of 50%.

The last column of Table IV presents the total results for the higher-order two-loop VP correction,

$$\delta E_{\text{VP}23+} = \langle V_{23} \rangle_{\text{pnt}} + \langle V_{25} \rangle_{\text{pnt}} + \langle V_{27} \rangle_{\text{pnt}} + \langle V_{23} + V_{25} + V_{27} \rangle_{\text{FNS}}. \quad (9)$$

The uncertainty due to the omitted higher-order terms (V_{29} , etc.) is not shown explicitly but included in the total uncertainty in the last column. It was estimated by scaling the $\langle V_{27} \rangle$ contribution by the factor $2 \langle V_{27} \rangle / \langle V_{25} \rangle$.

Our result for hydrogen, $G(1\alpha) = 0.192$, is close to the analytical $Z = 0$ value obtained by Krachkov and Lee, $G(0\alpha) = 0.1954 \dots$ [55]. In the high- Z region, our results are consistent with previous estimates. In particular, for the $1s$ state of uranium, Ref. [15] estimated $G(92\alpha) = \pm 1.3$, whereas we now obtain $G(92\alpha) = 0.169(4)$. It is remarkable that the calculated

TABLE V. Individual two-loop vacuum-polarization contributions to transition energies in Li-like bismuth and uranium (in eV). Subscripts “ext” and “pnt” indicate results obtained for the extended-size and the point nuclear models; “FNS” denotes the finite-nuclear-size correction. Uncertainties due to nuclear charge radii and models are now shown.

Term	$2p_{3/2}-2s, Z = 83$	$2p_{1/2}-2s, Z = 92$
$\langle V_{21} \rangle_{\text{ext}}$	0.06718	0.10111
$\langle V_1, V_1 \rangle_{\text{ext}}$	0.01573	0.03501
$\langle V_{23} \rangle_{\text{pnt}}$	-0.00276	-0.00474(1)
$\langle V_{25} \rangle_{\text{pnt}}$	-0.00036	-0.00082
$\langle V_{27} \rangle_{\text{pnt}}$	-0.00009	-0.00025(1)
$\langle V_{23+} \rangle_{\text{FNS}}$	0.00009(5)	0.00034(20)
Sum	0.07979(6)	0.13066(27)
Reference [12]	0.083(25)	0.136(46)

correction turned out to be an order of magnitude smaller than previously anticipated.

In Table V, we collect all two-loop VP contributions to transition energies of Li-like bismuth and uranium. The two leading terms—those arising from the Källén-Sabry potential V_{21} and from the second-order iteration of the one-loop VP potential (V_1, V_1)—were previously evaluated in Ref. [15]. The remaining entries in Table V represent higher-order two-loop VP corrections calculated in this work.

Table VI summarizes our numerical results for the higher-order two-loop VP correction $\delta E_{\text{VP}23+}$ for the $1s$, $2s$, $2p_{1/2}$,

TABLE VI. The higher-order two-loop vacuum-polarization correction $\delta E_{\text{VP}23+}$ for different states of hydrogenlike ions in terms of the function $G(Z\alpha)$ defined by Eq. (8).

Z	$1s$	$2s$	$2p_{1/2}$	$2p_{3/2}$
1	0.1915(7)	0.191(2)		
2	0.1881(5)	0.1882(8)		
3	0.1849(3)	0.1850(4)		
5	0.1789(2)	0.1789(3)	0.0001	
7	0.1735(1)	0.1735(1)	0.0002	0.0001
10	0.1662(1)	0.1664	0.0004	0.0002
15	0.1562	0.1567	0.0009	0.0004
20	0.1481	0.1491	0.0015	0.0007
25	0.1417	0.1434	0.0022	0.0010
30	0.1366	0.1392	0.0031	0.0013
35	0.1328(1)	0.1364(1)	0.0042	0.0016
40	0.1300(1)	0.1350(1)	0.0054	0.0019
45	0.1283(1)	0.1348(1)	0.0069	0.0023
50	0.1275(2)	0.1359(2)	0.0087	0.0026
55	0.1277(3)	0.1384(3)	0.0109	0.0030
60	0.1289(4)	0.1425(5)	0.0134	0.0034
65	0.1311(6)	0.1482(7)	0.0166	0.0038
70	0.1346(9)	0.156(1)	0.0204(1)	0.0042
75	0.139(1)	0.166(2)	0.0252(1)	0.0046
80	0.146(2)	0.179(3)	0.0313(2)	0.0050
83	0.151(3)	0.189(4)	0.0357(4)	0.0053
90	0.165(5)	0.217(7)	0.049(1)	0.0060
92	0.169(6)	0.227(8)	0.054(1)	0.0062
100	0.195(12)	0.28(2)	0.081(4)	0.0071(1)

TABLE VII. Theoretical contributions to transition energies in Li-like bismuth and uranium (in eV). All theory except two-loop vacuum polarization (VPVP) is from Ref. [6]. When two uncertainties are specified, the first is the purely theoretical uncertainty, whereas the second is due to the nuclear radius. The nuclear charge radii used are 5.5211(26) fm for bismuth and 5.8571(33) fm for uranium [60].

	Term	$2p_{3/2}-2s$, $^{209}\text{Bi}^{80+}$	$2p_{1/2}-2s$, $^{238}\text{U}^{89+}$	Reference
Structure		2814.395(3)(26)	322.286(5)(34)	
One-loop QED		−27.486(1)	−42.929(1)	
Screened one-loop QED		1.140(3)	1.193(16)	
Two-loop QED	SESE	0.141	0.296	
	SEVP	−0.095	−0.188	
	SVPE	−0.002(31)	−0.004(66)	
	VPVP	0.080	0.131	This work
Screened two-loop QED		−0.007(5)	−0.012(9)	
Nuclear recoil		−0.062(2)	−0.063(3)	
Nuclear polarization and deformation		0.013(13)	0.058(20)	
Theory		2788.116(35)(26)	280.767(72)(34)	
Previous theory		2788.12(7)	280.76 (14)	[12]
Experiment		2788.14(4)	280.645(15)	[57,63]
			280.516(99)	[58]
			280.59(10)	[59]

and $2p_{3/2}$ states of hydrogenlike ions. These results extend calculations of two-loop corrections reported in Ref. [15] and complete the treatment of the two-loop vacuum polarization effect.

We now turn to the experimental consequences of our calculations. Table VII summarizes individual theoretical contributions to the transition energies in Li-like bismuth and uranium, for which accurate experimental results are available. For a comprehensive summary of various theoretical corrections in Li-like ions we refer the reader to the recent study in Ref. [6]. As can be seen from Table VII, after our calculation of the two-loop vacuum-polarization (VPVP) correction, the main theoretical uncertainty for both bismuth and uranium now arises from the last uncalculated two-loop QED correction, namely, the self-energy with the VP insertion in the photon line (SVPE).

We observe that the updated theoretical predictions of the transition energies have approximately 2 times smaller uncertainties than the earlier results of Ref. [12]. The agreement with experiment is excellent in the case of bismuth. For uranium, there is a slight tension between the theoretical and experimental values (1.5σ with the experiment [57], 2.0σ with that of Ref. [58], and 1.4σ with Ref. [59]). A possible explanation for this tension is underestimated uncertainty in the currently accepted nuclear charge radius of ^{238}U as listed in the tabulation [60]. This interpretation is consistent with the recent criticism by Ohayon [61], who argued that the model dependence of the nuclear charge distribution was not properly accounted for in Ref. [60]. A similar issue was recently identified for the doubly magic nucleus of ^{208}Pb , where a state-of-the-art reanalysis of historical muonic spectroscopy data led to a 3σ shift in the accepted nuclear radius [62].

V. SUMMARY

We performed calculations of Coulomb corrections to the leading-order two-loop vacuum-polarization potential derived

70 years ago by Källén and Sabry [24]. Specifically, we derived the two-loop vacuum-polarization potentials V_{23} , V_{25} , and V_{27} that are induced by Feynman diagrams with three, five, and seven Coulomb interactions inside the vacuum-polarization loop, respectively. The potentials were computed in the momentum representation and stored on a grid. Furthermore, we evaluated the expectation values of these potentials with the reference-state wave function and obtained the corresponding energy shifts for H-like ions for a wide range of nuclear charges Z . In the limit of small Z , our results agree with the analytical result of Krachkov and Lee [55].

Our calculation eliminates one of the two largest uncertainties in theoretical values of the two-loop Lamb shift and represents an important step towards completing the long-standing project of calculating the full set of one-electron two-loop QED effects.

A comparison of the updated theoretical predictions for the $2p_{j-2s}$ transition energies in bismuth and uranium with available experiments results yielded some of the best tests of bound-state QED theory in the strong nuclear binding field. We found excellent agreement in the case of bismuth but a small tension of 1.4 – 2.0σ for uranium, which may stem from the insufficient knowledge of the nuclear charge radius.

In the future, it might be worthwhile to obtain the potentials V_{2j} in the coordinate representation, which is much more convenient for practical applications than the momentum one. This could be achieved through a numerical Fourier transformation, but it requires further knowledge of the behavior of the potentials near $\mathbf{p} = 0$ and $\mathbf{p} = \infty$.

DATA AVAILABILITY

The data that support the findings of this article are not publicly available. The data are available from the authors upon reasonable request.

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