

Exact two-loop vacuum polarization correction to the Lamb shift in hydrogenlike ions

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Abstract. We present a calculation scheme for the two-loop vacuum polarization correction of order α^2 to the Lamb shift of hydrogenlike high- Z atoms. The interaction with the external Coulomb field is taken into account to all orders in $(Z\alpha)$. By means of a modified potential approach the problem is reduced to the evaluation of effective one-loop vacuum polarization potentials. An expression for the energy shift is deduced within the framework of partial wave decomposition performing appropriate subtractions. Exact results for the two-loop vacuum polarization contribution to the Lamb shift of K- and L-shell electron states in hydrogenlike Lead and Uranium are presented.

PACS. 31.10.+z Theory of electronic structure, electronic transitions, and chemical binding – 31.30.-i Corrections to electronic structure – 31.30.Jv Relativistic and quantum electrodynamic effects in atoms and molecules

1 Introduction

Recent experimental progress in the spectroscopy of highly charged heavy ions [1–4] demands theoretical predictions for the Lamb shift, which should include the complete set of QED radiative corrections of order α^2 but accounting for all orders $(Z\alpha)$ in the interaction with the strong external Coulomb field. For low- Z elements, a potential expansion with respect to powers in $(Z\alpha)$ is legitimate and all α^2 -corrections have recently been calculated up to the order of $\alpha^2(Z\alpha)^5$ [5, 6]. However, for systems under consideration in recent Lamb-shift measurements such as Gold or Uranium, a value for the effective coupling $Z\alpha > 0.5$ already indicates that $Z\alpha$ -expansion in the regime of large Z becomes inadequate. Instead, exact electron propagators and wave functions in the external Coulomb field of extended nuclei have to be used in calculations of all second-order diagrams (Fig. 1). Meanwhile, calculational approaches are available for most of these QED effects (see the work of Persson *et al.* [7] and cited references). However, the calculations are not yet complete.

1. Exact numerical evaluations of the complete set of two-photon self-energy contributions remains as a major challenge, although recent progress has been made in deriving renormalized expressions for the resulting energy shifts [12]. The lack of numerical results for these contributions represents a major uncertainty in theoretical pre-

dictions for the Lamb shift aiming for a relative precision of 10^{-6} for the total electron binding energy.

2. Exact evaluation schemes, which also treat the loops involved to all orders in $(Z\alpha)$, have been developed [14] only for the combined self energy - vacuum polarization corrections SEVPabc and the two-loop ladder vacuum polarization diagram VPVPa (see Fig. 1). Values for the VPVPa correction for large Z -numbers have been tabulated recently [8]. The self energy-vacuum polarization S(VP)E (Fig. 1) is calculated by employing the Uehling-approximation for the loop [7]. Calculation of the higher-order contribution to this diagram are presently in progress.

3. Until now, the two-loop diagram VPVPb as well as the self energy corrected one-loop vacuum polarization contribution VPVPc (Fig. 1) where calculated only to lowest order in $(Z\alpha)$ utilizing the Källén-Sabry polarization function [11, 9, 10].

Aiming towards the completion of the exact evaluation of all QED-radiative corrections of order α^2 , we shall present a calculation scheme which allows the higher-order $(Z\alpha)$ -contribution of the two-loop vacuum polarization correction VPVPb to be determined. Recognizing that the diagram we wish to calculate is part of the complete “dressed” one-loop vacuum polarization allows us to reduce the problem to the evaluation of effective one-loop corrections where the renormalization procedure is known [13, 15].

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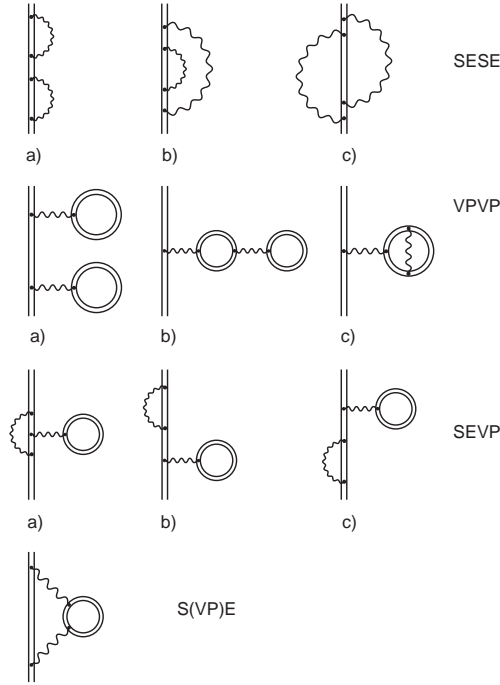


Fig. 1. QED corrections of order α^2 in hydrogenlike atoms. The double lines indicate wave functions and propagators in the external Coulomb field of the nucleus.

Section 2 contains a general discussion of “dressed” electron propagators in arbitrary, classical external fields and of the induced vacuum polarization. In Section 3 we specify the formulae to the situation in hydrogenlike ions. The subtraction scheme for deducing the two-loop correction from various effective one-loop contributions will be introduced. Section 4 briefly reviews the renormalization procedure. An expression for the renormalized energy shift due to the higher-order (in $(Z\alpha)$) part is derived. This consists of two terms which require a different numerical treatment. In order to compare the effect due to higher orders in $(Z\alpha)$ we also present results for the two-loop correction in Uehling approximation, which will be derived in Section 5. In section 6 we will calculate the effect of the higher-order contribution to the Lamb shift in hydrogenlike Lead and Uranium.

Throughout this paper, units will be used where $\hbar = m_0 = 1$ and $e^2 = \alpha$.

2 Dressed electron propagators and one-loop vacuum polarization

We start with a brief discussion of the concept of “dressed” electron propagators and of the corresponding “dressed” one-loop vacuum polarization (VP). Some general formulae will be derived, which will be employed in the next section.

We shall adopt the term “dressed” electron (positron) line ψ for an electron (positron) moving in an arbitrary, external electromagnetic field A_μ . The wave function that

accounts for the interaction with this external field is a solution of the Dirac equation:

$$[i\partial_x - e\mathcal{A}(x) - m]\psi(x) = 0. \quad (1)$$

Choosing free electron lines as a reference, we shall refer to the state ψ as “ A -dressed” electron line. Similarly, an electron interacting with the external Coulomb-potential $V^C = eA_0^C$ generated by the (bare) nuclear charge density distribution may be called a “Coulomb-dressed” electron. In general situations it is appropriate to divide the total external field A_μ into two parts A_μ^e and \tilde{A}_μ , *i.e.*:

$$A_\mu(x) = A_\mu^e(x) + \tilde{A}_\mu(x), \quad (2)$$

where *e.g.* the second term \tilde{A}_μ may be considered a perturbation. Accordingly, considering electron states ϕ in the external field A_μ^e as unperturbed states, we may then call these states ψ “ \tilde{A} -dressed”. The propagators $\mathcal{S}_F^A(x, x')$ and $S_F^e(x, x')$ describing electrons in the external field A_μ respectively A_μ^e are defined by

$$\begin{aligned} [i\partial_x - e\mathcal{A}(x) - m]\mathcal{S}_F^A(x, x') &= \delta(x - x'), \\ [i\partial_x - e\mathcal{A}^e(x) - m]S_F^e(x, x') &= \delta(x - x'). \end{aligned} \quad (3)$$

Note that they also satisfy the equations

$$\begin{aligned} \mathcal{S}_F^A(x, x') [i\partial_{x'} + e\mathcal{A}(x') + m] &= -\delta(x - x'), \\ S_F^e(x, x') [i\partial_{x'} + e\mathcal{A}^e(x') + m] &= -\delta(x - x'), \end{aligned} \quad (4)$$

where the (adjoint) Dirac-operators are acting to the left. In analogy to the Dyson equation defining dressed propagators in terms of improper self-energy insertions *etc.* we postulate an equation of the form

$$\begin{aligned} \mathcal{S}_F^A(x, x') &= S_F^e(x, x') \\ &+ \int d^4x_1 d^4x_2 S_F^e(x, x_1) \tilde{\mathcal{K}}(x_1, x_2) S_F^e(x_2, x'), \end{aligned} \quad (5)$$

with a kernel $\tilde{\mathcal{K}}$. With the aid of equations (3 and 4) we can solve for the kernel:

$$\tilde{\mathcal{K}}(x, x') = e\tilde{A}(x) \delta(x - x') + e\tilde{A}(x) \mathcal{S}_F^A(x, x') e\tilde{A}(x'). \quad (6)$$

The kernel $\tilde{\mathcal{K}}(x, x')$ contains the fully dressed propagator \mathcal{S}_F^A . Equation (6) is verified by acting on Equation (5) with the Dirac-operator from the right and with the adjoint Dirac-operator to the left. Insertion of the kernel (6) into Equation (5) leads to an equation for the exact propagator \mathcal{S}_F^A (we may call it “ \tilde{A} -dressed” propagator when taking S_F^e as the reference) which can be solved iteratively. The exact propagator \mathcal{S}_F^A appears as the sum of three terms: the unperturbed external field propagator S_F^e , a term describing a single-scattering with the additional external field \tilde{A}_μ and a higher-order term which accounts for multiple-scattering contributions. Given this representation for \mathcal{S}_F^A a formal expression for the corresponding

one-loop vacuum-polarization current induced by the total external field A_μ can be derived. For later purposes we will already specialize to the case of static external fields. Since the propagators are homogeneous in time, one obtains:

$$\begin{aligned} \mathcal{J}^{A\mu}(\mathbf{r}) &= ie \int \frac{dE}{2\pi} \text{Tr} [\gamma^\mu S_F^A(\mathbf{r}, \mathbf{r}, E)] \\ &= ie \int \frac{dE}{2\pi} \left\{ \text{Tr} [\gamma^\mu S_F^e(\mathbf{r}, \mathbf{r}, E)] \right. \\ &+ \int d^3\mathbf{r}_1 \text{Tr} [\gamma^\mu S_F^e(\mathbf{r}, \mathbf{r}_1, E) e\tilde{A}(\mathbf{r}_1) S_F^e(\mathbf{r}_1, \mathbf{r}, E)] \\ &+ \int d^3\mathbf{r}_1 d^3\mathbf{r}_2 \text{Tr} [\gamma^\mu S_F^e(\mathbf{r}, \mathbf{r}_1, E) \\ &\quad \times e\tilde{A}(\mathbf{r}_1) S_F^A(\mathbf{r}_1, \mathbf{r}_2, E) e\tilde{A}(\mathbf{r}_2) S_F^e(\mathbf{r}_2, \mathbf{r}, E)] \left. \right\}. \end{aligned} \quad (7)$$

Putting aside questions about renormalization for a moment, this formally exact equation implies that the one-loop vacuum polarization $\mathcal{J}^{A\mu}$ induced by the total field A_μ is given as a sum of three terms: a part induced by the external field A_μ^e , a single-interaction contribution and a third part taking into account multiple interactions with the additional external field \tilde{A}_μ .

The representation of the propagator S_F^A and of the induced vacuum polarization $\mathcal{J}^{A\mu}$ derived above are not unique. The reason for this is provided by the fact that the decomposition of the total external field (Eq. (2)) is completely arbitrary. In particular, we could have chosen the free-field configuration as unperturbed reference. Consequently, the external field propagator S_F^e in the defining equation (5) has to be replaced by the free Feynman propagator S_F^0 leading to a similar kernel (Eq. (6)) which will contain the total external field A_μ . In this case equation (7) takes the form

$$\begin{aligned} \mathcal{J}^{A\mu}(\mathbf{r}) &= ie \int \frac{dE}{2\pi} \left\{ \int d^3\mathbf{r}_1 \text{Tr} [\gamma^\mu S_F^0(\mathbf{r} - \mathbf{r}_1, E) \right. \\ &\quad \times e\tilde{A}(\mathbf{r}_1) S_F^0(\mathbf{r}_1 - \mathbf{r}, E)] \\ &+ \int d^3\mathbf{r}_1 d^3\mathbf{r}_2 \text{Tr} [\gamma^\mu S_F^0(\mathbf{r} - \mathbf{r}_1, E) e\tilde{A}(\mathbf{r}_1) S_F^A(\mathbf{r}_1, \mathbf{r}_2, E) \\ &\quad \times e\tilde{A}(\mathbf{r}_2) S_F^0(\mathbf{r}_2 - \mathbf{r}, E)] \left. \right\}. \end{aligned} \quad (8)$$

The free closed-loop contribution vanishes in accordance with the Furry-theorem. The induced vacuum polarization itself gives rise to a modification \mathcal{A}_μ of the total external field:

$$\mathcal{A}_\mu(\mathbf{r}) = \int d^3\mathbf{r}' D_{\mu\nu}(\mathbf{r} - \mathbf{r}', 0) \mathcal{J}^{A\nu}(\mathbf{r}'). \quad (9)$$

The free photon propagator is given by (in Feynman gauge)

$$\begin{aligned} D_{\mu\nu}(\mathbf{r} - \mathbf{r}', 0) &= g_{\mu\nu} D(\mathbf{r} - \mathbf{r}', 0) \\ &= -g_{\mu\nu} \int \frac{d^3\mathbf{k}}{(2\pi)^3} e^{-i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} \frac{1}{-\mathbf{k}^2 + i\varepsilon} \\ &= g_{\mu\nu} \frac{1}{\pi} \int_0^\infty dk \sum_{\ell, m} 4\pi Y_{\ell m}(\hat{r}) Y_{\ell m}^*(\hat{r}') j_\ell(kr) j_\ell(kr'). \end{aligned} \quad (10)$$

The last line of the expression above specifies the partial wave decomposition of the photon propagator. A spherically symmetric, static external potential $V = eA_0$ induces only a static vacuum polarization charge density \mathcal{J}^{A0} which will also be spherically symmetric. It gives rise to an effective one-loop VP-potential:

$$\mathcal{V}^A(r) = \frac{e}{\pi} \int dk j_0(kr) \int dr' r'^2 j_0(kr') \mathcal{J}^{A0}(r'). \quad (11)$$

3 Subtraction scheme

The general considerations of the previous section may have already anticipated how we are going to deduce the two-loop vacuum polarization correction. The basic idea is to derive this contribution from an effective one-loop vacuum polarization \mathcal{V}^A , which is dressed with the renormalized first-order vacuum polarization potential $V_{\text{ren}}^{\text{VP}}$ induced by the external Coulomb field V^C of the nucleus. At first we need to specialize equations (7) to (11) to the situation of bound-state QED. In the presence of a static, spherically symmetric nuclear charge density, we specify the total external field (Eq. (2)) as the sum of the (bare) external Coulomb potential V^C and the renormalized, first-order vacuum polarization potential $V_{\text{ren}}^{\text{VP}}$:

$$V(r) = eA_0(r) = V^C(r) + V_{\text{ren}}^{\text{VP}}(r). \quad (12)$$

The one-loop potential is obtained from

$$\begin{aligned} V_{\text{ren}}^{\text{VP}}(r) &= e\tilde{A}_0(r) \\ &= i\alpha \int d^3\mathbf{r}' D(\mathbf{r} - \mathbf{r}', 0) \left\{ \int \frac{dE}{2\pi} \text{Tr} [\gamma^0 S_F^C(\mathbf{r}', \mathbf{r}', E)] \right\}_{\text{ren}} \end{aligned} \quad (13)$$

after renormalization. S_F^C denotes the electron propagator in the external Coulomb field. In view of equations (7) and (11) the VP-dressed one-loop vacuum polarization potential formally reads

$$\begin{aligned} \mathcal{V}(r) &= i\alpha \int d^3\mathbf{r}' D(\mathbf{r} - \mathbf{r}', 0) \int \frac{dE}{2\pi} \text{Tr} [\gamma^0 S_F^V(\mathbf{r}', \mathbf{r}', E)] \\ &= i\alpha \int d^3\mathbf{r}' D(\mathbf{r} - \mathbf{r}', 0) \int \frac{dE}{2\pi} \left\{ \text{Tr} [\gamma^0 S_F^C(\mathbf{r}', \mathbf{r}', E)] \right. \\ &\quad + \int d^3\mathbf{r}_1 \text{Tr} [\gamma^0 S_F^C(\mathbf{r}', \mathbf{r}_1, E) \gamma^0 V_{\text{ren}}^{\text{VP}}(r_1) S_F^C(\mathbf{r}_1, \mathbf{r}', E)] \\ &\quad + \int d^3\mathbf{r}_1 d^3\mathbf{r}_2 \text{Tr} [\gamma^0 S_F^C(\mathbf{r}', \mathbf{r}_1, E) \gamma^0 V_{\text{ren}}^{\text{VP}}(r_1) \\ &\quad \times S_F^V(\mathbf{r}_1, \mathbf{r}_2, E) \gamma^0 V_{\text{ren}}^{\text{VP}}(r_2) S_F^C(\mathbf{r}_2, \mathbf{r}', E)] \left. \right\}. \end{aligned} \quad (14)$$

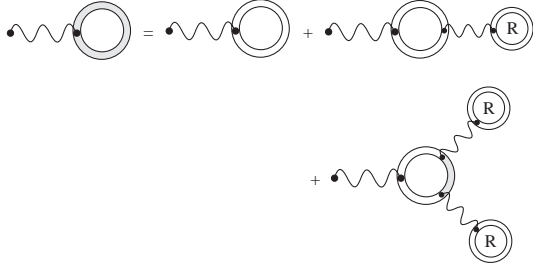


Fig. 2. VP-dressed one-loop vacuum polarization potential (indicated by shadowed lines). The “R” inside of the external VP-loops refers to the *renormalized* one-loop VP-potential $V_{\text{ren}}^{\text{VP}}$ induced by the external Coulomb field of the nucleus, which appears as additional external potential.

A graphical representation of the VP-dressed one-loop potential is depicted in Figure 2. The two-loop vacuum polarization correction we are interested in appears as the second term of the decomposition (Eq. (14)) together with the ordinary one-loop vacuum polarization (first term). The third term accounts for all multiple interaction terms and is at least of order $\alpha^4(Z\alpha)^3$, since the additional potential $V_{\text{ren}}^{\text{VP}}$ contributes with a leading order $\alpha(Z\alpha)$ (Uehling-term). Thus, it is legitimate to neglect this higher-order part. Consequently, we identify as the renormalized two-loop potential

$$\mathcal{U}_{\text{ren}}^{\text{VPVPb}}(r) \simeq i\alpha \int d^3\mathbf{r}' D(\mathbf{r} - \mathbf{r}', 0) \times \left\{ \left(\int \frac{dE}{2\pi} \text{Tr} [\gamma^0 \mathcal{S}_{\text{F}}^{\text{V}}(\mathbf{r}', \mathbf{r}', E)] \right) - \left(\int \frac{dE}{2\pi} \text{Tr} [\gamma^0 \mathcal{S}_{\text{F}}^{\text{C}}(\mathbf{r}', \mathbf{r}', E)] \right) \right\}_{\text{ren}} \quad (15)$$

after appropriate renormalizations have been applied to the right-hand side of the above equation. Note, however, that the formal expression for the effective one-loop vacuum polarization density (first term in the curly brackets) already contains the renormalized one-loop potential $V_{\text{ren}}^{\text{VP}}$, assuming that the renormalization of the exterior VP-loops can be performed separately. This issue will be addressed in the next section. We are now in the position to write down the energy shift of a bound electron state ϕ_{A} due to the exact two-loop correction:

$$\Delta E_{\text{A}}^{\text{VPVPb}} = \langle \phi_{\text{A}} | \mathcal{U}_{\text{ren}}^{\text{VPVPb}} | \phi_{\text{A}} \rangle. \quad (16)$$

In order to deduce exclusively the contribution $\Delta E_{\text{A}}^{\text{VPVPb}}$ (h.o.) arising from higher orders in $(Z\alpha)$, one has to subtract the corresponding two-loop contribution evaluated in the Uehling-approximation.

4 Renormalization

Taking the above into consideration, the problem of renormalization of the exact two-loop potential

$$\mathcal{U}^{\text{VPVPb}}(r) = i\alpha \int d^3\mathbf{r}' D(\mathbf{r} - \mathbf{r}', 0) \int d^3\mathbf{r}_1 \times \int \frac{dE}{2\pi} \text{Tr} [\gamma^0 \mathcal{S}_{\text{F}}^{\text{C}}(\mathbf{r}', \mathbf{r}_1, E) \gamma^0 \mathcal{S}_{\text{F}}^{\text{C}}(\mathbf{r}_1, \mathbf{r}', E)] \quad (17) \times \int d^3\mathbf{r}_2 D(\mathbf{r}_1 - \mathbf{r}_2, 0) \int \frac{dE'}{2\pi} \text{Tr} [\gamma^0 \mathcal{S}_{\text{F}}^{\text{C}}(\mathbf{r}_2, \mathbf{r}_2, E')]$$

as it is derived from standard perturbation expansion of the S -matrix in bound-state QED (see Gell-Mann-Low-Sucher formalism) now reduces to the problem of renormalization of the one-loop vacuum polarization. This is suggested by equations (14) and (15). It relies on the fact, that the external VP-loop is properly taken into account in terms of a VP-dressed effective one-loop, where the external VP-loop may be replaced by the renormalized first-order potential $V_{\text{ren}}^{\text{VP}}$. This is supported by the notion that the electron (positron) experiences the effective nuclear charge modified by the induced vacuum polarization cloud. Procedures for renormalization of one-loop potentials involved in equation (15) are well known from the evaluation of the energy shift due to the first-order vacuum polarization in external Coulomb fields. We adopt the partial wave decomposition approach together with the subtraction scheme developed in [13,15] and apply it to equation (15). These references provide a self-contained description of the evaluation of the exact one-loop vacuum polarization. In order to perform similar steps as in the case of the ordinary Coulomb-dressed VP-loop, we employ the equivalent representation according to equation (8)

$$\mathcal{V}(r) = i\alpha \int d^3\mathbf{r}' D(\mathbf{r} - \mathbf{r}', 0) \int \frac{dE}{2\pi} \times \left\{ \int d^3\mathbf{r}_1 \text{Tr} [\gamma^0 \mathcal{S}_{\text{F}}^{\text{O}}(\mathbf{r}' - \mathbf{r}_1, E) \gamma^0 V(r_1) \mathcal{S}_{\text{F}}^{\text{O}}(\mathbf{r}_1 - \mathbf{r}', E)] + \int d^3\mathbf{r}_1 d^3\mathbf{r}_2 \text{Tr} [\gamma^0 \mathcal{S}_{\text{F}}^{\text{O}}(\mathbf{r}' - \mathbf{r}_1, E) \gamma^0 V(r_1) \mathcal{S}_{\text{F}}^{\text{V}}(\mathbf{r}_1, \mathbf{r}_2, E) \times \gamma^0 V(r_2) \mathcal{S}_{\text{F}}^{\text{O}}(\mathbf{r}_2 - \mathbf{r}', E)] \right\}, \quad (18)$$

where V denotes the total external potential (Eq. (12)). Figure 3 shows the diagrammatic representation of equation (18). Further evaluation requires a partial wave decomposition of all the propagators

$$\mathcal{S}_{\text{F}}^{\text{V}}(\mathbf{r}, \mathbf{r}', E) = \sum_{n\kappa\mu} \frac{\psi_{n\kappa\mu}(\mathbf{r}) \bar{\psi}_{n\kappa}(\mathbf{r}')}{E - \mathcal{E}_{n,\kappa}(1 - i\eta)}, \quad \mathcal{S}_{\text{F}}^{\text{e}}(\mathbf{r}, \mathbf{r}', E) = \sum_{n\kappa\mu} \frac{\phi_{n\kappa\mu}(\mathbf{r}) \bar{\phi}_{n\kappa\mu}(\mathbf{r}')}{E - E_{n,\kappa}(1 - i\eta)}, \quad \mathcal{S}_{\text{F}}^{\text{O}}(\mathbf{r} - \mathbf{r}', E) = \sum_{p,\kappa,\mu} \frac{\varphi_{p\kappa\mu}(\mathbf{r}) \bar{\varphi}_{p\kappa\mu}(\mathbf{r}')}{E - \varepsilon_{p,\kappa}(1 - i\eta)}. \quad (19)$$

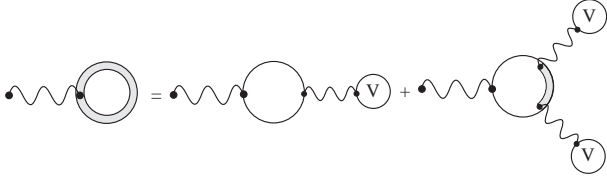


Fig. 3. V -dressed one-loop vacuum polarization potential (indicated by shadowed lines) according to the decomposition (7). \textcircled{V} symbolizes interactions with the total (renormalized) external potential (Eq. (12)).

together with equation (10) for the photon propagator. According to the partial wave renormalization prescription developed in [15] the renormalized one-loop potential \mathcal{V}_{ren} is obtained as the sum of the finite “Wichmann-Kroll”-type contribution $\mathcal{V}_{\mathcal{F}_2}$ and of the renormalized “Uehling”-type potential $\mathcal{V}_{\mathcal{F}_1}$. We are lead to the following expressions:

$$\begin{aligned} \mathcal{V}_{\mathcal{F}_2}(r) &= -\frac{\alpha}{\pi} \int dk j_0(kr) \\ &\times \sum_{|\kappa|=1}^{|\kappa_{\text{max}}|} \left\{ \sum_n \text{sign}(\mathcal{E}_{n,\kappa}) \langle \psi_{n\kappa} | j_0(kr') | \psi_{n\kappa} \rangle \right. \\ &\left. - 4 \sum_p^+ \sum_{p'}^- \frac{\langle \varphi_{p\kappa} | j_0(kr') | \varphi_{p'\kappa} \rangle \langle \varphi_{p'\kappa} | V | \varphi_{p\kappa} \rangle}{\varepsilon_{p,\kappa} - \varepsilon_{p',\kappa}} \right\}, \\ \mathcal{V}_{\mathcal{F}_1}(r) &= \int_0^\infty dr' 4\pi r'^2 [e\rho^V(r')] f(r, r'), \end{aligned} \quad (20)$$

together with the radial kernel

$$\begin{aligned} f(r, r') &= -\frac{2\alpha}{3\pi} \int_1^\infty d\xi \sqrt{1 - \frac{1}{\xi^2}} \left(1 + \frac{1}{2\xi^2} \right) \\ &\times \left[\Theta(r - r') \frac{e^{-2r\xi}}{r\xi} \frac{\sinh(2r'\xi)}{2r'\xi} \right. \\ &\left. + \Theta(r' - r) \frac{e^{-2r'\xi}}{r'\xi} \frac{\sinh(2r\xi)}{2r\xi} \right] \\ &= -\frac{\alpha}{3\pi r'} \left(\frac{1}{2r} \right) [\chi_2(2|r - r'|) - \chi_2(2(r + r'))], \\ \chi_n(z) &= \int_1^\infty d\xi \sqrt{1 - \frac{1}{\xi^2}} \left(1 + \frac{1}{2\xi^2} \right) \frac{e^{-z\xi}}{\xi^n}. \end{aligned} \quad (21)$$

ρ^V denotes the sum of the (bare) nuclear charge density ρ_{nuc} and of the renormalized first-order vacuum polarization charge density $\rho_{\text{ren}}^{\text{VP}}$ induced by the Coulomb field of the nucleus. Equations (20) and (21) are analogous to expressions one has to deal with when deriving the renormalized, exact one-loop potential equation (13). Performing now the subtraction as implied by equation (15), we

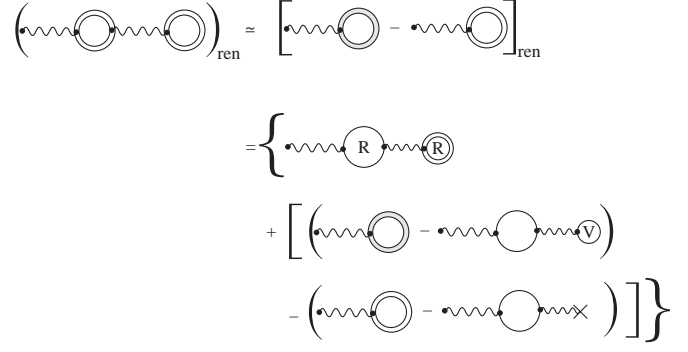


Fig. 4. Diagrammatic representation of the subtraction scheme for deducing the renormalized two-loop vacuum polarization potential according to equations (22) to (24). The first term in curly brackets stands for the part $\mathcal{U}_{\mathcal{F}_1}^{\text{VPVPb}}$ and the second term in square brackets symbolizes the Wichmann-Kroll-type potential $\mathcal{U}_{\mathcal{F}_2}^{\text{VPVPb}}$.

identify the renormalized two-loop vacuum polarization potential:

$$\mathcal{U}_{\text{ren}}^{\text{VPVPb}}(r) = \mathcal{U}_{\mathcal{F}_1}^{\text{VPVPb}}(r) + \mathcal{U}_{\mathcal{F}_2}^{\text{VPVPb}}(r), \quad (22)$$

$$\mathcal{U}_{\mathcal{F}_1}^{\text{VPVPb}}(r) = \int_0^\infty dr' 4\pi r'^2 [e\rho_{\text{ren}}^{\text{VP}}(r')] f(r, r'), \quad (23)$$

$$\begin{aligned} \mathcal{U}_{\mathcal{F}_2}^{\text{VPVPb}}(r) &\simeq -\frac{\alpha}{\pi} \int dk j_0(kr) \\ &\times \sum_{|\kappa|=1}^{|\kappa_{\text{max}}|} \left\{ \left[\sum_n \text{sign}(\mathcal{E}_{n,\kappa}) \langle \psi_{n\kappa} | j_0(kr') | \psi_{n\kappa} \rangle \right. \right. \\ &\left. - 4 \sum_p^+ \sum_{p'}^- \frac{\langle \varphi_{p\kappa} | j_0(kr') | \varphi_{p'\kappa} \rangle \langle \varphi_{p'\kappa} | V | \varphi_{p\kappa} \rangle}{\varepsilon_{p,\kappa} - \varepsilon_{p',\kappa}} \right] \\ &- \left[\sum_n \text{sign}(E_{n,\kappa}) \langle \phi_{n\kappa} | j_0(kr') | \phi_{n\kappa} \rangle \right. \\ &\left. - 4 \sum_p^+ \sum_{p'}^- \frac{\langle \varphi_{p\kappa} | j_0(kr') | \varphi_{p'\kappa} \rangle \langle \varphi_{p'\kappa} | V^{\text{C}} | \varphi_{p\kappa} \rangle}{\varepsilon_{p,\kappa} - \varepsilon_{p',\kappa}} \right] \left. \right\}. \end{aligned} \quad (24)$$

The term $\mathcal{U}_{\mathcal{F}_1}^{\text{VPVPb}}$ denotes the finite (renormalized) Uehling-type potential generated by the Uehling part of the renormalized first-order vacuum polarization charge density. The term $\mathcal{U}_{\mathcal{F}_2}^{\text{VPVPb}}$ summarizes the finite part of the Wichmann-Kroll-type potential. Since the sum over partial waves terminates at some finite $|\kappa_{\text{max}}|$ each contribution in square brackets becomes well defined. The procedure described in equations (22) to (24) for deducing the renormalized exact two-loop vacuum polarization potential is depicted in Figure 4.

For numerical evaluations, however, the representation (Eq. (24)) of the potential $\mathcal{U}_{\mathcal{F}_2}^{\text{VPVPb}}$ is rather cumbersome since it involves terms given as multiple summations over the free Dirac spectrum. A representation which is more convenient for numerical calculations can be introduced as follows: at first, we combine the one-potential terms

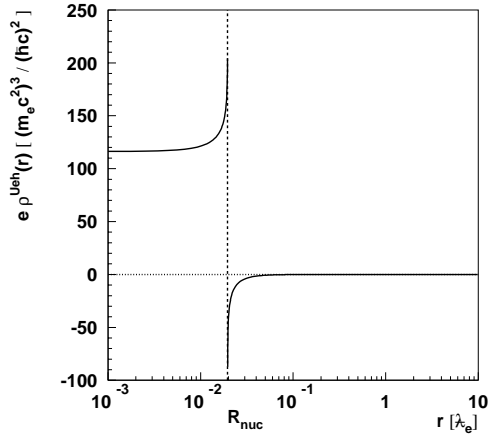


Fig. 5. Uehling-vacuum polarization charge density $e\rho_{\text{ren}}^{\text{Ueh}}$ induced by the extended external charge of a Uranium nucleus (uniform sphere model) as a function of the radial distance r . Natural units are used.

in equation (24) to a one-potential term involving the renormalized one-loop vacuum potential $V_{\text{ren}}^{\text{VP}}$ only. Secondly, the resulting one-potential term is replaced by the completely VP-dressed (free) one-loop potential assuming that the effects due to multiple-interaction contributions, which are at least of order $\alpha(\alpha(Z\alpha))^3$, are negligible. Thus we obtain the alternative representation:

$$\begin{aligned} \mathcal{U}_{\mathcal{F}_2}^{\text{VPVPb}}(r) &\simeq -\frac{\alpha}{\pi} \int dk j_0(kr) \\ &\times \sum_{|\kappa|=1}^{|\kappa_{\text{max}}|} \left\{ \sum_n \text{sign}(\mathcal{E}_{n,\kappa}) \langle \psi_{n\kappa} | j_0(kr') | \psi_{n\kappa} \rangle \right. \\ &\quad - \sum_n \text{sign}(E_{n,\kappa}) \langle \phi_{n\kappa} | j_0(kr') | \phi_{n\kappa} \rangle \\ &\quad \left. - \sum_n \text{sign}(\tilde{\varepsilon}_{n,\kappa}) \langle \tilde{\varphi}_{n\kappa} | j_0(kr') | \tilde{\varphi}_{n\kappa} \rangle \right\}, \end{aligned} \quad (25)$$

where the states $\tilde{\varphi}_{n\kappa}$ are solutions of the Dirac equation with the external potential $V_{\text{ren}}^{\text{VP}}$ and corresponding energy eigenvalues $\tilde{\varepsilon}_{n,\kappa}$.

Having derived the renormalized potential $\mathcal{U}_{\text{ren}}^{\text{VPVPb}}$, the corresponding energy shift of a bound electron state ϕ_A in the external Coulomb field can be evaluated according to equation (16). It is convenient to divide the total energy shift resulting from the exact two-loop vacuum polarization into the following three contributions:

$$\begin{aligned} \Delta E_A^{\text{VPVPb}} &= \langle \phi_A | \mathcal{U}_{\mathcal{F}_1, \text{Ueh}}^{\text{VPVPb}} | \phi_A \rangle + \langle \phi_A | \mathcal{U}_{\mathcal{F}_1, \text{WK}}^{\text{VPVPb}} | \phi_A \rangle \\ &\quad + \langle \phi_A | \mathcal{U}_{\mathcal{F}_2}^{\text{VPVPb}} | \phi_A \rangle \\ &= \Delta E_A^{\text{VPVPb}}(\mathcal{F}_1, \text{Ueh}) + \Delta E_A^{\text{VPVPb}}(\mathcal{F}_1, \text{WK}) \\ &\quad + \Delta E_A^{\text{VPVPb}}(\mathcal{F}_2), \end{aligned} \quad (26)$$

which we shall evaluate separately. The first energy contribution in the above equation may be called *Uehling-in-Uehling* contribution, since the corresponding part of the potential (23) originates from the Uehling part $\rho_{\text{ren}}^{\text{Ueh}}$ of the renormalized vacuum polarization. Similarly, we may refer to the second term in (26) as *Wichmann-Kroll-in-Uehling* contribution, since it accounts for the effect of the Wichmann-Kroll part $\rho_{\text{ren}}^{\text{WK}}$ of the vacuum-polarization loop. Finally, the third term takes into account the Wichmann-Kroll-type potential (25).

5 Two-loop contribution in Uehling approximation

Being interested primarily in the contribution to the energy shift due to higher orders in $(Z\alpha)$, we should subtract the Uehling-in-Uehling contribution, where the exact vacuum polarization loops are replaced by free fermion loops. Taking a uniform sphere model for the nuclear charge distribution, *i.e.* $\rho_{\text{nuc}} = (3Ze/4\pi R_0^3) \Theta(R_0 - r)$, the latter reads:

$$\begin{aligned} \mathcal{U}_{\mathcal{F}_1, \text{Ueh}}^{\text{VPVPb}}(r) &= \int_0^\infty dr' 4\pi r'^2 [e\rho_{\text{ren}}^{\text{Ueh}}(r')] f(r, r'), \\ [e\rho_{\text{ren}}^{\text{Ueh}}(r)] &= \left(\frac{3Z\alpha}{4\pi R_0^3} \right) \frac{2\alpha}{3\pi} \frac{R_0}{r} \\ &\quad \times \int_1^\infty d\xi \sqrt{1 - \frac{1}{\xi^2}} \left(1 + \frac{1}{2\xi^2} \right) \frac{1}{\xi} \\ &\quad \times \left\{ \Theta(R_0 - r) \left(1 + \frac{1}{2R_0\xi} \right) \sinh(2r\xi) e^{-2R_0\xi} \right. \\ &\quad \left. - \Theta(r - R_0) \left[\cosh(2R_0\xi) - \frac{\sinh(2R_0\xi)}{2R_0\xi} \right] e^{-2r\xi} \right\}. \end{aligned} \quad (27)$$

The expression for $\rho_{\text{ren}}^{\text{Ueh}}$ may be cast into the more familiar form:

$$\begin{aligned} [e\rho_{\text{ren}}^{\text{Ueh}}(r)] &= \left(\frac{Z\alpha}{4\pi R_0^2} \right) \frac{\alpha}{\pi r} \\ &\quad \times \left\{ \text{sign}(R_0 - r) \chi_1(2|R_0 - r|) - \chi_1(2(R_0 + r)) \right. \\ &\quad \left. + \frac{1}{2R_0} [\chi_2(2|R_0 - r|) - \chi_2(2(R_0 + r))] \right\}. \end{aligned} \quad (28)$$

This vacuum polarization charge density is plotted in Figure 5. It is easily verified that the induced Uehling density (Eq. (28)) possesses a logarithmic singularity at the nuclear radius, which originates from the first term in the curly brackets. Integrating the Uehling charge density over the interior of the nucleus we obtain the finite induced

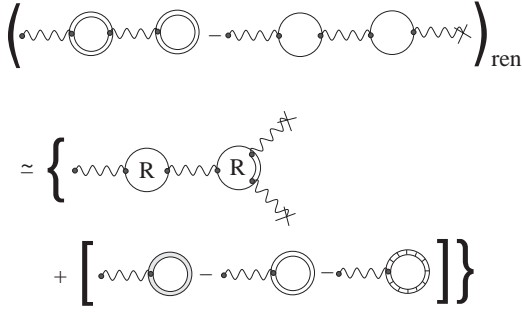


Fig. 6. Diagrammatic representation the subtraction scheme for deducing the higher-order in $(Z\alpha)$ part of the renormalized two-loop vacuum polarization potential $\mathcal{U}_{\text{ren}}^{\text{VPVPb}}$. The first term in curly brackets stands for the part $\mathcal{U}_{\mathcal{F}1, \text{WK}}^{\text{VPVPb}}$ and the second term in square brackets represents the Wichmann-Kroll-type potential $\mathcal{U}_{\mathcal{F}2}^{\text{VPVPb}}$ according to equation (25). The third one-loop potential involves Dirac states in the presence of the vacuum polarization potential $V_{\text{ren}}^{\text{VP}}$ only.

vacuum charge

$$\begin{aligned} eQ^{\text{int}}(R_0) &= \int_0^{R_0} dr' 4\pi r'^2 [e\rho_{\text{ren}}^{\text{Ueh}}(r')] = \frac{Z\alpha}{2R_0} \frac{\alpha}{\pi} \\ &\times \left[\chi_2(0) + \chi_2(4R_0) + \frac{\chi_3(4R_0)}{R_0} + \frac{\chi_4(4R_0) - \chi_4(0)}{(2R_0)^2} \right] \\ &= - \int_{R_0}^{\infty} dr' 4\pi r'^2 [e\rho_{\text{ren}}^{\text{Ueh}}(r')] = -eQ^{\text{ext}}(R_0) \end{aligned} \quad (29)$$

which is exactly cancelled by the total induced charge in the exterior region Q^{ext} .

The corresponding energy correction to the binding energy $\Delta E_A^{\text{VPVPb}}(\mathcal{F}1, \text{Ueh})$ is part of the Källén-Sabry correction [10] and will be calculated separately.

6 Evaluation

We now turn to the evaluation of the higher-order $(Z\alpha)$ -contribution of the two-loop vacuum polarization to the Lamb shift of strongly bound electrons

$$\Delta E_A^{\text{VPVPb}}(\text{h.o.}) = \langle \phi_A | (\mathcal{U}_{\mathcal{F}1, \text{WK}}^{\text{VPVPb}} + \mathcal{U}_{\mathcal{F}2}^{\text{VPVPb}}) | \phi_A \rangle, \quad (30)$$

where the Uehling-in-Uehling part is subtracted. Thus the effect of all higher orders in $(Z\alpha)$ in the interaction with the external Coulomb potential contributing to the exact two-loop correction proceeds in two separate steps. Accordingly, we only need to calculate the renormalized Uehling-potential generated exclusively by the induced Wichmann-Kroll charge density

$$\mathcal{U}_{\mathcal{F}1, \text{WK}}^{\text{VPVPb}}(r) = \int_0^{\infty} dr' 4\pi r'^2 [e\rho_{\text{ren}}^{\text{WK}}(r')] f(r, r'), \quad (31)$$

and the renormalized Wichmann-Kroll-type Potential $\mathcal{U}_{\mathcal{F}2}^{\text{VPVPb}}$ according to the subtraction scheme (Eq. (25)).

As a first step towards the evaluation of the energy correction (30) we consider the Wichmann-Kroll-in Uehling

contribution $\Delta E_A^{\text{VPVPb}}(\mathcal{F}1, \text{WK})$. This correction to the Lamb shift of the bound state ϕ_A is related to the change of the Uehling potential (Eq. (31)) arising from the Wichmann-Kroll part of the induced vacuum polarization. At first we wish to derive an estimate for this correction to the Lamb shift of the ground state in hydrogenlike Lead and Uranium.

The Wichmann-Kroll charge density $\rho_{\text{ren}}^{\text{WK}}$ is calculated based on the partial wave decomposition of the Coulomb propagator and of the free propagator as developed in reference [13]. It is obtained from

$$\begin{aligned} e\rho_{\text{ren}}^{\text{WK}}(r) &= \frac{\alpha}{\pi} \int_0^{\infty} \frac{du}{2\pi} \sum_{|\kappa|=1}^{\infty} |\kappa| \Re \left\{ \sum_{j=1}^2 G_{\kappa}^{jj}(r, r, iu) \right. \\ &\quad \left. + \int_0^{\infty} dr' r'^2 V^{\text{C}}(r') \sum_{j,k=1}^2 [F_{\kappa}^{j,k}(r, r', iu)]^2 \right\}, \end{aligned} \quad (32)$$

where the summation over κ is terminated at some maximum value $|\kappa_{\text{max}}|$. The quantities G_{κ}^{jj} and $F_{\kappa}^{j,k}$ denote the partial wave decompositions of the free and the bound propagators. Apart from the long-range tail where the Wichmann-Kroll vacuum polarization charge density is positive, a strongly pronounced maximum of negative charge density occurs in the vicinity of the nuclear surface (see Ref. [13]). Integrating over this r -range one obtains a total induced negative charge

$$Q_-^{\text{WK}} = eZ^{\text{WK}} = \int_0^{r^-} dr 4\pi \rho_{\text{ren}}^{\text{WK}}(r). \quad (33)$$

Since the Wichmann-kroll density is strongly localized near the nuclear surface it acts almost like an additional negatively charged spherical shell surrounding the nucleus. A strongly bound S -electron experiences the reduced nuclear charge. This suggests replacing the corresponding potential $\mathcal{U}_{\mathcal{F}1, \text{WK}}^{\text{VPVPb}}$ by the Uehling potential generated by a spherical shell carrying the negative charge Q_-^{WK} as an approximation. In this case the integral (Eq. (31)) can be evaluated immediately. If we further employ a spherical shell model for the nuclear charge distribution, a simple scaling law is derived. This relates the energy shift $\Delta E_A^{\text{VPVPb}}(\mathcal{F}1, \text{WK})$ and the first-order Uehling correction $\Delta E_A^{\text{VP}}(\text{Ueh})$ according to:

$$\Delta E_A^{\text{VPVPb}}(\mathcal{F}1, \text{WK}) \simeq \frac{Z^{\text{WK}}}{Z} \Delta E_A^{\text{VP}}(\text{Ueh}). \quad (34)$$

The validity of this scaling law is supported by the fact that the numerical results for the Uehling correction do not depend significantly upon details of the extended nuclear charge distribution. With the scaling law at hand we have an additional tool for testing the numerical results for the Wichmann-Kroll-in-Uehling contribution for strongly bound electrons.

The complete evaluation of the Wichmann-Kroll-type contribution $\Delta E_A^{\text{VPVPb}}(\mathcal{F}2)$ will be performed numerically

Table 1. Estimate of the “Wichmann-Kroll in Uehling” contribution to the $1S_{1/2}$ -Lamb shift in hydrogenlike Lead and Uranium. The values given for the first-order Uehling correction $E_A^{\text{VP}}(\text{Ueh})$ are calculated assuming a uniform sphere model for the nuclear charge density [7]. The Wichmann-Kroll density $\rho_{\text{ren}}^{\text{WK}}$ is calculated for a spherical shell model [8].

system	$\Delta E_{1S_{1/2}}^{\text{VP}}(\text{Ueh})$ [eV]	Z^{WK}	$\Delta E_{1S_{1/2}}^{\text{VPVPb}}(\mathcal{F}1, \text{WK})$ [eV]
$^{238}_{92}\text{U}$	-93.58	-0.006	0.0061
$^{208}_{82}\text{Pb}$	-50.70	-0.004	0.0024

Table 2. The results for the two-loop vacuum polarization contribution in Uehling approximation $\Delta E_A^{\text{VPVPb}}(\mathcal{F}1, \text{Ueh})$ (first term of Eq. (26)) in comparison with the exact two-loop correction $\Delta E_A^{\text{VPVPb}}$ to the Lamb shift of strongly bound electrons in hydrogenlike Lead and Uranium. The higher-order contributions $\Delta E_A^{\text{VPVPb}}(\mathcal{F}1, \text{WK})$ (Eq. (34)) and $\Delta E_A^{\text{VPVPb}}(\mathcal{F}2)$ (second and third terms of Eq. (26)) are listed separately. Energies are given in units of eV.

system	state	$\Delta E_A^{\text{VPVPb}}(\mathcal{F}1, \text{Ueh})$	$\Delta E_A^{\text{VPVPb}}$	$\Delta E_A^{\text{VPVPb}}(\mathcal{F}1, \text{WK})$	$\Delta E_A^{\text{VPVPb}}(\mathcal{F}2)$
$^{238}_{92}\text{U}$	$1S_{1/2}$	-0.1150	-0.1530	0.0040	-0.0420
	$2S_{1/2}$	-0.0220	-0.0286	0.00074	-0.0073
	$2P_{1/2}$	-0.0023	-0.0036	0.000079	-0.0014
$^{208}_{82}\text{Pb}$	$1S_{1/2}$	-0.0520	-0.0685	0.0015	-0.0180
	$2S_{1/2}$	-0.0092	-0.0118	0.00027	-0.0029
	$2P_{1/2}$	-0.0006	-0.0010	0.000018	-0.0004

according to the subtraction scheme introduced by equation (24) respectively (25). Figure 6 illustrates the subtraction scheme we applied for numerical calculations. The numerical evaluation utilizes the very precise computer codes developed by Mohr *et al.* [13] for generating the Wichmann-Kroll part of the vacuum polarization density and those by Persson *et al.* [15] for representing the potential $\mathcal{U}_{\mathcal{F}2}^{\text{VPVPb}}$ in terms of partial waves.

7 Results and discussion

The scaling law (Eq. (34)) derived above for the “Wichmann-Kroll in Uehling” part $\Delta E_A^{\text{VPVPb}}(\mathcal{F}1, \text{WK})$ may only be useful as test for its complete numerical calculation. In order to employ the scaling law the first-order Uehling correction $E_A^{\text{VP}}(\text{Ueh})$ and the Wichmann-Kroll charge density ρ^{WK} need to be determined. This can be achieved by means of very accurate numerical procedures developed earlier (see *e.g.* [13, 15, 8] and references therein). For a discussion of technical details encountered with the evaluation of $\rho_{\text{ren}}^{\text{WK}}$ we refer to [8]. The total induced negative charge number $Z_{\text{ren}}^{\text{WK}}$ is obtained by integrating the Wichmann-Kroll density from the origin $r = 0$ up to $r = r_-$ where $\rho_{\text{ren}}^{\text{WK}}$ changes its sign. Table 1 gives numerical results for the first-order Uehling correction, the induced negative charge number and for the corresponding energy shifts $\Delta E_A^{\text{VPVPb}}(\mathcal{F}1, \text{WK})$ according to the scaling law for the $1S$ -ground state of hydrogenlike Lead and Uranium respectively. The energy correction is repulsive, since the induced charge is negative.

Let us compare the effect of the higher-order contribution to the two-loop correction $\Delta E_A^{\text{VPVPb}}(\text{h.o.})$ defined by equation (30) with the one obtained in Uehling approximation $\Delta E_A^{\text{VPVPb}}(\mathcal{F}1, \text{Ueh})$. The latter is tabulated in

the first column of Table 2 for K- and L- shell electrons in hydrogenlike Lead and Uranium. This Uehling-in-Uehling contribution is attractive and amounts to less than 20% of the total Källén-Sabry correction to the Lamb shift as tabulated in [10]. The results for the exact two-loop correction are tabulated in the second column of Table 2.

In comparison with the exact numerical results for the Wichmann-Kroll-in-Uehling contribution as presented in the third column of Table 2 the scaling law indeed gives the right order of magnitude but leads to a systematic overestimation due to the neglect of the long-range tail of $\rho_{\text{ren}}^{\text{WK}}$. The numerical results for the Wichmann-Kroll-type contribution $\Delta E_A^{\text{VPVPb}}(\mathcal{F}2)$, which have been obtained according to the representation (Eq. (25)), are presented in the last column of Table 2. As for the Uehling-in-Uehling correction this contribution carries the same overall sign, *i.e.* it also acts attractive. It comprises about 40% of the two-loop diagram evaluated in Uehling approximation. This result also indicates that higher-order ($Z\alpha$) contributions to the one-loop polarization insertion of the photon propagator may be not small compared with the Uehling approximation. Accordingly, it may be not surprising at all, if the higher-order contribution to the S(VP)E - correction (see Fig. 1) may turn out to be important as well.

Even in the case of Uranium the order of magnitude for the total higher-order part $\Delta E_A^{\text{VPVPb}}(\text{h.o.})$ (see Table 2) is about $\sim 10^{-2}$ eV for the $1S$ -state, which indicates that the effect of the higher-order contributions to the two-loop vacuum polarization alone are far too small to be detected *via* Lamb-shift measurements with current accuracies. Furthermore, this correction is about one order of magnitude below the natural limitations for tests of QED set by nuclear polarization effects [16]. It might also be instructive to compare this effect with the uncertainties

of the 1S-energy level caused by the uncertainties in the determination of the nuclear radii. The rms-radius for Uranium is given by $\langle r^2 \rangle_U^{1/2} = 5.8604(23)$ fm [17] and leads to an uncertainty of about $\delta E_{1S}^U \sim 0.1$ eV. The current status of Lamb shift predictions is presented in [18]. Although a complete numerical evaluation of the exact Källén-Sabry diagrams, i.e., the higher-order contributions of the self-energy-corrected one-loop diagram VPVPc remain to be performed, the goals of this paper have been achieved:

1. We have presented a calculational scheme for evaluating the two-loop vacuum polarization corrections to all orders in the interaction with the external Coulomb potential. The problem is reduced to the evaluation of an effective one-loop correction. Thus, the partial wave decomposition can be employed in a similar way as it has been used successfully in calculations of the ordinary first-order vacuum polarization correction.

2. Numerical results for exact two-loop vacuum polarization correction to the Lamb shift of K- and L-shell electrons in hydrogenlike Lead and Uranium have been obtained. It turns out to be below the natural limits set by nuclear polarization effects and by the uncertainties of nuclear parameters.

3. Although the effect of the higher-order contributions to the two-loop diagram turn out to be small a further uncertainty in Lamb-shift calculations has been eliminated. Aiming for a relative precision of 10^{-6} of theoretical predictions of the binding energy we conjecture that the still unknown exact two-photon self energy corrections remain the major source of uncertainties.

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