9-1-1997

# Lamb Shift of 3P and 4P States and the Determination of $\alpha$

Ulrich D. Jentschura
*Missouri University of Science and Technology*, ulj@mst.edu

Gerhard Soff

Peter J. Mohr



## Recommended Citation

U. D. Jentschura et al., "Lamb Shift of 3P and 4P States and the Determination of α," *Physical Review A - Atomic, Molecular, and Optical Physics*, vol. 56, no. 3, pp. 1739-1755, American Physical Society (APS), Sep 1997.
The definitive version is available at https://doi.org/10.1103/PhysRevA.56.1739

# Lamb shift of $3P$ and $4P$ states and the determination of $\alpha$

U. D. Jentschura,[1,*] G. Soff,[1] and P. J. Mohr[2,†]
[1]*Institut für Theoretische Physik, TU Dresden, Mommsenstraße 13, 01062 Dresden, Germany*
[2]*Atomic Physics Division, National Institute of Standards and Technology (NIST), Gaithersburg, Maryland 20899-0001*
(Received 6 March 1997)

The fine-structure interval of $P$ states in hydrogenlike systems can be determined theoretically with high precision, because the energy levels of $P$ states are only slightly influenced by the structure of the nucleus. Therefore a measurement of the fine structure may serve as an excellent test of QED in bound systems, or alternatively as a means of determining the fine-structure constant $\alpha$ with very high precision. In this paper an improved analytic calculation of higher-order binding corrections to the one-loop self-energy of $3P$ and $4P$ states in hydrogenlike systems with a low nuclear charge number $Z$ is presented. The method of calculation has been described earlier by Jentschura and Pachucki [Phys. Rev. A **54**, 1853 (1996)], and is applied here to the excited $P$ states. Because of the more complicated nature of the wave functions and the bound-state poles corresponding to decay of the excited states, the calculations are more complex. Comparison of the analytic results to the extrapolated numerical data for high-$Z$ ions [Mohr and Kim, Phys. Rev. A **45**, 2727 (1992)] serves as an independent test of the analytic evaluation. Theoretical values for the Lamb shift of the $P$ states and for the fine-structure splittings are given. [S1050-2947(97)08408-4]

PACS number(s): 12.20.Ds, 31.30.Jv, 06.20.Jr

## I. INTRODUCTION

Evaluations of the radiative corrections in higher order for bound states are an involved task because of the appearance of a multitude of terms, and because of the difficulties associated with bound-state formalism. In this paper, we present an improved calculation of higher-order corrections to the one-loop self-energy of an electron in an excited $3P$ or $4P$ state [1,2].

For the contribution $\delta E_{\rm SE}$ of the one-loop radiative correction to the Lamb shift of a bound electron, we have the following nonanalytic expansion in powers of $Z$ times the fine-structure constant $\alpha$,

$$\delta E_{\rm SE}=\frac{\alpha}{\pi}\frac{(Z\alpha)^4 m}{n^3}F, \tag{1}$$

where

$$F=A_{4,1}\ln(Z\alpha)^{-2}+A_{4,0}+(Z\alpha)A_{5,0}+(Z\alpha)^2 \times[A_{6,2}\ln^2(Z\alpha)^{-2}+A_{6,1}\ln(Z\alpha)^{-2}+A_{6,0}+(Z\alpha)G_{\rm SE,7}]. \tag{2}$$

The remainder function $G_{\rm SE,7}$ is of order 1, and is comprised of the terms $A_{7,0}$ and higher coefficients. Corrections $A_{4,1}$, $A_{5,0}$, and $A_{6,2}$ vanish for $P$ states. The terms $A_{4,0}$ (see, e.g., Ref. [3]) and $A_{6,1}$ [3,4] are known analytically. The term $A_{4,0}$ contains the Bethe logarithm which has been evaluated to 12 significant figures [5,6]. Results have not been obtained for $A_{6,0}$ coefficients. In this paper, we present an evaluation of the $A_{6,0}$ coefficients for the $3P_{1/2}$, $3P_{3/2}$, $4P_{1/2}$, and $4P_{3/2}$ states. The results lead to improved values for the Lamb shift of the respective states, and to a new theoretical value for the fine-structure splitting. We give an explicit formula for the fine structure of the $2P$, $3P$, and $4P$ states as a function of the fine-structure constant $\alpha$, which can be used to obtain a value of $\alpha$ from experimental data.

In this paper, we briefly compare some of the methods that have been developed for the treatment of the one-loop problem. We give a brief account and illustrate the usefulness of the $\epsilon$ method [1,7] for analytic evaluations. We then describe the evaluation of the high-energy part to the self-energy, with a focus on details of the integration procedure. We then proceed to the low-energy part. Results of the calculation are given, and specific contributions are discussed in detail.

## II. VARIOUS METHODS OF TREATMENT OF THE ONE-LOOP SELF-ENERGY

Using units in which $\hbar=c=1$ and $e^2=4\pi\alpha$, we can write the integral corresponding to the one-loop self energy of an electron bound in a Coulomb field,

$$\delta E_{\rm SE}=\lim_{M\to\infty}-ie^2\int_{C_F}\frac{d\omega}{2\pi}\int\frac{d^3\mathbf{k}}{(2\pi)^3}D^{\rm reg}_{\mu,\nu}(k^2,M) \times\left\langle\overline{\psi}\left|\gamma^\mu\frac{1}{\not p-\not k-m-\gamma^0 V}\gamma^\nu\right|\psi\right\rangle-\langle\overline{\psi}|\delta m(M)|\psi\rangle, \tag{3}$$

where $D^{\rm reg}_{\mu,\nu}(k^2,M)$ is the Pauli-Villars regularized photon propagator (in the Feynman gauge, we have $D^{\rm reg}_{\mu\nu}(k^2,M)$

*Electronic address: ulj@nist.gov
†Electronic address: mohr@nist.gov

 

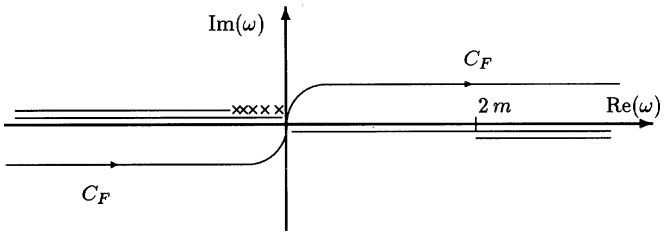


FIG. 1. Feynman contour for $\omega$ integration (one-loop self-energy). Lines directly below and above the real axis denote branch cuts from the photon and electron propagators. Crosses denote poles originating from the discrete spectrum of the electron propagator.

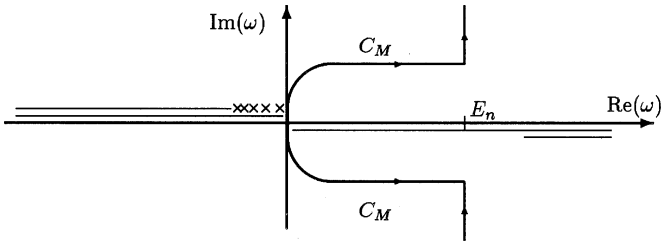


FIG. 2. Mohr's contour for evaluating the one-loop self-energy contribution to the Lamb shift.

$=-g_{\mu\nu}[1/k^2-1/(k^2-M^2)]$). The term $\delta m(M)$ in Eq. (3) is the one-loop mass counter term as a function of $M$, $\delta m(M)=\alpha(3/4\pi)m[\ln(M^2/m^2)+\frac{1}{2}]$. $\overline{\psi}=\psi^\dagger\gamma^0$ denotes the Dirac adjoint. It is straightforward to derive Eq. (3) with the Feynman rules of QED. By rescaling all variables to the electron mass scale,

$$\omega\to m\omega', \quad \mathbf{k}\to m\mathbf{k}', \quad p\to mp',$$

$$V\to mV', \quad M\to mM', \tag{4}$$

we have

$$\delta E_{\rm SE}=-ie^2m\int_{C_F}\frac{d\omega'}{2\pi}\int\frac{d^3\mathbf{k}'}{(2\pi)^3}\left[\frac{1}{k'^2}-\frac{1}{k'^2-M'^2}\right]$$
$$\times\left\langle\overline{\psi}\left|\gamma^\mu\frac{1}{\not p'-\not k'-1-\gamma^0V'}\gamma_\mu\right|\psi\right\rangle$$
$$-\langle\overline{\psi}|\delta m(M')|\psi\rangle. \tag{5}$$

In this paper we will use variables rescaled to the electron mass, and suppress the prime of the rescaled variables in the sequel. Note that in our system of units, we have (e.g.) for the Bohr radius of the atom $a_{\rm Bohr}=1/(Z\alpha)$. By contrast, in atomic units, which are used, for example, in Ref. [8], we would have the Bohr radius of length unity.

The analytic properties of the propagators determine the location of the poles in the integrand in Eq. (3), as indicated in Fig. 1. The original Feynman prescription calls for integrating the photon energy along the contour $C_F$. For the actual evaluation of the Lamb shift, however, a different contour of integration is used by most authors. Taking advantage of the analytic properties of the integrand and of Jordan's lemma, one can change the Feynman contour in the complex plane without changing the result of the calculation. Here we compare the contour used in Bethe's original derivation of the Lamb shift, the contour used by Mohr in Refs. [9–12], and the contour used in Pachucki's $\epsilon$ method, which is used in this paper.

Mohr's and Pachucki's methods both depend on a division of the calculation into low- and high-energy parts. Mohr's method relies on the contour $C_M$ in Fig. 2. His low-energy part is determined by the part of the contour $C_M$ where $\mathrm{Re}(\omega)<E_n$. The residues of the poles of the photon propagator only contribute to low-energy part in this case. It can be shown that the low-energy part is given by the formula

$$\Delta E_L=\lim_{\delta\to0+}\left[\frac{\alpha}{\pi}E_n-\frac{\alpha}{4\pi^2}\int_{k<E_n}d^3k\frac{1}{k}\left(\delta^{ij}-\frac{k^ik^j}{k^2}\right)\right.$$
$$\left.\times\left\langle\psi\left|\alpha^ie^{i\mathbf{k}\cdot\mathbf{r}}\frac{1}{H_D-E_n+k-i\delta}\alpha^je^{-i\mathbf{k}\cdot\mathbf{r}}\right|\psi\right\rangle\right] \tag{6}$$

[cf. Eq. (3.8) in Ref. [9]; $H_D$ is the Dirac Hamiltonian]. This contribution contains terms of lower order in $(Z\alpha)$ than $(Z\alpha)^4$. The spurious lower-order terms cancel when the low- and high-energy parts are added in that method. The high-energy part is obtained by Wick rotating the Feynman contour for $\omega$ integration along the line with $\mathrm{Re}(\omega)=E_n$. In the nonrelativistic limit, expression (6) corresponds (up to the term $\alpha/\pi E_n$) to what would be expected to be the self energy of the electron in terms of traditional second-order perturbation theory due to transverse modes of the electromagnetic field,

$$\Delta E_L^{(2)}=\mathrm{Re}(\Delta E_L)-\frac{\alpha}{\pi}E_n$$
$$=\sum_{n'}P\int_{k<K}d^3k\sum_{\lambda=1,2}\frac{e^2}{4m^2}\int d^3r\,\frac{|\psi_{n'}^\dagger(\mathbf{x})[\nabla\cdot\boldsymbol{\epsilon}_\lambda(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{r}}+e^{i\mathbf{k}\cdot\mathbf{r}}\nabla\cdot\boldsymbol{\epsilon}_\lambda(\mathbf{k})]\psi_{n'}(\mathbf{x})|^2}{E_n-E_{n'}-k}, \tag{7}$$

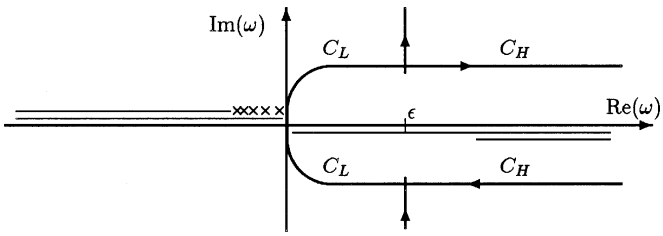


FIG. 3. The $\omega$-integration contour used by Pachucki and in the calculation presented in this paper. For the divergent terms in the high-energy part, we use the Wick-rotated contour given by the lines extending to $\epsilon \pm i\infty$. For the naively convergent terms, we use the original contour $C_H$ which extends to $+\infty \pm i\delta$.

where

$$\sum_{\lambda=1,2} \epsilon_\lambda^i(\mathbf{k})\epsilon_\lambda^j(\mathbf{k}) = \delta^{ij} - \frac{k^i k^j}{k^2}. \tag{8}$$

$K$ in Eq. (7) is an appropriate energy cutoff to make the expression finite (for a derivation of Eq. (7) cf. Ref. [13], Eqs. (7-112)–(7-115), *ibid.*, where in the relativistic case one has to substitute $\boldsymbol{\alpha}$ for $1/i\nabla$). In Mohr's method, $K$ corresponds to $E_n$. Bethe's derivation of the Lamb shift, which gave the right scaling of the effect of the self-energy and correctly identified $A_{4,1}$, but did not include the contribution to the Lamb shift of order $\alpha/\pi(Z\alpha)^4$ due to the anomalous magnetic moment, comprised the expression given in Eq. (7), but with a major modification. Bethe subtracted from Eq. (7) the contribution that would modify the energy (or mass) of a free electron due to its self-interaction. This contribution would make a contribution to the rest mass of any electron, and thus would be unobservable. In our terminology, Bethe's nonrelativistic (NR) expression would be written

$$\delta E_L^{2,\mathrm{NR}} = -P\frac{2\alpha}{3\pi}\int_0^{K=m} dk\; k\langle\phi|\frac{p^i}{m}\left[\frac{1}{H_S-(E_\phi-k)} - \frac{1}{k}\right]\frac{p^i}{m}|\phi\rangle, \tag{9}$$

where $H_S$ is the Schrödinger Hamiltonian, $\phi$ is the nonrelativistic wave function, and the subtracted term $-1/k$ in the integrand corresponds to the portion of mass renormalization attributable to the low-energy part. By taking the principal value ($P$), we identify the real part of Eq. (9) as the energy shift, whereas the imaginary part corresponds to the decay width of the state $|\phi\rangle$. Using the subtraction, Bethe disposed of the spurious lower-order terms and obtained a finite expression.

In Pachucki's method (see Fig. 3), an expression similar to Eq. (7) is obtained in the nonrelativistic limit for the low-energy part, but with an upper cutoff epsilon for the photon energy. This cutoff epsilon separates the low- and the high-energy parts. In the dipole approximation $\exp(i\mathbf{k}\cdot\mathbf{r})\to 1$, one obtains the expression

$$\delta E_L = -\frac{2\alpha}{3\pi}\int_0^{\epsilon} dk\; k\langle\phi|\frac{p^i}{m}\frac{1}{H_S-(E_\phi-k)}\frac{p^i}{m}|\phi\rangle \tag{10}$$

for the low-energy part in leading order. The renormalization term $-1/k$ is gone, and the upper cutoff has been changed from $K=m$ to $K=\epsilon$. The justification for leaving out the renormalization term is intimately linked to the special series expansion prescription used by Pachucki.

Pachucki's method relies on the fact that the low- and high-energy parts may formally be regarded as functions of the fine-structure constant $\alpha$ and the cutoff parameter $\epsilon$. Their sum, however, the self-energy of the electron $\delta E$,

$$\delta E(\alpha) = E_L(\alpha,\epsilon) + E_H(\alpha,\epsilon), \tag{11}$$

does not depend on $\epsilon$, provided the high- and low-energy parts are expanded first in $\alpha$, and then in $\epsilon$ (the order of expansion plays a crucial role in that case).

Another important point in Pachucki's method is that the spurious lower-order terms which were present in Mohr's calculation vanish in the limit $\epsilon\to 0$, so we do not need to take them into account. For example, in Mohr's calculation, the first spurious term $(\alpha/\pi)E_n$ originated from a trivial integration $\int_0^{E_n} dk\,\alpha/\pi = (\alpha/\pi)E_n$. In Pachucki's method, we would change the upper limit of integration to $\epsilon$ and calculate $\lim_{\epsilon\to 0}\int_0^{\epsilon} dk\,\alpha/\pi = 0$. That means by choosing the $\epsilon$ prescription, we not only make the expression for the low-energy part separately finite, but also dispose of the spurious lower-order terms. That is the principal reason why Pachucki's method is well suited for an analytic calculation of higher-order corrections to the one-loop self-energy.

The choice of $\epsilon$ remains arbitrary to a certain extent (it has to be because we analytically expand in $\epsilon$, and thus require arbitrariness). However, we must put some restraints on the magnitude of $\epsilon$. In the high-energy part, we expand the propagator of the bound electron in powers of the binding field $V$. We initially assume a fixed value for $\epsilon$ which prevents infrared problems, but since eventually $\epsilon\to 0$, this expansion is regarded as a formal expansion that is not necessarily convergent. However, $\epsilon$ may not be arbitrarily large. If we let $\epsilon > 2m$, we enclose poles not only from the photon propagator, but also from the negative spectrum of the Dirac-Coulomb propagator, which would significantly alter our expression for the low-energy part. It is also required that in the entire domain of the low-energy part, an expansion of the expression

$$\exp(i\mathbf{k}\cdot\mathbf{r})$$

in the matrix element

$$\langle\psi|\alpha^i e^{i\mathbf{k}\cdot\mathbf{r}}\frac{1}{H_D-E_n-k-i\delta}\alpha^j e^{-i\mathbf{k}\cdot\mathbf{r}}|\psi\rangle$$

in powers of $\mathbf{k}\cdot\mathbf{r}$ corresponds to an expansion in powers of $Z\alpha$ [this requirement justifies the so-called dipole approximation, in which we replace $\exp(i\mathbf{k}\cdot\mathbf{r})$ by unity to obtain the lowest-order contribution to the self-energy]. The order of magnitude of $r$ is $1/(Z\alpha)$ in natural units. Thus we require $\epsilon < (Z\alpha)$. The dominant contribution is then determined by the region in which the photon energy $k\equiv\omega = O((Z\alpha)^2)$, so that $\mathbf{k}\cdot\mathbf{r} = O(Z\alpha)$. In this paper we consider the relativistic corrections up to relative order $(Z\alpha)^2$. This corresponds to

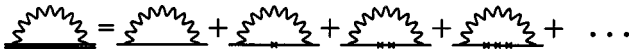

FIG. 4. Expansion of the bound electron self-energy in powers of the binding field.

expanding $\exp(i\mathbf{k}\cdot\mathbf{r})$ up to $(\mathbf{k}\cdot\mathbf{r})^2$. Our restrictions on the magnitude of $\epsilon$ do not compromise the validity of analytic expansion in the parameter $\epsilon$.

### III. HIGH-ENERGY PART

The high-energy part of the radiative correction is given by

$$E_H = -ie^2 m \int_{C_H} \frac{d\omega}{2\pi} \int \frac{d^3\mathbf{k}}{(2\pi)^3} \left[ \frac{1}{k^2} - \frac{1}{k^2 - M^2} \right] \times \langle \overline{\psi} | \gamma^\mu \frac{1}{\not p - \not k - 1 - \gamma^0 V} \gamma_\mu | \psi \rangle - \langle \overline{\psi} | \delta m(M) | \psi \rangle, \tag{12}$$

where we have used the Feynman gauge for the photon propagator $[D_{\mu\nu}(k) = -g_{\mu\nu}/k^2]$ and the Pauli-Villars regularization prescription

$$\frac{1}{k^2 + i\delta} \to \frac{1}{k^2 + i\delta} - \frac{1}{k^2 - M^2 + i\delta}. \tag{13}$$

Note that we may leave out the $i\epsilon$ prescription when integrating along $C_H$, since we take the difference of the integrand infinitesimally above and below the real axis on $C_H$. Along the positive real axis, the integrand has branch cuts due to the photon and electron propagators as depicted in Fig. 1. The expression given in Eq. (12) for $E_H$ is infrared divergent. In the evaluation, we start by calculating the matrix element

$$\widetilde{P} = \langle \overline{\psi} | \gamma^\mu \frac{1}{\not p - \not k - m - \gamma^0 V} \gamma_\mu | \psi \rangle \tag{14}$$

up to the order of $(Z\alpha)^6$. As outlined in Ref. [1], this can be achieved by first expanding the electron propagator in powers of the binding Coulomb field $V$. This leads to three-vertex, double-vertex, single-vertex, and zero-vertex parts. The expansion can be diagrammatically represented as in Fig. 4. The resulting expressions are subsequently expanded in powers of the spatial electron momenta $p^i$. This procedure is feasible for $P$ states because, up to order $(Z\alpha)^6$, all of the resulting matrix elements converge. After performing the algebra of the Dirac matrices, the resulting matrix elements on the $P$ state are evaluated by symbolic procedures written in the computer algebra system MATHEMATICA [14]. For the evaluation, we first expand the wave function (given by the exact solution to the Dirac-Coulomb equation) in powers of $(Z\alpha)$, then we apply operators in coordinate space representation, and finally integrate the resulting expressions with the help of a set of rules that apply to standard integrals. The integrands which are to be evaluated for the matrix elements have lengths of up to 2000 terms.

We use a parametric representation of the mass counter term to allow for local cancellation of the divergences. It can be shown that

$$\delta m(M) = -ie^2 m \int_{C_H} \frac{d\omega}{2\pi} \int \frac{d^3\mathbf{k}}{(2\pi)^3} \times \left[ \frac{1}{\omega^2 - \mathbf{k}^2} - \frac{1}{\omega^2 - \mathbf{k}^2 - M^2} \right] \frac{2(\omega+1)}{\omega^2 - \mathbf{k}^2 - 2\omega} \tag{15}$$

is a suitable parametric representation of the mass counter term along the contour $C_H$. The portion of mass renormalization along the contour $C_L$ vanishes in the limit $\epsilon \to 0$, and we have

$$\delta m(M) = -ie^2 m \int_{C_F} \frac{d\omega}{2\pi} \int \frac{d^3\mathbf{k}}{(2\pi)^3} \times \left[ \frac{1}{k^2 + i\epsilon} - \frac{1}{k^2 - M^2 + i\epsilon} \right] \frac{2(\omega+1)}{\omega^2 - \mathbf{k}^2 - 2\omega} = \alpha \frac{3m}{4\pi} \ln(M^2) + \tfrac{1}{2}]. \tag{16}$$

Therefore, by (locally) subtracting the expression

$$\delta m_l = \frac{2(\omega+1)}{\omega^2 - \mathbf{k}^2 - 2\omega} \langle \overline{\psi} | \psi \rangle$$

before the final $d\omega\, d^3\mathbf{k}[1/(\omega^2 - \mathbf{k}^2) - 1/(\omega^2 - \mathbf{k}^2 - M^2)]$ integration in Eq. (12), we can subtract the divergences associated with mass renormalization.

Note that $\delta m_l$ contains the matrix element $\langle \overline{\psi} | \psi \rangle$, which is state dependent. Using the virial theorem for the Dirac-Coulomb equation ($\langle \boldsymbol{\alpha} \cdot \mathbf{p} \rangle = -\langle V \rangle$), we have $\langle \overline{\psi} | \psi \rangle = E_\psi$, where $E_\psi$ is the dimensionless Dirac energy of the state $\psi$.

We give here the result for the renormalized matrix element

$$\widetilde{P}_{\rm ren} = \widetilde{P} - \delta m_l \tag{17}$$

up to $(Z\alpha)^6$ in terms of $\mathbf{k}$ and $\omega$. We have, for the $3P_{1/2}$ state,

$$\widetilde{P}_{\rm ren}(3P_{1/2})=(Z\alpha)^2[-8\mathbf{k}^2+4\mathbf{k}^4+6\mathbf{k}^2\omega-3\mathbf{k}^4\omega+12\omega^2-10\mathbf{k}^2\omega^2-6\omega^3+6\mathbf{k}^2\omega^3+6\omega^4-3\omega^5]/[27(\mathbf{k}^2+2\omega-\omega^2)^3]$$
$$+(Z\alpha)^4[-128\mathbf{k}^4+48\mathbf{k}^6+24\mathbf{k}^8+96\mathbf{k}^4\omega+2\mathbf{k}^6\omega-9\mathbf{k}^8\omega+256\mathbf{k}^2\omega^2-156\mathbf{k}^4\omega^2-90\mathbf{k}^6\omega^2-168\mathbf{k}^2\omega^3+46\mathbf{k}^4\omega^3$$
$$+36\mathbf{k}^6\omega^3-16\omega^4+240\mathbf{k}^2\omega^4+126\mathbf{k}^4\omega^4+72\omega^5-98\mathbf{k}^2\omega^5-54\mathbf{k}^4\omega^5-132\omega^6-78\mathbf{k}^2\omega^6+50\omega^7+36\mathbf{k}^2\omega^7+18\omega^8$$
$$-9\omega^9]/[324(\mathbf{k}^2+2\omega-\omega^2)^5]+(Z\alpha)^6[-1\,044\,992\mathbf{k}^6+516\,224\mathbf{k}^8+319\,032\mathbf{k}^{10}+32\,340\mathbf{k}^{12}+587\,776\mathbf{k}^4\omega$$
$$+1\,716\,736\mathbf{k}^6\omega+26\,320\mathbf{k}^8\omega-65\,310\mathbf{k}^{10}\omega-8085\mathbf{k}^{12}\omega-358\,400\mathbf{k}^2\omega^2+4\,218\,368\mathbf{k}^4\omega^2-3\,461\,600\mathbf{k}^6\omega^2$$
$$-1\,372\,476\mathbf{k}^8\omega^2-177\,870\mathbf{k}^{10}\omega^2+1\,469\,440\mathbf{k}^2\omega^3-9\,185\,344\mathbf{k}^4\omega^3+1\,027\,600\mathbf{k}^6\omega^3+357\,630\mathbf{k}^8\omega^3$$
$$+48\,510\mathbf{k}^{10}\omega^3+1\,075\,200\omega^4-9\,354\,240\mathbf{k}^2\omega^4+10\,195\,136\mathbf{k}^4\omega^4+2\,348\,976\mathbf{k}^6\omega^4+404\,250\mathbf{k}^8\omega^4$$
$$-3\,978\,240\omega^5+15\,638\,560\mathbf{k}^2\omega^5-3\,365\,600\mathbf{k}^4\omega^5-777\,420\mathbf{k}^6\omega^5-121\,275\mathbf{k}^8\omega^5+7\,869\,120\omega^6$$
$$-12\,272\,960\mathbf{k}^2\omega^6-2\,002\,392\mathbf{k}^4\omega^6-485\,100\mathbf{k}^6\omega^6-8\,571\,360\omega^7+3\,543\,120\mathbf{k}^2\omega^7+839\,580\mathbf{k}^4\omega^7$$
$$+161\,700\mathbf{k}^6\omega^7+5\,023\,200\omega^8+852\,600\mathbf{k}^2\omega^8+323\,400\mathbf{k}^4\omega^8-1\,231\,440\omega^9-450\,870\mathbf{k}^2\omega^9-121\,275\mathbf{k}^4\omega^9$$
$$-145\,740\omega^{10}-113\,190\mathbf{k}^2\omega^{10}+96\,390\omega^{11}+48\,510\mathbf{k}^2\omega^{11}+16\,170\omega^{12}-8085\omega^{13}]/[612\,360(\mathbf{k}^2+2\omega-\omega^2)^7]; \quad (18)$$

for the $3P_{3/2}$ state,

$$\widetilde{P}_{\rm ren}(3P_{3/2})=(Z\alpha)^2[-8\mathbf{k}^2+4\mathbf{k}^4+6\mathbf{k}^2\omega-3\mathbf{k}^4\omega+12\omega^2-10\mathbf{k}^2\omega^2-6\omega^3+6\mathbf{k}^2\omega^3+6\omega^4-3\omega^5]/[27(\mathbf{k}^2+2\omega-\omega^2)^3]$$
$$+(Z\alpha)^4[-128\mathbf{k}^4+32\mathbf{k}^6+8\mathbf{k}^8+32\mathbf{k}^4\omega-26\mathbf{k}^6\omega-3\mathbf{k}^8\omega+192\mathbf{k}^2\omega^2-68\mathbf{k}^4\omega^2-30\mathbf{k}^6\omega^2-56\mathbf{k}^2\omega^3+42\mathbf{k}^4\omega^3$$
$$+12\mathbf{k}^6\omega^3-112\omega^4+42\mathbf{k}^4\omega^4+24\omega^5-6\mathbf{k}^2\omega^5-18\mathbf{k}^4\omega^5+36\omega^6-26\mathbf{k}^2\omega^6-10\omega^7+12\mathbf{k}^2\omega^7+6\omega^8$$
$$-3\omega^9]/[324(\mathbf{k}^2+2\omega-\omega^2)^5]+(Z\alpha)^6[-4\,179\,968\mathbf{k}^6+516\,608\mathbf{k}^8+224\,616\mathbf{k}^{10}+12\,180\mathbf{k}^{12}+2\,351\,104\mathbf{k}^4\omega$$
$$+243\,712\mathbf{k}^6\omega-1\,022\,336\mathbf{k}^8\omega-103\,110\mathbf{k}^{10}\omega-3045\mathbf{k}^{12}\omega-1\,433\,600\mathbf{k}^2\omega^2+8\,960\,000\mathbf{k}^4\omega^2+667\,456\mathbf{k}^6\omega^2$$
$$-539\,868\mathbf{k}^8\omega^2-66\,990\mathbf{k}^{10}\omega^2+4\,157\,440\mathbf{k}^2\omega^3-2\,845\,696\mathbf{k}^4\omega^3+1\,703\,632\mathbf{k}^6\omega^3+370\,230\mathbf{k}^8\omega^3$$
$$+18\,270\mathbf{k}^{10}\omega^3+4\,300\,800\omega^4-17\,297\,280\mathbf{k}^2\omega^4-3\,980\,704\mathbf{k}^4\omega^4+135\,408\mathbf{k}^6\omega^4+152\,250\mathbf{k}^8\omega^4$$
$$-10\,752\,000\omega^5+10\,612\,000\mathbf{k}^2\omega^5-619\,136\mathbf{k}^4\omega^5-449\,820\mathbf{k}^6\omega^5-45\,675\mathbf{k}^8\omega^5+15\,408\,960\omega^6-99\,680\mathbf{k}^2\omega^6$$
$$+586\,824\mathbf{k}^4\omega^6-182\,700\mathbf{k}^6\omega^6-10\,647\,840\omega^7+216\,720\mathbf{k}^2\omega^7+159\,180\mathbf{k}^4\omega^7+60\,900\mathbf{k}^6\omega^7+2\,896\,320\omega^8$$
$$-543\,480\mathbf{k}^2\omega^8+121\,800\mathbf{k}^4\omega^8-278\,880\omega^9+65\,730\mathbf{k}^2\omega^9-45\,675\mathbf{k}^4\omega^9+136\,500\omega^{10}-42\,630\mathbf{k}^2\omega^{10}$$
$$-42\,210\omega^{11}+18\,270\mathbf{k}^2\omega^{11}+6090\omega^{12}-3045\omega^{13}]/[2\,449\,440(\mathbf{k}^2+2\omega-\omega^2)^7]; \quad (19)$$

for the $4P_{1/2}$ state,

$$\widetilde{P}_{\rm ren}(4P_{1/2})=(Z\alpha)^2[-8\mathbf{k}^2+4\mathbf{k}^4+6\mathbf{k}^2\omega-3\mathbf{k}^4\omega+12\omega^2-10\mathbf{k}^2\omega^2-6\omega^3+6\mathbf{k}^2\omega^3+6\omega^4-3\omega^5]/[48(\mathbf{k}^2+2\omega-\omega^2)^3]$$
$$+(Z\alpha)^4[-2944\mathbf{k}^4+1072\mathbf{k}^6+520\mathbf{k}^8+2080\mathbf{k}^4\omega-10\mathbf{k}^6\omega-195\mathbf{k}^8\omega+5760\mathbf{k}^2\omega^2-3412\mathbf{k}^4\omega^2-1950\mathbf{k}^6\omega^2$$
$$-3640\mathbf{k}^2\omega^3+1050\mathbf{k}^4\omega^3+780\mathbf{k}^6\omega^3-560\omega^4+5040\mathbf{k}^2\omega^4+2730\mathbf{k}^4\omega^4+1560\omega^5-2070\mathbf{k}^2\omega^5-1170\mathbf{k}^4\omega^5$$
$$-2700\omega^6-1690\mathbf{k}^2\omega^6+1030\omega^7+780\mathbf{k}^2\omega^7+390\omega^8-195\omega^9]/[15\,360(\mathbf{k}^2+2\omega-\omega^2)^5]+(Z\alpha)^6$$
$$\times[-41\,518\,080\mathbf{k}^6+20\,285\,056\mathbf{k}^8+12\,019\,560\mathbf{k}^{10}+1\,140\,300\mathbf{k}^{12}+21\,790\,720\mathbf{k}^4\omega+67\,517\,184\mathbf{k}^6\omega$$
$$-1\,295\,056\mathbf{k}^8\omega-2\,875\,250\mathbf{k}^{10}\omega-285\,075\mathbf{k}^{12}\omega-13\,189\,120\mathbf{k}^2\omega^2+164\,921\,344\mathbf{k}^4\omega^2-138\,538\,016\mathbf{k}^6\omega^2$$
$$-50\,829\,380\mathbf{k}^8\omega^2-6\,271\,650\mathbf{k}^{10}\omega^2+53\,975\,040\mathbf{k}^2\omega^3-357\,889\,728\mathbf{k}^4\omega^3+50\,610\,672\mathbf{k}^6\omega^3+14\,327\,250\mathbf{k}^8\omega^3$$
$$+1\,710\,450\mathbf{k}^{10}\omega^3+39\,567\,360\omega^4-357\,683\,200\mathbf{k}^2\omega^4+404\,953\,920\mathbf{k}^4\omega^4+81\,291\,280\mathbf{k}^6\omega^4+14\,253\,750\mathbf{k}^8\omega^4$$
$$-147\,302\,400\omega^5+601\,024\,480\mathbf{k}^2\omega^5-153\,435\,296\mathbf{k}^4\omega^5-28\,556\,500\mathbf{k}^6\omega^5-4\,276\,125\mathbf{k}^8\omega^5+294\,387\,520\omega^6$$
$$-485\,016\,000\mathbf{k}^2\omega^6-59\,093\,160\mathbf{k}^4\omega^6-17\,104\,500\mathbf{k}^6\omega^6-325\,403\,680\omega^7+160\,218\,800\mathbf{k}^2\omega^7$$
$$+28\,458\,500\mathbf{k}^4\omega^7+5\,701\,500\mathbf{k}^6\omega^7+198\,315\,040\omega^8+17\,532\,200\mathbf{k}^2\omega^8+11\,403\,000\mathbf{k}^4\omega^8-56\,099\,120\omega^9$$

$$-14\,180\,250\mathbf{k}^2\omega^9-4\,276\,125\mathbf{k}^4\omega^9-920\,500\omega^{10}-3\,991\,050\mathbf{k}^2\omega^{10}+2\,826\,250\omega^{11}+1\,710\,450\mathbf{k}^2\omega^{11}$$
$$+570\,150\omega^{12}-285\,075\omega^{13}]/[51\,609\,600(\mathbf{k}^2+2\omega-\omega^2)^7]; \tag{20}$$

and, for the $4P_{3/2}$ state,

$$\widetilde{P}_{\rm ren}(4P_{3/2})=(Z\alpha)^2[-8\mathbf{k}^2+4\mathbf{k}^4+6\mathbf{k}^2\omega-3\mathbf{k}^4\omega+12\omega^2-10\mathbf{k}^2\omega^2-6\omega^3+6\mathbf{k}^2\omega^3+6\omega^4-3\omega^5]/[48(\mathbf{k}^2+2\omega-\omega^2)^3]$$
$$+(Z\alpha)^4[-2944\mathbf{k}^4+752\mathbf{k}^6+200\mathbf{k}^8+800\mathbf{k}^4\omega-570\mathbf{k}^6\omega-75\mathbf{k}^8\omega+4480\mathbf{k}^2\omega^2-1652\mathbf{k}^4\omega^2-750\mathbf{k}^6\omega^2$$
$$-1400\mathbf{k}^2\omega^3+970\mathbf{k}^4\omega^3+300\mathbf{k}^6\omega^3-2480\omega^4+240\mathbf{k}^2\omega^4+1050\mathbf{k}^4\omega^4+600\omega^5-230\mathbf{k}^2\omega^5-450\mathbf{k}^4\omega^5+660\omega^6$$
$$-650\mathbf{k}^2\omega^6-170\omega^7+300\mathbf{k}^2\omega^7+150\omega^8-75\omega^9]/[15\,360(\mathbf{k}^2+2\omega-\omega^2)^5]+(Z\alpha)^6[-41\,518\,080\mathbf{k}^6$$
$$+5\,273\,472\mathbf{k}^8+2\,372\,328\mathbf{k}^{10}+132\,300\mathbf{k}^{12}+21\,790\,720\mathbf{k}^4\omega+3\,438\,848\mathbf{k}^6\omega-10\,087\,504\mathbf{k}^8\omega-1\,069\,810\mathbf{k}^{10}\omega$$
$$-33\,075\mathbf{k}^{12}\omega-13\,189\,120\mathbf{k}^2\omega^2+88\,747\,008\mathbf{k}^4\omega^2+4\,454\,624\mathbf{k}^6\omega^2-5\,916\,484\mathbf{k}^8\omega^2-727\,650\mathbf{k}^{10}\omega^2$$
$$+37\,847\,040\mathbf{k}^2\omega^3-29\,007\,552\mathbf{k}^4\omega^3+18\,082\,288\mathbf{k}^6\omega^3+3\,870\,930\mathbf{k}^8\omega^3+198\,450\mathbf{k}^{10}\omega^3+39\,567\,360\omega^4$$
$$-163\,681\,280\mathbf{k}^2\omega^4-34\,772\,416\mathbf{k}^4\omega^4+2\,115\,344\mathbf{k}^6\omega^4+1\,653\,750\mathbf{k}^8\omega^4-98\,918\,400\omega^5+100\,285\,920\mathbf{k}^2\omega^5$$
$$-8\,639\,904\mathbf{k}^4\omega^5-4\,785\,620\mathbf{k}^6\omega^5-496\,125\mathbf{k}^8\omega^5+143\,286\,080\omega^6-1\,740\,480\mathbf{k}^2\omega^6+5\,429\,592\mathbf{k}^4\omega^6$$
$$-1\,984\,500\mathbf{k}^6\omega^6-99\,145\,760\omega^7+3\,382\,960\mathbf{k}^2\omega^7+1\,829\,380\mathbf{k}^4\omega^7+661\,500\mathbf{k}^6\omega^7+26\,784\,800\omega^8$$
$$-5\,400\,920\mathbf{k}^2\omega^8+1\,323\,000\mathbf{k}^4\omega^8-2\,737\,840\omega^9+563\,430\mathbf{k}^2\omega^9-496\,125\mathbf{k}^4\omega^9+1\,400\,140\omega^{10}$$
$$-463\,050\mathbf{k}^2\omega^{10}-408\,310\omega^{11}+198\,450\mathbf{k}^2\omega^{11}+66\,150\omega^{12}-33\,075\omega^{13}]/[51\,609\,600(\mathbf{k}^2+2\omega-\omega^2)^7]. \tag{21}$$

Having calculated $\widetilde{P}$, we finally integrate along $C_H$ to obtain the result for $E_H$,

$$E_H=-ie^2m\int_{C_H}\frac{d\omega}{2\pi}\int\frac{d^3\mathbf{k}}{(2\pi)^3}\left[\frac{1}{\omega^2-\mathbf{k}^2}-\frac{1}{\omega^2-\mathbf{k}^2-M^2}\right]\widetilde{P}_{\rm ren}. \tag{22}$$

Note that as $\widetilde{P}_{\rm ren}=\widetilde{P}-\delta m_l$, both $\widetilde{P}$ as well as the local mass renormalization term $\delta m_l$ are properly integrated with the regularized photon propagator.

The final integrations with respect to the photon momenta are done in a different way for the terms in $\widetilde{P}_{\rm ren}$, which require regularization and those which do not. The terms which require regularization are integrated covariantly by Feynman parameter techniques and a subsequent Wick rotation. These terms are not integrated along $C_H$, but rather along $C_H'$. They are not infrared divergent, so we may put $\epsilon=0$ for these terms. Those terms which do not require regularization are integrated in an essentially noncovariant way. The $d^3\mathbf{k}$ integration is carried out first, then we proceed to the $d\omega$ integration.

The integration procedure for the terms which require regularization is as follows. We isolate those terms in $(\widetilde{P}-\delta m_l)$ which would be ultraviolet divergent if integrated with the unregularized photon propagator. We denote these terms by $\widetilde{P}^{\rm div}_{\rm ren}$. We then evaluate

$$\delta E_{\rm div}=\int_{C_H}\frac{d\omega}{2\pi}\int\frac{d^3\mathbf{k}}{(2\pi)^3}\,\frac{1}{\omega^2-\mathbf{k}^2}[\widetilde{P}^{\rm div}_{\rm ren}].$$

All terms in $\widetilde{P}^{\rm div}_{\rm ren}$ require regularization.

By simple power-counting arguments, it can be shown that $\widetilde{P}^{\rm div}_{\rm ren}$ is exactly the sum of those terms of order $k^n$ where $n\geqslant -2$ for large $k$. Therefore, the terms contributing to $\widetilde{P}^{\rm div}_{\rm ren}$ can easily be isolated. The terms in $\widetilde{P}_{\rm div}$, can obviously be written as the sum of terms of the form

$$\widetilde{P}_{\rm div}=\sum_i\frac{p_i(|\mathbf{k}|,\omega)}{[\mathbf{k}^2+2\omega-\omega^2]^{n_i}}, \tag{23}$$

where $p_i$ is a polynomial in $|\mathbf{k}|$ and $\omega$ and $\deg(p_i)\geqslant n_i-2$. The entirely covariant integration procedure for the divergent terms will be outlined here. The terms in Eq. (23) need to be multiplied by the factors $1/(\omega^2-\mathbf{k}^2)$ and $1/(\omega^2-\mathbf{k}^2-M^2)$ from the regularized photon propagator. We use Feynman parameters in the form

$$\frac{1}{AB^n}=\int_0^1 dx\,\frac{nx^{n-1}}{[A(1-x)+Bx]^{n+1}} \tag{24}$$

to join the denominators. Identifying $A_1=-\omega^2+\mathbf{k}^2$, $A_2=-\omega^2+\mathbf{k}^2+M^2$, and $B=\mathbf{k}^2+2\omega-\omega^2$, we have for the contribution from the unrenormalized photon propagator $1/(\omega^2-\mathbf{k}^2)$,

$$A_1(1-x)+Bx=-\widetilde{k}^2+D_1, \tag{25}$$

where

$$\widetilde{k}=(\widetilde{\omega},\mathbf{k})=(\omega-x,\mathbf{k}),\quad D_1=x^2 \tag{26}$$

and for the contribution from the renormalization part of the photon propagator

$$A(1-x)+Bx=-\tilde{k}^2+D_2, \tag{27}$$

where

$$D_2=x^2+M(1-x). \tag{28}$$

The energy shift due to the divergent terms is then proportional to

$$\sum_i \int_0^1 dx \int d\tilde{\omega}\, d^3k \frac{n_i x^{n_i-1} p_i(|\mathbf{k}|,\tilde{\omega})}{-\tilde{k}^2+D},$$

where $D$ represents either of the terms $D_1$ or $D_2$ and it is understood that the contribution from these two terms must be subtracted to obtain the final result. Performing the Wick rotation

$$\tilde{\omega}\rightarrow i\omega,$$

we have

$$-\tilde{k}^2=\omega^2+\mathbf{k}^2=k_e^2+D,$$

where $k_e$ is the Euclidean 4-vector $k_e=(\omega,\mathbf{k})$. We then obtain the energy shift due to the divergent terms proportional to

$$\sum_i \int_0^1 dx \int d^4k_e \frac{n_i x^{n_i-1} p_i(|\mathbf{k}|,\omega)}{k_e^2+D}.$$

The (straightforward) angular part of these integrals can be done by parametrizing the Euclidean 4-space as $\omega=k_e\cos\gamma$, $k^1=k_e\sin\gamma\sin\theta\cos\phi$, $k^2=k_e\sin\gamma\sin\theta\sin\phi$, and $k_3=k_e\sin\gamma\cos\theta$. We then have $\omega=k_e\cos\gamma$, $|\mathbf{k}|=k_e\sin\gamma$. For the average over the four-dimensional angle, we utilize the formulas

$$\int \frac{d\Omega_e^{(4)}}{2\pi^2}\cos^2\gamma=\frac{1}{4}, \quad \int \frac{d\Omega_e^{(4)}}{2\pi^2}\cos^4\gamma=\frac{1}{8},$$

$$\int \frac{d\Omega_e^{(4)}}{2\pi^2}\cos^6\gamma=\frac{5}{64}.$$

The remaining radial part of the integrals can be evaluated with the help of the formulas

$$\int_0^\infty dk_e\, k_e^3 \frac{1}{(k_e^2+D)^\beta}=\frac{1}{2D^{\beta-2}(\beta-1)(\beta-2)}; \quad (\beta>2)$$

and

$$\int_0^\Lambda dk_e\, k_e^3 \frac{1}{(k_e^2+D)^2}=\frac{1}{2}\ln\left(\frac{\Lambda}{D}\right)+O\left(\frac{1}{\Lambda}\right)^2.$$

It is easy to prove that the dependence on the temporary upper cutoff $\Lambda$ disappears when the contribution due to the unregularized and the regularization part of the photon propagator are subtracted ($D_1$ and $D_2$).

As the final step, we integrate over the parameter $x$ introduced in Eq. (24), and subsequently investigate the resulting expression in the limit $M\rightarrow\infty$. The respective expressions vanish as $M\rightarrow\infty$ for all states considered in this paper. This fact is intimately linked to our using the entirely covariant Feynman parameter approach for the integration of the divergent terms. If we had used a noncovariant scheme of integration, as in Ref. [7], then we would have had to take into account finite correction terms to obtain the correct result for the Lamb shift. Note that the (divergent) spurious terms of order $(Z\alpha)^2$, which are present in all of the matrix elements $\tilde{P}_{\rm ren}$, vanish after we have performed the $d^4k$ integration in the way outlined above, which includes final expansion in the $\epsilon$ parameter.

The terms in $\tilde{P}_{\rm ren}^{\rm fin}$ which are finite when integrated with the unrenormalized photon propagator do not need regularization. It is easy to see that $\tilde{P}_{\rm ren}^{\rm fin}$ can be written as the sum of terms of the form

$$\tilde{P}_{\rm ren}^{\rm fin}=\sum_j \frac{q_j(|\mathbf{k}|,\omega)}{[\mathbf{k}^2+2\omega-\omega^2]^{n_j}}, \tag{29}$$

where $q_j$ is a polynomial in $|\mathbf{k}|$ and $\omega$ whose degree is less than $2n_j-2$ to insure ultraviolet convergence. For the $4P_{1/2}$ state, e.g., $\tilde{P}_{\rm ren}^{\rm fin}$ is given by

$$\begin{aligned}
P_{\rm ren}^{\rm fin}=&(Z\alpha)^2[-4\mathbf{k}^2+3\mathbf{k}^2\omega+6\omega^2-3\omega^3]/[24(\mathbf{k}^2+2\omega-\omega^2)^3]+(Z\alpha)^4[-1472\mathbf{k}^4+536\mathbf{k}^6+1040\mathbf{k}^4\omega-5\mathbf{k}^6\omega+2880\mathbf{k}^2\omega^2\\
&-1706\mathbf{k}^4\omega^2-1820\mathbf{k}^2\omega^3+525\mathbf{k}^4\omega^3-280\omega^4+2520\mathbf{k}^2\omega^4+780\omega^5-1035\mathbf{k}^2\omega^5-1350\omega^6+515\omega^7]/[7680(\mathbf{k}^2+2\omega\\
&-\omega^2)^5]+(Z\alpha)^6[-20\,759\,040\mathbf{k}^6+10\,142\,528\mathbf{k}^8+6\,009\,780\mathbf{k}^{10}+10\,895\,360\mathbf{k}^4\omega+33\,758\,592\mathbf{k}^6\omega-647\,528\mathbf{k}^8\omega\\
&-1\,437\,625\mathbf{k}^{10}\omega-6\,594\,560\mathbf{k}^2\omega^2+82\,460\,672\mathbf{k}^4\omega^2-69\,269\,008\mathbf{k}^6\omega^2-25\,414\,690\mathbf{k}^8\omega^2+26\,987\,520\mathbf{k}^2\omega^3\\
&-178\,944\,864\mathbf{k}^4\omega^3+25\,305\,336\mathbf{k}^6\omega^3+7\,163\,625\mathbf{k}^8\omega^3+19\,783\,680\omega^4-178\,841\,600\mathbf{k}^2\omega^4+202\,476\,960\mathbf{k}^4\omega^4\\
&+40\,645\,640\mathbf{k}^6\omega^4-73\,651\,200\omega^5+300\,512\,240\mathbf{k}^2\omega^5-76\,717\,648\mathbf{k}^4\omega^5-14\,278\,250\mathbf{k}^6\omega^5+147\,193\,760\omega^6\\
&-242\,508\,000\mathbf{k}^2\omega^6-29\,546\,580\mathbf{k}^4\omega^6-162\,701\,840\omega^7+80\,109\,400\mathbf{k}^2\omega^7+14\,229\,250\mathbf{k}^4\omega^7+99\,157\,520\omega^8\\
&+8\,766\,100\mathbf{k}^2\omega^8-28\,049\,560\omega^9-7\,090\,125\mathbf{k}^2\omega^9-460\,250\omega^{10}+1\,413\,125\omega^{11}]/[25\,804\,800(\mathbf{k}^2+2\omega-\omega^2)^7].
\end{aligned} \tag{30}$$

We have to calculate

$$\delta E_H = -ie^2 m \int_{C_H} \frac{d\omega}{2\pi} \int \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{1}{\omega^2 - \mathbf{k}^2} [\widetilde{P}^{\rm fin}_{\rm ren}].$$

The quantity $F_H$ defined by

$$E_H = \frac{\alpha}{\pi} m \frac{(Z\alpha)^4}{n^3} F_H \tag{31}$$

in Eq. (2) may be expressed as

$$F_H = [n^3/(Z\alpha)^4] \int_{C_H} d\omega \mathcal{F}(\omega), \tag{32}$$

where

$$\mathcal{F}(\omega) = \frac{1}{2\pi i} \int d|\mathbf{k}| \frac{\mathbf{k}^2}{\omega^2 - \mathbf{k}^2} \widetilde{P}^{\rm fin}_{\rm ren}(\omega, |\mathbf{k}|).$$

One can dispose of the factors $\mathbf{k}^2$ in the numerator of the integrand using the following procedure. First write $\mathbf{k}^2$ as

$$\mathbf{k}^2 = Y - 2\omega + \omega^2,$$

so $Y = \mathbf{k}^2 + 2\omega - \omega^2$ corresponds to the denominator in Eq. (29). The resulting expression is subsequently expanded. The powers of $Y$ cancel, and the result does not carry powers of $\mathbf{k}$ in the numerator.

The integrand in $\mathcal{F}(\omega)$ can be written as the sum of terms of the form

$$\mathcal{F}(\omega) = \frac{1}{2\pi i} \int d|\mathbf{k}| \left( \sum_j a_j \frac{\omega^{n_j}}{\omega^2 - \mathbf{k}^2} \frac{1}{(\mathbf{k}^2 + 2\omega - \omega^2)^{m_j}} \right), \tag{33}$$

with suitable coefficients $a_j$. The $d|\mathbf{k}|$ integration can then be carried out using the formula

$$\begin{aligned} &\frac{1}{2\pi i} \int_{-\infty}^{\infty} d|\mathbf{k}| \frac{1}{\omega^2 - \mathbf{k}^2} \frac{1}{\mathbf{k}^2 + \Omega} \\ &\quad = \frac{-1}{2\ \mathrm{sgn}(\mathrm{Im}(\omega))(\omega^2 + \Omega)\omega} + \frac{(-1)^{n-1}}{(n-1)!} \frac{\partial^{n-1}}{\partial \Omega^{n-1}} \\ &\qquad \times \left[ \frac{i}{2\sqrt{\Omega}} \frac{1}{\omega^2 + \Omega} \right], \end{aligned} \tag{34}$$

where sgn is the sign function defined as

$$\mathrm{sgn}(x) = \begin{cases} 1 & x \geqslant 0 \\ -1 & x < 0. \end{cases} \tag{35}$$

We identify

$$\Omega = 2\omega - \omega^2 \tag{36}$$

in order to carry out the integration in Eq. (33). The formula Eq. (34) deserves some comments. We are integrating along the real axis. Because $\omega$ and $\Omega$ both have an infinitesimal imaginary part all along the contour of integration $C_H$, the positions of the poles of the integrand are well defined.

The branch cuts of the function $\mathcal{F}(\omega)$ can be readily identified. Due to the term $\mathrm{sgn}(\mathrm{Im}(\omega))\omega$ in the first term on the right-hand side in Eq. (34), there is a branch cut along the positive real axis. This branch cut is caused by the photon propagator. Due to the term $\sqrt{\Omega}$ in the second term on the right-hand side in Eq. (34), there is also a branch cut along the line where the expression $\Omega = 2\omega - \omega^2$ assumes negative real values. This branch cut extends from $\omega = 2$ along the positive real axis to $\omega = \infty$. It is caused by the Dirac-Coulomb propagator (see Fig. 1).

It can be explicitly checked that the function $\mathcal{F}(\omega)$ satisfies the equation

$$\mathcal{F}(\omega^*) = -\mathcal{F}(\omega)^*. \tag{37}$$

We can divide the contour $C_H$ in an upper contour $C_H^u$ which extends from $\epsilon + i0^+$ to $\infty + i0^+$, and a lower contour $C_H^l$ which extends from $\infty - i0^+$ to $\epsilon - i0^+$. We then have, due to Eq. (37),

$$\begin{aligned} \int_{C_H} d\omega\ \mathcal{F}(\omega) &= \int_{C_H^l} d\omega\ \mathcal{F}(\omega) + \int_{C_H^u} d\omega\ \mathcal{F}(\omega) \\ &= \int_{\epsilon}^{\infty} d\omega\ \mathcal{F}(\omega + i0^+) + \int_{\infty}^{\epsilon} d\omega\ \mathcal{F}(\omega - i0^+) \\ &= \int_{\epsilon}^{\infty} d\omega\ \mathcal{F}(\omega + i0^+) + \int_{\epsilon}^{\infty} d\omega\ \mathcal{F}(\omega + i0^+)^* \\ &= \int_{C_H^u} d\omega\ \mathcal{F}(\omega) + \mathrm{c.c.} \end{aligned} \tag{38}$$

We restrict ourselves therefore to the upper contour $C_H^u$, and understand that the complete result is the sum of the integral along the upper contour plus its complex conjugate.

We then perform a change of variable to proceed to the final $d\omega$ integration. Defining

$$u = \frac{\sqrt{\Omega} + i\omega}{\sqrt{\Omega} - i\omega} \tag{39}$$

and

$$\mathcal{U}(u) = \frac{d\omega}{du} \mathcal{F}(\omega), \tag{40}$$

we have

$$F_H = n^3/(Z\alpha)^4 \int_{u(C_H)} du\ \mathcal{U}(u). \tag{41}$$

Note that

$$u = \frac{\sqrt{\mathrm{Re}(2\omega - \omega^2)} + i\omega}{\sqrt{\mathrm{Re}(2\omega - \omega^2)} - i\omega} \quad \text{for} \quad \omega \in C_H^U, \mathrm{Re}(\omega) \in [\epsilon, 2), \tag{42}$$

whereas

$$u=\frac{\sqrt{\mathrm{Re}(\omega^2-2\omega)}-\omega}{\sqrt{\mathrm{Re}(\omega^2-2\omega)}+\omega} \quad \text{for} \quad \omega\in C_H^U, \mathrm{Re}(\omega)\in[2,\infty), \tag{43}$$

where the argument of the square root is written in such a way as to represent a positive real quantity in the two above equations. So $u(\omega=0)=1$, $u(\omega=2)=-1$, $u(\infty+i0^+)=0$, and $u\in[-1,0)$ for $\omega\in C_H^U, \mathrm{Re}(\omega)\in[2,\infty)$. So for $\omega\in C_H^U$, $\mathrm{Re}(\omega)\in[\epsilon,2)$, $u$ has a nonvanishing imaginary part, whereas for $\omega\in C_H^U$, $\mathrm{Re}(\omega)\in[2,\infty)$, $u$ is a real quantity. The mapping $\omega\to u$ is one on one for $\omega\in C_H^U$.

Note that if we had chosen the lower contour $C_H^L$, then $u(\infty-i0^+)=-\infty$. In that case, the above substitution would not have had the desired property $u\to 0$ for $\omega\to\infty$.

On $C_H^U$, $\omega$ and $\sqrt{\Omega}$ can be expressed as functions of $u$ according to

$$\omega=-\frac{1}{2}\frac{1-u^2}{u},$$

$$\sqrt{\Omega}=-\frac{i}{2}\frac{(1-u)(1+u)}{(-u)},$$

i.e., $\sqrt{\Omega}$ extends along the negative imaginary axis for $\mathrm{Re}(\omega)>2$, $u\in[-1,0]$. The result for $\mathcal{U}(u)$ ($4P_{1/2}$ state) is

$$\begin{aligned}\mathcal{U}(u)=&(Z\alpha)^2\left[-\frac{1}{192}-\frac{1}{96(-1+u)^2}\right]+(Z\alpha)^4\left[-\frac{47}{20\,480}+\frac{23}{10\,240(-1+u)^4}+\frac{23}{10\,240(-1+u)^3}+\frac{79}{40\,960(-1+u)^2}\right.\\&\left.+\frac{13}{2048(1+u)^4}-\frac{13}{2048(1+u)^3}+\frac{113}{24\,576(1+u)^2}\right]+(Z\alpha)^6\left[-\frac{141\,737}{41\,287\,680}-\frac{39\,173}{20\,643\,840(-1+u)^6}\right.\\&-\frac{39\,173}{10\,321\,920(-1+u)^5}-\frac{2\,228\,617}{206\,438\,400(-1+u)^4}-\frac{3\,485\,527}{206\,438\,400(-1+u)^3}-\frac{4\,685\,519}{330\,301\,440(-1+u)^2}\\&-\frac{499}{46\,080(-1+u)}-\frac{343u}{614\,400}+\frac{1267}{65\,536(1+u)^8}-\frac{3801}{65\,536(1+u)^7}+\frac{11\,765}{131\,072(1+u)^6}-\frac{2715}{32\,768(1+u)^5}\\&\left.+\frac{69\,651}{1\,310\,720(1+u)^4}-\frac{28\,021}{1\,310\,720(1+u)^3}+\frac{89\,779}{15\,728\,640(1+u)^2}\right].\end{aligned} \tag{44}$$

The next step in the calculation is the $u$ integration,

$$F_H=[n^3/(Z\alpha)^4]\int_{u(\epsilon+i0^+)}^0 du\ \mathcal{U}(u)+\text{c.c.}, \tag{45}$$

where

$$u(\epsilon+i0^+)=1+i\sqrt{2}\epsilon-\epsilon-\frac{i\epsilon^{3/2}}{2\sqrt{2}}+O(\epsilon)^{5/2}. \tag{46}$$

It is useful to define

$$\tilde{\epsilon}=1-u(\epsilon+i0^+)=-i\sqrt{2\epsilon}+\epsilon+\frac{i\epsilon^{3/2}}{2\sqrt{2}}+O(\epsilon)^{5/2}. \tag{47}$$

Note that the $\epsilon$ prescription calls for carrying out the $u$ integration from $u(\epsilon+i0^+)$ to 0, and subsequently expanding the result in powers of $\epsilon$ up to $\epsilon^0$. For those terms which are finite when integrated from 1 to 0 we may carry out this integration without regarding the dependence on $\epsilon$. For instance,

$$\int_{u(\epsilon+i0^+)}^0 du\frac{1}{(1+u)^n}=\frac{1-2^{1-n}}{n-1}+O(\sqrt{\epsilon}), \tag{48}$$

so, in the limit $\epsilon\to 0$, the $\epsilon$-dependent term vanishes. Terms of the form $1/(1-u)^n$, however, introduce a divergence in $1/\tilde{\epsilon}$. We have

$$\int_{u(\epsilon+i0^+)}^0 du\frac{1}{(1-u)^n}=\frac{\tilde{\epsilon}^{1-n}-1}{n-1}. \tag{49}$$

We then add to the result of this integration the complex conjugate, and subsequently expand in powers of $\epsilon$. This procedure is illustrated with some examples. For the terms proportional to $1/(1-u)^2$, we have

$$\int_{u(\epsilon+i0^+)}^0 du\frac{1}{(1-u)^2}=1-\frac{1}{\tilde{\epsilon}}, \tag{50}$$

so

$$\int_{u(\epsilon+i0^+)}^0 du\frac{1}{(1-u)^2}+\text{c.c.}$$

$$=2-\frac{1}{\tilde{\epsilon}}-\frac{1}{\tilde{\epsilon}^*}$$

$$= 2 - \frac{1}{-i\sqrt{2\epsilon} + \epsilon + O(\epsilon)^{3/2}} - \frac{1}{i\sqrt{2\epsilon} + \epsilon O(\epsilon)^{3/2}}$$

$$= 2 - \left( \frac{i}{\sqrt{2\epsilon}} + \frac{1}{2} + O(\epsilon)^{1/2} \right) - \left( -\frac{i}{\sqrt{2\epsilon}} + \frac{1}{2} + O(\epsilon)^{1/2} \right)$$

$$= 2 - 1 + O(\epsilon)^{1/2} = 1 + O(\epsilon)^{1/2}. \tag{51}$$

For terms proportional to $1/(1-u)$, we have

$$\int_{u(\epsilon + i0^+)}^{0} du \frac{1}{(1-u)} = \ln(\tilde{\epsilon}), \tag{52}$$

so

$$\int_{u(\epsilon + i0^+)}^{0} du \frac{1}{1-u} + \text{c.c.}$$

$$= \ln(\tilde{\epsilon}) + \ln(\tilde{\epsilon}^*)$$

$$= \ln[-i\sqrt{2\epsilon} + O(\epsilon)] + \ln[i\sqrt{2\epsilon} + O(\epsilon)]$$

$$= -i\frac{\pi}{2} + i\frac{\pi}{2} + 2\ln(\sqrt{2\epsilon}) + O(\epsilon)^{1/2}$$

$$= \ln 2 + \ln\epsilon + O(\epsilon)^{1/2}. \tag{53}$$

Note that for constant terms, this results in

$$\int_{u(\epsilon + i0^+)}^{0} du \times \text{const} + \text{c.c.} = -2 \times \text{const} + O(\epsilon)^{1/2}. \tag{54}$$

Using the results Eqs. (51) and (54), it is easy to show that the spurious terms of order $(Z\alpha)^2$ in expression (44) vanish after the final $u$ integration.

The final result for the high-energy part ($4P_{1/2}$ state) is

$$F_H(4P_{1/2}) = -\frac{1}{6} + (Z\alpha)^2 \left[ \frac{24\,409}{86\,400} - \frac{499}{720}(\ln 2 + \ln\epsilon) - \frac{23}{90\epsilon} \right]. \tag{55}$$

Here we give the complete results for the high-energy parts of the other states treated in this paper:

$$F_H(3P_{1/2}) = -\frac{1}{6} + (Z\alpha)^2 \left[ \frac{6191}{24\,300} - \frac{268}{405}(\ln 2 + \ln\epsilon) - \frac{20}{81\epsilon} \right], \tag{56}$$

$$F_H(3P_{3/2}) = \frac{1}{12} + (Z\alpha)^2 \left[ \frac{67\,903}{194\,400} - \frac{148}{405}(\ln 2 + \ln\epsilon) - \frac{20}{81\epsilon} \right], \tag{57}$$

$$F_H(4P_{3/2}) = \frac{1}{12} + (Z\alpha)^2 \left[ \frac{31\,399}{86\,400} - \frac{137}{360}(\ln 2 + \ln\epsilon) - \frac{23}{90\epsilon} \right]. \tag{58}$$

## IV. LOW-ENERGY PART

The low-energy part of the energy shift originates from low-energy virtual photons. The energy of the photons is comparable in magnitude to the binding energy of the electron [order $(Z\alpha)^2$]. Therefore it is impossible to expand the electron propagator in powers of the binding field. We have to treat the binding field nonperturbatively. An expansion in powers of $(Z\alpha)$ is accomplished by considering the spatial momenta of the virtual photon and the electron momenta as expansion parameters.

Choosing the Coulomb gauge for the photon propagator, one finds that only the spatial elements of this propagator contribute [1]. The $\omega$ integration along $C_L$ is performed first, which leads to the following expression for $E_L$:

$$E_L = -e^2 P \int_{|\mathbf{k}|<\epsilon} \frac{d^3k}{(2\pi)^3 2|\mathbf{k}|} \delta^{T,ij} \times \langle \psi | \alpha^i e^{i\mathbf{k}\cdot\mathbf{r}} \frac{1}{H_D - (E_\psi - \omega)} \alpha^j e^{-i\mathbf{k}\cdot\mathbf{r}} | \psi \rangle \qquad (\omega \equiv |\mathbf{k}|). \tag{59}$$

$H_D$ denotes the Dirac-Coulomb Hamiltonian $H_D = \boldsymbol{\alpha}\cdot\mathbf{p} + \beta m + V$, $\delta^T$ is the transverse delta function, and $\alpha^i$ refers to the Dirac $\alpha$ matrices. The principal value of the above integral is the real quantity corresponding to the energy shift in one-loop order. The imaginary part of the $C_L$ integration, which leads to the decay width of the state, has been dropped in Eq. (59). In the matrix element

$$P^{ij} = \langle \psi | \alpha^i e^{i\mathbf{k}\cdot\mathbf{r}} \frac{1}{H_D - (E_\psi - \omega)} \alpha^j e^{-i\mathbf{k}\cdot\mathbf{r}} | \psi \rangle, \tag{60}$$

we introduce a unitary Foldy-Wouthuysen transformation $U$,

$$P^{ij} = \langle U\psi | (U\alpha^i e^{i\mathbf{k}\cdot\mathbf{r}} U^+) \frac{1}{U[H_D - (E_\psi - \omega)]U^+} \times (U\alpha^j e^{-i\mathbf{k}\cdot\mathbf{r}} U^+) | U\psi \rangle. \tag{61}$$

The lower components of the Foldy-Wouthuysen transformed Dirac wave function $\psi$ vanish up to $(Z\alpha)^2$, so that we may approximate $|U\psi\rangle$ by

$$|U\psi\rangle = |\phi\rangle + |\delta\phi\rangle \quad \text{with} \quad \langle \phi | \delta\phi \rangle = 0, \tag{62}$$

where $|\phi\rangle$ is the nonrelativistic (Schrödinger-Pauli) wave function, and $|\delta\phi\rangle$ is the relativistic correction.

We define an operator acting on the spinors as even if it does not mix upper and lower components of spinors, and we call the odd operator odd if it mixes upper and lower components. The Foldy-Wouthuysen (FW) Hamiltonian consists of even operators only. For the upper left $2\times2$ submatrix of this Hamiltonian, we find the result [13]

$$H_{\rm FW} = U[H_D - (E_\psi - \omega)]U^+ = m + H_S + \delta H, \tag{63}$$

where $H_S$ refers to the Schrödinger Hamiltonian, and $\delta H$ is the relativistic correction,

$$\delta H = -\frac{(\mathbf{p})^4}{8m^3} + \frac{\pi(Z\alpha)}{2m^2}\delta(\mathbf{r}) + \frac{(Z\alpha)}{4m^2 r^3}\boldsymbol{\sigma}\cdot\mathbf{L}. \tag{64}$$

It is interesting to note the reason why we can ignore the lower $2\times2$ submatrix of the FW Hamiltonian in our scheme

of calculation. The lower $2\times2$ submatrix contains the terms $-m-(E_\psi-\omega)\approx-2m$ as the dominating $(Z\alpha)^0$ contribution. Therefore the integral vanishes in the limit $\epsilon\to0$. This can be checked by considering the integral in Eq. (59), inserting a spectral resolution for the Dirac-Coulomb propagator, and performing the integral over $d^3k$ after suitable angular averaging. The upper $2\times2$ submatrix has no $(Z\alpha)^0$ contribution, because terms proportional to $m$ and $E_\psi$ cancel. This submatrix contributes to the Lamb shift. Now we turn to the calculation of the Foldy-Wouthuysen transform of the operators $\alpha^i\exp(\mathbf{k}\cdot\mathbf{r})$. The expression $U\alpha^i\exp(i\mathbf{k}\cdot\mathbf{r})U^+$ is to be calculated. Assuming that $\omega=|\mathbf{k}|$ is of the order $O((Z\alpha)^2)$, we may expand the expression $U\alpha^ie^{i\mathbf{k}\cdot\mathbf{r}}U^+$ in powers of $(Z\alpha)$. The result of the calculation is

$$\begin{aligned}U\alpha^ie^{i\mathbf{k}\cdot\mathbf{r}}U^+=&\alpha^i\Big[1+i(\mathbf{k}\cdot\mathbf{r})-\tfrac{1}{2}(\mathbf{k}\cdot\mathbf{r})^2\Big]-\frac{1}{2m^2}p^i(\boldsymbol{\alpha}\cdot\mathbf{p})\\&+\gamma^0\frac{p^i}{m}\Big[1+i(\mathbf{k}\cdot\mathbf{r})-\tfrac{1}{2}(\mathbf{k}\cdot\mathbf{r})^2\Big]-\gamma^0\frac{1}{2m^3}p^i\mathbf{p}^2\\&-\frac{1}{2m^2}\frac{\alpha}{r^3}(\mathbf{r}\times\boldsymbol{\Sigma})^i+\frac{1}{2m}\gamma^0(\mathbf{k}\cdot\mathbf{r})(\mathbf{k}\times\boldsymbol{\Sigma})^i\\&-\frac{i}{2m}\gamma^0(\mathbf{k}\times\boldsymbol{\Sigma})^i.\end{aligned}\tag{65}$$

In the limit $\epsilon\to0$ the odd operators in the above expression do not contribute to the self-energy in $(Z\alpha)^2$ relative order, because, up to $(Z\alpha)^2$ relative order, these operators only join the upper components of the wave function with the lower components of the Dirac-Coulomb Hamiltonian. This contribution vanishes, as described. So one can neglect the odd operators. By using symmetry arguments, it can be shown easily that the last term in the above expression (proportional to $\mathbf{k}\times\boldsymbol{\Sigma}$) also does not contribute to the Lamb shift in $(Z\alpha)^2$ relative order for $\epsilon\to0$.

Because we can ignore odd operators, and because the lower components of the Foldy-Wouthuysen transformed wave function vanish, we keep only the upper left $2\times2$ submatrix of Eq. (65), and we write $U\alpha^ie^{i\mathbf{k}\cdot\mathbf{r}}U^+$ as

$$\begin{aligned}U\alpha^ie^{i\mathbf{k}\cdot\mathbf{r}}U^+\simeq&\frac{p^i}{m}\Big[1+i(\mathbf{k}\cdot\mathbf{r})-\tfrac{1}{2}(\mathbf{k}\cdot\mathbf{r})^2\Big]-\frac{1}{2m^3}p^i\mathbf{p}^2\\&-\frac{1}{2m^2}\frac{\alpha}{r^3}(\mathbf{r}\times\boldsymbol{\sigma})^i+\frac{1}{2m}(\mathbf{k}\cdot\mathbf{r})(\mathbf{k}\times\boldsymbol{\sigma})^i.\end{aligned}\tag{66}$$

This can be rewritten as

$$U\alpha^ie^{i\mathbf{k}\cdot\mathbf{r}}U^+=\frac{p^i}{m}e^{i\mathbf{k}\cdot\mathbf{r}}+\delta y^i,\tag{67}$$

where $\delta y^i$ is of order $(Z\alpha)^3$. It is understood that the term $(p^i/m)e^{i\mathbf{k}\cdot\mathbf{r}}$ is also expanded up to the order $(Z\alpha)^3$. Denoting the Schrödinger energy by $E$ [$E=-(Z\alpha)^2m/n^2$ for $nP$ states] and the first relativistic correction to $E$ by $\delta E$, we can thus write the matrix element $P^{ij}$ as

$$\begin{aligned}P^{ij}=&\langle\phi+\delta\phi|\left[\frac{p^i}{m}e^{i\mathbf{k}\cdot\mathbf{r}}+\delta y^i\right]\\&\times\frac{1}{H_S-(E-\omega)+\delta H-\delta E}\left[\frac{p^j}{m}e^{-i\mathbf{k}\cdot\mathbf{r}}+\delta y^j\right]|\phi+\delta\phi\rangle.\end{aligned}\tag{68}$$

We now define the dimensionless quantity

$$P=\frac{m}{2}\delta^{T,ij}P^{ij}.\tag{69}$$

Up to $(Z\alpha)^2$, we can write the matrix element $P$ as the sum of the contributions [Eqs. (70)–(75)]. The leading contribution (the ''nonrelativistic dipole'') is given by

$$P_{\rm nd}=\frac{1}{3m}\langle\phi|p^i\frac{1}{H_S-(E-\omega)}p^i|\phi\rangle.\tag{70}$$

The other contributions to $P$ are [1] as follows:

(i) the nonrelativistic quadrupole,

$$P_{\rm nq}=\frac{1}{3m}\langle\phi|p^ie^{i\mathbf{k}\cdot\mathbf{r}}\frac{1}{H_S-(E-\omega)}p^ie^{-i\mathbf{k}\cdot\mathbf{r}}|\phi\rangle-P_{\rm nd};\tag{71}$$

(ii) the corrections to the current $\alpha^i$ from the Foldy-Wouthuysen transformation,

$$P_{\delta y}=\delta^{T,ij}\langle\phi|\delta y^i\frac{1}{H_S-(E-\omega)}p^je^{-i\mathbf{k}\cdot\mathbf{r}}|\phi\rangle;\tag{72}$$

(iii) the contribution due to the relativistic Hamiltonian,

$$P_{\delta H}=-\frac{1}{3m}\langle\phi|p^i\frac{1}{H_S-(E-\omega)}\delta H\frac{1}{H_S-(E-\omega)}p^i|\phi\rangle;\tag{73}$$

(iv) the contribution due to the relativistic correction to the energy,

$$P_{\delta E}=\frac{1}{3m}\langle\phi|p^i\frac{1}{H_S-(E-\omega)}\delta E\frac{1}{H_S-(E-\omega)}p^i|\phi\rangle;\tag{74}$$

and

(v) the contribution due to the relativistic correction to the wave function,

$$P_{\delta\phi}=\frac{2}{3m}\langle\delta\phi|p^i\frac{1}{H_S-(E-\omega)}p^i|\phi\rangle.\tag{75}$$

Almost all of the above contributions are calculated using a coordinate space representation of the Schrödinger Coulomb propagator given in Refs. [1] and [15]. Formulas given in Refs. [17] and [16] prove useful for the summation over the intermediate quantum numbers. For the nonrelativistic quadrupole contribution, however, we use the momentum-space representation due to Schwinger [19],

$$G(\mathbf{p},\mathbf{p}',\Omega)=4\pi mX^3\left(\frac{ie^{i\pi\tau}}{2\sin\pi\tau}\right)\int_1^{0^+}d\rho\ \rho^{-\tau}\frac{d}{d\rho}\frac{1-\rho^2}{\rho}\frac{1}{[X^2(\mathbf{p}-\mathbf{p}')^2+(\mathbf{p}^2+X^2)(\mathbf{p}'^2+X^2)(1-\rho)^2/(4\rho)]^2},\qquad(76)$$

where $X=\sqrt{-2m\Omega}$, $\tau=m\alpha/X$. For noninteger $\tau$, one may replace the complex integration around the origin (in the positive sense) by a much simpler integral:

$$\left(\frac{ie^{i\pi\tau}}{2\sin\pi\tau}\right)\int_1^{0^+}d\rho\ \rho^{-\tau}g(\rho)\to\int_0^1 d\rho\ \rho^{-\tau}g(\rho).\qquad(77)$$

We then perform the calculation of $P_{\rm NQ}$ in momentum space using formulas given in the paper by Gavrila and Costescu [18]. The momentum-space wave functions of $P$ states were given in Ref. [19]. Calculations for $P_{\rm NQ}$ become increasingly complex. It should be noted that in the case of the $4P$ wave function, one has to deal with intermediate expressions of up to 20 000 terms. We do not describe these calculations in any further detail. Evaluations for this part of the calculation were done on IBM RISC/6000 and SGI POWER ONYX systems with the help of the computer algebra system MATHEMATICA [14].

The final $\omega$ integration is done by a change of variable

$$\omega\to t\quad\text{where}\quad t=\frac{1}{\sqrt{1+(2n^2\omega)/[(Z\alpha)^2m]}}\qquad(78)$$

($t=0$ corresponds to $\omega=\infty$, and $t=1$ corresponds to $\omega=0$). As an example for a $P$ matrix element, we give here the result for a contribution to $P_{\delta H}(4P_{1/2})$, caused by the Russell-Saunders coupling term in the Foldy-Wouthuysen transformed Dirac Hamiltonian:

$$\begin{aligned}
P_{\mathbf{L}\cdot\mathbf{S}}(4P_{1/2})&=\langle\phi|p^i\frac{1}{H_S-(E_\phi-\omega)}\left[\frac{\alpha}{4m^2r^3}\boldsymbol{\sigma}\cdot\mathbf{L}\right]\frac{1}{H_S-(E_\phi-\omega)}p^i|\phi\rangle\\
&=(Z\alpha)^2[16\,384F_{366}(t)t^6(-1+2t)(1+2t)(-1+4t)(1+4t)(-5+9t^2)^2]/[(675(-1+t)^2(1+t)^{14}]+(Z\alpha)^2\\
&\times[8192\Phi_{23}(t)t^6(-1+2t)(1+2t)(-1+4t)(1+4t)(-5+9t^2)^2]/[675(-1+t)^2(1+t)^{14}]\\
&-(Z\alpha)^2[16\,384\Psi_{63}(t)t^6(-1+2t)(1+2t)(-1+4t)(1+4t)(-5+9t^2)^2]/[675(-1+t)^2(1+t)^{14}]\\
&-(Z\alpha)^2[16F_4(t)t^5(-5+9t^2)(5+9t^2)]/[45(-1+t)^5(1+t)^5]-(Z\alpha)^2[4096\gamma t^7(1+2t)(1+4t)\\
&\times(-5+9t^2)^2(-630+2988t-22\,677t^2+322\,539t^3-1\,308\,681t^4+5\,929\,071t^5-20\,884\,413t^6\\
&+53\,752\,275t^7-124\,047\,785t^8+233\,683\,811t^9-362\,131\,987t^{10}+489\,361\,437t^{11}-552\,966\,475t^{12}\\
&+526\,774\,701t^{13}-433\,556\,447t^{14}+298\,335\,889t^{15}-171\,601\,869t^{16}+84\,114\,837t^{17}-33\,425\,148t^{18}\\
&+10\,588\,500t^{19}-2\,811\,264t^{20}+536\,448t^{21}-64\,512t^{22}+9216t^{23})]/[675(-2+t)(-1+t)^8(1+t)^24\\
&\times(-3+2t)(-7+4t)(-5+4t)(-3+4t)]+(Z\alpha)^2[t^4(54\,385\,222\,500+13\,984\,771\,500t\\
&+15\,573\,367\,761\,525t^2+137\,704\,964\,619\,600t^3-1\,186\,676\,073\,750\,825t^4-891\,514\,989\,328\,950t^5\\
&-18\,753\,057\,125\,404\,875t^6+257\,731\,557\,911\,828\,220t^7-644\,138\,132\,939\,443\,685t^8\\
&-162\,189\,845\,176\,905\,698t^9+5\,703\,957\,333\,855\,251\,853t^{10}-40\,461\,889\,136\,476\,779\,376t^{11}\\
&+179\,879\,463\,449\,806\,219\,483t^{12}-470\,465\,622\,621\,377\,811\,686t^{13}+722\,355\,119\,079\,050\,313\,441t^{14}\\
&-285\,989\,274\,333\,023\,499\,852t^{15}-2\,287\,627\,466\,701\,513\,790\,137t^{16}+8\,721\,622\,433\,626\,707\,698\,710t^{17}\\
&-17\,878\,002\,921\,800\,012\,898\,021t^{18}+22\,584\,212\,519\,300\,184\,263\,992t^{19}\\
&-11\,732\,105\,237\,171\,234\,433\,515t^{20}-22\,234\,628\,025\,915\,862\,014\,322t^{21}\\
&+73\,751\,337\,137\,966\,874\,205\,423t^{22}-118\,367\,926\,111\,467\,660\,583\,708t^{23}\\
&+122\,509\,973\,591\,672\,089\,703\,233t^{24}-68\,708\,753\,123\,836\,196\,116\,438t^{25}
\end{aligned}$$

$$
\begin{aligned}
&-27\,553\,239\,135\,523\,122\,581\,409t^{26}+126\,820\,257\,213\,436\,783\,378\,720t^{27}\\
&-189\,954\,960\,243\,232\,498\,928\,039t^{28}+199\,312\,481\,720\,191\,257\,908\,238t^{29}\\
&-164\,901\,212\,087\,123\,003\,552\,709t^{30}+112\,286\,946\,900\,261\,699\,896\,044t^{31}\\
&-64\,112\,830\,789\,916\,243\,409\,479t^{32}+30\,834\,230\,557\,497\,197\,343\,734t^{33}\\
&-12\,455\,975\,426\,801\,658\,077\,884t^{34}+4\,211\,137\,005\,166\,537\,183\,048t^{35}\\
&-1\,183\,248\,309\,588\,246\,704\,096t^{36}+270\,125\,031\,800\,068\,986\,496t^{37}\\
&-48\,193\,573\,673\,016\,712\,704t^{38}+6\,583\,393\,931\,443\,034\,112t^{39}\\
&-691\,086\,520\,295\,792\,640t^{40}+41\,007\,381\,492\,105\,216t^{41}+1\,314\,475\,331\,420\,160t^{42})]/\\
&[425\,250(-2+t)^2(-1+t)^{10}(1+t)^{24}(-3+2t)^2(-1+2t)(-7+4t)^2(-5+4t)^2(-3+4t)^2(-1+4t)]\\
&+(Z\alpha)^2[8192t^8(-1+2t)(-1+4t)(-5+9t^2)^2(3+6t+3t^2+8t^3)\ln[2/(1+t)]]/[675(-1+t)^{12}(1+t)^6]\\
&+(Z\alpha)^2\{16G_4(t)t^5(-5+9t^2)(-1125+2400t+145\,390t^2-19\,200\gamma t^2-148\,320t^3-2\,026\,412t^4\\
&+418\,560\gamma t^4+1\,027\,200t^5+7\,316\,050t^6-1\,920\,000\gamma t^6-1\,382\,400t^7-7\,444\,143t^8+2\,211\,840\gamma t^8\\
&-19\,200t^2\ln[2/(1+t)]+418\,560t^4\ln[2/(1+t)]-1\,920\,000t^6\ln[2/(1+t)]\\
&+2\,211\,840t^8\ln[2/(1+t)])\}/[10\,125(-1+t)^8\\
&\times(1+t)^8]+(Z\alpha)^2[256t^7(-5+9t^2)^2(8+45t-305t^2-175t^3+283t^4-265t^5+3421t^6+395t^7\\
&+433t^8)\ln[(2t)/(1+t)]]/[675(-1+t)^12(1+t)^7], \qquad (79)
\end{aligned}
$$

where

$$F_4(t)={}_2F_1\{1,-4t,1-4t,[(t-1)/(t+1)]^2\}, \qquad (80)$$

$$G_4(t)={}_2F_1[1,-4t,1-4t,(t-1)/(t+1)], \qquad (81)$$

$$F_{366}(t)=t^2\sum_{k=6}^{\infty}\frac{[(t-1)/(t+1)]^k}{3-4t+k}\times\frac{\partial}{\partial b}({}_2F_1)[-k,6,6,2/(1+t)], \qquad (82)$$

$$\Phi_{23}(t)=\sum_{k=6}^{\infty}\frac{[(t-1)/(t+1)]^{2k}}{(3-4t+k)^2}, \qquad (83)$$

$$\Psi_{63}(t)=\sum_{k=6}^{\infty}\frac{[(t-1)/(t+1)]^{2k}}{(3-4t+k)}\Psi(k+6), \qquad (84)$$

where $\Psi$ denotes the logarithmic derivative of the $\Gamma$ function. The quadratic singularity in the result for $P_{\mathbf{L}\cdot\mathbf{S}}(4P_{1/2})$ in Eq. (79) at $t=\frac{3}{4}$ [given by the $(-3+4t)^2$ term in the denominator of the purely rational function] corresponds to the decay into the $3D$ state. One can check explicitly that the insertion of corresponding intermediate states in the spectral decomposition of the propagators necessitates the existence of quadratic singularities in the $P$ matrix elements, and that the quadratic singularities occur only in the matrix elements with two propagators. The quadratic singularities are a consequence of the perturbative treatment of $\delta H$ in the propagator $1/[H_S+\delta H-(E_\phi+\delta E-\omega)]$ [expansion in $\delta H$ is not allowed in the vicinity of a pole of the resolvent $G(E)=1/(H_S-E)$]. The integration procedure for the quadratic singularities is as follows: first we isolate and calculate analytically the integral of the term that gives rise to the singularity (as a function of $t$), then we take the difference of the edge terms at $t=1$ and 0. This procedure takes back the effect of the perturbative treatment, and assigns the correct value to the $t$ integral. As the final step, we subtract the term that gave rise to the quadratic singularity, and proceed with the rest of the terms in the usual way described in Ref. [1].

The integration procedure deserves some further comments. We also encounter in the matrix elements singularities of linear type at $t=\frac{1}{4}$, $\frac{1}{2}$, and $\frac{3}{4}$, which also correspond to the decay of the excited state. The residue taken at these singularities yields the decay width of the respective states. In order to obtain the principal value of the $t$ integral, one has to symmetrize the integrand around all the singularities. This is also accomplished by symbolic procedures written in the computer algebra language MATHEMATICA.

The results of the calculations have been checked in many ways. An important cross-check is the cancellation of $\epsilon$-divergent terms in the sum of the high- and low-energy parts. By considering the expansion of the propagators in powers of $1/\omega$, the logarithmic singularities of all contribu-

TABLE I. Contributions of relative order $(Z\alpha)^2$ to the low-energy part $F_L$ for the $3P_{1/2}$ and $3P_{3/2}$ states.

| Contribution | $3P_{1/2}$ | $3P_{3/2}$ |
|---|---|---|
| $F_{\rm nq}$ | $-1.433\,010(1)+248/405\,\ln(\epsilon/(Z\alpha)^2)$ | $-1.433\,010(1)+248/405\,\ln(\epsilon/(Z\alpha)^2)$ |
| $F_{\delta y}$ | $0.922\,653(1)-20/81\,\ln(\epsilon/(Z\alpha)^2)$ | $0.629\,717(1)-20/81\,\ln(\epsilon/(Z\alpha)^2)$ |
| $F_{\delta H}$ | $0.356\,318(1)-73/324\,\ln(\epsilon/(Z\alpha)^2)$ | $0.333\,053(1)-55/324\,\ln(\epsilon/(Z\alpha)^2)$ |
| $F_{\delta E}$ | $0.040\,651\,9(1)+1/36\,\ln(\epsilon/(Z\alpha)^2)$ | $0.013\,551(1)+1/108\,\ln(\epsilon/(Z\alpha)^2)$ |
| $F_{\delta\phi}$ | $-0.830\,340(1)+40/81\,\ln(\epsilon/(Z\alpha)^2)$ | $-0.236\,869(1)+13/108\,\ln(\epsilon/(Z\alpha)^2)$ |
| sum | $-0.94\,378(1)+268/405\,\ln(\epsilon/(Z\alpha)^2)$ | $-0.69\,356(1)+148/405\,\ln(\epsilon/(Z\alpha)^2)$ |

tions can be calculated individually, and agree with the results obtained from complete evaluation.

The contributions to the low-energy part $F_L$ in $(Z\alpha)^2$ relative order are given in Tables I and II. Summing all contributions, we obtain the following complete results for the contribution of the low energy parts $F_L$:

$$F_L(3P_{1/2})=-\frac{4}{3}\ln k_0(3P)+(Z\alpha)^2 \times\left[-0.943\,78(1)+\frac{20}{81\epsilon}+\frac{268}{405}\ln\frac{\epsilon}{(Z\alpha)^2}\right], \tag{85}$$

$$F_L(3P_{3/2})=-\frac{4}{3}\ln k_0(3P)+(Z\alpha)^2 \times\left[-0.693\,56(1)+\frac{20}{81\epsilon}+\frac{148}{405}\ln\frac{\epsilon}{(Z\alpha)^2}\right], \tag{86}$$

$$F_L(4P_{1/2})=-\frac{4}{3}\ln k_0(4P)+(Z\alpha)^2 \times\left[-0.997\,80(1)+\frac{23}{90\epsilon}+\frac{499}{720}\ln\frac{\epsilon}{(Z\alpha)^2}\right], \tag{87}$$

and

$$F_L(4P_{3/2})=-\frac{4}{3}\ln k_0(4P)+(Z\alpha)^2 \times\left[-0.730\,57(1)+\frac{23}{90\epsilon}+\frac{137}{360}\ln\frac{\epsilon}{(Z\alpha)^2}\right]. \tag{88}$$

## V. RESULTS AND EVALUATION OF THE LAMB SHIFT

Summing the contributions from the high- and low-energy parts, we obtain the following results for the scaled $F$ function defined in Eq. (2):

$$F(3P_{1/2})=-\tfrac{1}{6}-\tfrac{4}{3}\ln k_0(3P)+(Z\alpha)^2 \times\{-1.147\,68(1)+\tfrac{268}{405}\ln[(Z\alpha)^{-2}]\}, \tag{89}$$

$$F(3P_{3/2})=\tfrac{1}{12}-\tfrac{4}{3}\ln k_0(3P)+(Z\alpha)^2 \times\{-0.597\,56(1)+\tfrac{148}{405}\ln[(Z\alpha)^{-2}]\}, \tag{90}$$

$$F(4P_{1/2})=-\tfrac{1}{6}-\tfrac{4}{3}\ln k_0(3P)+(Z\alpha)^2 \times\{-1.195\,68(1)+\tfrac{499}{720}\ln[(Z\alpha)^{-2}]\}, \tag{91}$$

$$F(4P_{3/2})=\tfrac{1}{12}-\tfrac{4}{3}\ln k_0(3P)+(Z\alpha)^2 \times\{-0.630\,94(1)+\tfrac{137}{360}\ln[(Z\alpha)^{-2}]\}. \tag{92}$$

The results obtained for $A_{4,0}$ and $A_{6,1}$ are in agreement with those previously known [3]. The values of the Bethe logarithms [5,6]

TABLE II. Contributions of relative order $(Z\alpha)^2$ to the low-energy part $F_L$ for the $4P_{1/2}$ and $4P_{3/2}$ states.

| Contribution | $4P_{1/2}$ | $4P_{3/2}$ |
|---|---|---|
| $F_{\rm nq}$ | $-1.512\,220(1)+229/360\,\ln(\epsilon/(Z\alpha)^2)$ | $-1.512\,220(1)+229/360\,\ln(\epsilon/(Z\alpha)^2)$ |
| $F_{\delta y}$ | $0.966\,398(1)-23/90\,\ln(\epsilon/(Z\alpha)^2)$ | $0.662\,154(1)-23/90\,\ln(\epsilon/(Z\alpha)^2)$ |
| $F_{\delta H}$ | $0.364\,541(1)-2891/11\,520\,\ln(\epsilon/(Z\alpha)^2)$ | $0.342\,940(1)-439/2304\,\ln(\epsilon/(Z\alpha)^2)$ |
| $F_{\delta E}$ | $0.033\,550\,4(1)+13/768\,\ln(\epsilon/(Z\alpha)^2)$ | $0.012\,904(1)+5/768\,\ln(\epsilon/(Z\alpha)^2)$ |
| $F_{\delta\phi}$ | $-0.850\,066(1)+787/1440\,\ln(\epsilon/(Z\alpha)^2)$ | $-0.236\,345(1)+53/288\,\ln(\epsilon/(Z\alpha)^2)$ |
| sum | $-0.997\,80(1)+499/720\,\ln(\epsilon/(Z\alpha)^2)$ | $-0.730\,57(1)+137/360\,\ln(\epsilon/(Z\alpha)^2)$ |

$$\ln k_0(3P) = -0.038\,190\,23(1),$$

$$\ln k_0(4P) = -0.041\,954\,89(1) \tag{93}$$

could be verified numerically with a seven-figure accuracy from our analytic expressions by numerical (Gaussian) integration. For $A_{6,1}$, we use the following general formula which may be extracted from the work by Erickson and Yennie [Ref. [4], Eq. (4.4a) ibid., upon subtraction of the vacuum polarization contribution implicitly contained in the quoted equation]:

$$\begin{aligned} A_{6,1}(n,l,j) &= \frac{4}{3}\Bigg\{ (1-\delta_{l,0})\frac{8\{3-[l(l+1)]/n^2\}}{(2l-1)(2l)(2l+1)(2l+2)(2l+3)} \\ &+ \delta_{l,1}\left[1-\frac{1}{n^2}\right]\left[\frac{1}{10}+\frac{1}{4}\,\delta_{j,l-1/2}\right] + \delta_{l,0}\Bigg[-\frac{601}{240} \\ &- \frac{77}{60n^2} + 7\,\ln 2 + 3[\gamma - \ln n + \Psi(n+1)]\Bigg]\Bigg\}, \end{aligned} \tag{94}$$

where $\gamma$ is Euler's constant, and $\Psi$ refers to the logarithmic derivative of the $\Gamma$ function. For $P$ states ($l=1$), this formula reduces to

$$A_{6,1}(n,1,j) = \frac{4}{3}\left[\frac{1}{15}\left(3-\frac{2}{n^2}\right) + \left(1-\frac{1}{n^2}\right)\left(\frac{1}{10}+\frac{1}{4}\,\delta_{j,1/2}\right)\right], \tag{95}$$

and is in agreement with our results. From our results for $F$, we extract the following values for the coefficients $A_{6,0}$:

$$A_{6,0}(3P_{1/2}) = -1.147\,68(1), \quad A_{6,0}(3P_{3/2}) = -0.597\,56(1) \tag{96}$$

and

$$A_{6,0}(4P_{1/2}) = -1.195\,68(1), \quad A_{6,0}(4P_{3/2}) = -0.630\,94(1). \tag{97}$$

The results for $A_{6,0}$ are the main results of this work. They are in excellent agreement with data obtained from numerical calculations by one of the authors (P.J.M.) and Y. K. Kim [2]. Mohr and Kim calculated the $F$ function defined in Eq. (2) numerically for $Z \geqslant 10$, treating the binding field nonperturbatively. By extrapolating their numerical data [2] to the region of small $Z$, we obtain the following estimates for the remainder function $G_{\mathrm{SE},7}$ implicitly defined in Eq. (2):

$$G_{\mathrm{SE},7}(3P_{1/2}, Z=1) = 3.6 \pm 0.5,$$

$$G_{\mathrm{SE},7}(3P_{3/2}, Z=1) = 2.6 \pm 0.5 \tag{98}$$

and

$$G_{\mathrm{SE},7}(4P_{1/2}, Z=1) = 3.9 \pm 0.5,$$

$$G_{\mathrm{SE},7}(4P_{3/2}, Z=1) = 2.8 \pm 0.5. \tag{99}$$

The uncertainties in $G_{\mathrm{SE},7}$ are used to estimate the theoretical uncertainty from the one-loop contribution. When modeling the numerical data, it must be taken into account that, as noted by Karshenboim [20], $A_{7,1}$ coefficients vanish for $P$ states. Values of $A_{6,0}$ and $G_{\mathrm{SE},7}$ for $2P$ states are given in Ref. [1]. We use the following implicit definition of the Lamb shift $\mathcal{L}$:

$$E = m_r[f(n,j)-1] - \frac{m_r^2}{2(m+m_N)}[f(n,j)-1]^2 + \mathcal{L} + E_{\mathrm{hfs}}, \tag{100}$$

where $E$ is the energy level of the two-body system and $f(n,j)$ is the dimensionless Dirac energy, $m$ is the electron mass, $m_r$ is the reduced mass of the system, and $m_N$ is the nuclear mass. It should be noted that we consider the hfs-fs mixing term as a contribution to the hyperfine structure. The small hfs-fs-mixing correction, which is discussed in Ref. [21], mixes the $F=1$ sublevels of the $P_{1/2}$ and $P_{3/2}$ states and shifts the center of the hyperfine levels. It should be taken into account when the fine structure is deduced from precision experiments.

In order to calculate the Lamb shift, we include the Barker-Glover correction to hydrogen energy levels [22], which we refer to as the $(Z\alpha)^4$ recoil correction. We also include the $(Z\alpha)^5$ recoil correction calculated by Salpeter [23], and the results [24] for recoil corrections of order $(Z\alpha)^6 m_r/m_N$. The results for recoil corrections of order $(Z\alpha)^6 m_r/m_N$ have been confirmed by Pachucki (see Chap. 5 of Ref. [1]). We include contributions from the higher-order two-loop correction of order $(\alpha/\pi)^2(Z\alpha)^6\ln^2(Z\alpha)^{-2}$ corresponding to the $B_{6,2}$ coefficient [25], and for three-loop corrections in lowest order. The theoretical error from the two-loop contribution ($B_{6,1}$ and higher terms) is estimated as half the contribution from the recently calculated $B_{6,2}$ coefficient [25]. The higher-order contributions due to vacuum polarization of order $\alpha/\pi(Z\alpha)^6$ can be obtained by analyzing the small distance behavior of the Dirac wave function, i.e., by evaluating the matrix element of the Uehling potential (see e.g., [26]),

$$V_{\mathrm{VP}}(\mathbf{r}) = \frac{\alpha(Z\alpha)}{m^2}\left[-\frac{4}{15}\,\delta(\mathbf{r}) - \frac{1}{35}\,\frac{\nabla^2}{m^2}\,\delta(\mathbf{r}) + O(\nabla^4\delta(\mathbf{r}))\right], \tag{101}$$

with $P$-state wave functions expanded in powers of $Z\alpha$. We obtain the results

$$A_{60}^{\mathrm{vac}}(nP_{1/2}) = -\frac{3}{35}\,\frac{n^2-1}{n^2} \tag{102}$$

and

$$A_{60}^{\mathrm{vac}}(nP_{3/2}) = -\frac{2}{105}\,\frac{n^2-1}{n^2} \tag{103}$$

for the leading term. We have also evaluated the contribution of the Uehling potential numerically without expansion in $Z\alpha$, with the results

$$G_{U,7}(3P_{1/2}, Z=1) = 0.0455, \quad G_{U,7}(3P_{3/2}, Z=1) = 0.0249, \tag{104}$$

TABLE III. Contributions to the Lamb shift in kHz for the $3P_{1/2}$ and $3P_{3/2}$ states.

| Contribution | $3P_{1/2}$ (kHz) | $3P_{3/2}$ (kHz) |
|---|---|---|
| one-loop self-energy | −3477.349(5) | 4046.413(5) |
| two-loop self-energy | 7.705(23) | −3.782(23) |
| three-loop self-energy | −0.064 | 0.032 |
| vacuum polarization | −0.122 | −0.027 |
| $(Z\alpha)^4$ recoil | 0.641 | −0.320 |
| $(Z\alpha)^5$ recoil | −4.705(13) | −1.915(13) |
| $(Z\alpha)^6$ recoil | 0.139 | 0.139 |
| Sum for $3P$ | −3473.75(3) | 4037.75(3) |

and

$$G_{U,7}(4P_{1/2},Z=1)=0.0480, \quad G_{U,7}(4P_{3/2},Z=1)=0.0262, \tag{105}$$

where the function $G_{U,7}$ is defined in analogy with $G_{\mathrm{SE},7}$. The contribution of the higher-order terms is negligible compared to the uncertainty in the higher-order self-energy terms. The Wichmann-Kroll vacuum polarization contribution is expected to be of order $(Z\alpha)^2$ times the Uehling correction, and is not included here.

The above-mentioned contributions to the Lamb shift are listed in Tables III and IV for the states under investigation. It should be noted that the reduced mass dependence of the terms must be restored in low-$Z$ systems to obtain the correct value for the Lamb shift. Terms which are caused by the anomalous magnetic moment of the electron acquire a factor $(m_r/m_e)^2$ (where $m_r$ is the reduced mass of the system, and $m_e$ the mass of the electron), all other contributions to the Lamb shift acquire a factor $(m_r/m_e)^3$. In addition, the argument of the logarithms $\ln[(Z\alpha)^{-2}]$ must be replaced by $\ln[(m_e/m_r Z\alpha)^{-2}]$. The relevant formulas are also given in Ref. [3].

It should also be noted that for two- and three-loop corrections in respective lowest order $(\alpha/\pi)^2(Z\alpha)^4$ and $(\alpha/\pi)^3(Z\alpha)^4$, only the anomalous magnetic moment of the electron contributes to the Lamb shift for $P$ states, because the Dirac form factor $F_1(q^2)$ is infrared finite in two- and three-loop order. So it is only the contribution from the magnetic form factor $F_2(q^2=0)$ which persists. The calculation of the contribution to the Lamb shift is then straightforward.

TABLE IV. Contributions to the Lamb shift in kHz for the $4P_{1/2}$ and $4P_{3/2}$ states.

| Contribution | $4P_{1/2}$ (kHz) | $4P_{3/2}$ (kHz) |
|---|---|---|
| one-loop self-energy | −1403.102(2) | 1770.887(2) |
| two-loop self-energy | 3.252(10) | −1.594(10) |
| three-loop self-energy | −0.027 | 0.014 |
| vacuum polarization | −0.054 | −0.012 |
| $(Z\alpha)^4$ recoil | 0.270 | −0.135 |
| $(Z\alpha)^5$ recoil | −1.915(5) | −1.915(5) |
| $(Z\alpha)^6$ recoil | 0.061 | 0.061 |
| Sum for $4P$ | −1401.52(1) | 1767.30(1) |

We obtain the following theoretical results for the Lamb shift of $3P$ and $4P$ states:

$$\mathcal{L}(3P_{1/2})=-3473.75(3)\ \text{kHz}, \tag{106}$$

$$\mathcal{L}(3P_{3/2})=4037.75(3)\ \text{kHz}, \tag{107}$$

$$\mathcal{L}(4P_{1/2})=-1401.52(1)\ \text{kHz}, \tag{108}$$

$$\mathcal{L}(4P_{3/2})=1767.30(1)\ \text{kHz}. \tag{109}$$

The theoretical values for the fine-structure splitting, using the 1987 Cohen-Taylor value of $\alpha^{-1}=137.035\,989\,5(61)$ [27], are as follows:

$$\Delta E_{\mathrm{fs}}(3P)=3\,250\,089.8(3)\ \text{kHz}, \tag{110}$$

$$\Delta E_{\mathrm{fs}}(4P)=1\,371\,130.0(1)\ \text{kHz}. \tag{111}$$

For $2P$ states, the theoretical value is $\Delta E_{\mathrm{fs}}(2P)=10\,969\,043(1)$ kHz [1]. The uncertainty in the theoretical values for the fine-structure splitting is given by the uncertainty in $\alpha$. Any determination of the fine structure beyond the quoted uncertainty would yield a value of $\alpha$ improved with respect to the 1987 value. Given the scattering of available data for $\alpha$ [28], such a determination could be useful for checking the consistency of measurements coming from different fields of physics.

The formula for the fine structure as a function of $\alpha$ for atomic hydrogen $(Z=1)$ is as follows:

$$\begin{aligned}
\Delta E_{\mathrm{fs}}(n) &= E(nP_{3/2})-E(nP_{1/2}) \\
&= R_\infty\left\{ \alpha^2\left(\frac{y}{2n^3}-\frac{x^2y^3}{2n^3}\right)+\alpha^3\left(\frac{y^2}{2\pi n^3}\right)\right. \\
&\quad +\alpha^4\left(\frac{a_e^{(2)}y^2}{\pi^2 n^3}+\frac{7y}{32n^3}+\frac{9y}{16n^4}-\frac{3y}{4n^5}\right. \\
&\quad \left.+\frac{xy^2}{4n^5(1+x)}\right) \\
&\quad +\alpha^5\left[\frac{a_e^{(3)}y^2}{\pi^3 n^3}+\frac{2y^3}{\pi n^3}\left(\Delta A_{6,0}(n)+\frac{1}{15}\,\frac{n^2-1}{n^2}\right.\right. \\
&\quad \left.\left.-\frac{1}{3}\,\frac{n^2-1}{n^2}\ln(y^{-1}\alpha^{-2})\right)\right] \\
&\quad +\alpha^6\left(\frac{2y^3}{\pi n^3}\Delta G(n)+\frac{31y}{256n^3}+\frac{45y}{128n^4}+\frac{7y}{64n^5}\right. \\
&\quad \left.\left.-\frac{45y}{32n^6}+\frac{15y}{16n^7}\right)\right\}+\delta\mathcal{L}_{\mathrm{th}}(n),
\end{aligned} \tag{112}$$

where the theoretical uncertainty in the difference of the Lamb shift of $nP$ states is given by

$$\delta\mathcal{L}_{\rm th}(2)=80\ \text{Hz},\quad \delta\mathcal{L}_{\rm th}(3)=30\ \text{Hz},\quad \delta\mathcal{L}_{\rm th}(4)=10\ \text{Hz}. \tag{113}$$

The mass ratios are

$$x=m_e/m_p \quad \text{and} \quad y=m_r/m_e=1/(1+x). \tag{114}$$

$\Delta A_{6,0}(n)$ and $\Delta G(n)$ are defined as

$$\Delta A_{6,0}(n)=A_{6,0}(nP_{3/2})-A_{6,0}(nP_{1/2}),$$

$$\Delta G(n)=G_{\rm SE,7}(nP_{3/2})-G_{\rm SE,7}(nP_{1/2}). \tag{115}$$

For practical purposes, the $n$ dependence of $\Delta G_{\rm SE,7}(n)$ may be suppressed, because it is a very small contribution (in the 1-Hz range), and we may assume $\Delta G_{\rm SE,7}(n)\approx -1.0$. The two- and three-loop coefficients to the anomalous magnetic moment are given by [28]

$$a_2^{(e)}=-0.328\,478\,965,\quad a_3^{(e)}=1.181\,241\,56. \tag{116}$$

## VI. CONCLUSIONS

The analytic calculation of higher-order binding corrections to the Lamb shift of excited $P$ states has been described in this paper. We provide more accurate theoretical values of the Lamb shift for $3P$ and $4P$ states in hydrogenlike systems. We also give a formula for the fine structure as a function of $\alpha$ (for $2P$, $3P$, and $4P$ states), which may be used to determine $\alpha$ from an improved measurement of the fine structure.

With the possibility of substantial improvement in the precision of spectroscopic experiments (trapped atoms), a better determination of $\alpha$ from measurement of the fine structure might be within reach in the near future. Such a determination of the fine-structure constant $\alpha$, from the effect on which its name is based, would complement other high precision determinations from solid-state physics and the anomalous magnetic moment of the electron.

We note that there are deviations of experimental data for excited $nS$-$nP$ transitions from theory by more than one standard deviation but less than two standard deviations (see Ref. [21], and references therein). However, both the theory of the Lamb shift and spectroscopic techniques have improved since the measurements were made, so one might expect a more precise comparison of theory and experiment in the future. The present uncertainty in the theory would in principle allow a determination of the fine-structure constant with a relative uncertainty of less than five parts in $10^9$. However, at this level of precision additional theoretical work might be needed to address questions such as asymmetries in the natural line shape. We only mention that, for excited states, an experimental determination of the fine structure could be simplified by the slower decay (narrower line width) of the higher excited $P$ states [8].

## ACKNOWLEDGMENTS

The authors thank D.F.G. for continued support (Contract No. SO333/1-2). We would like to thank K. Pachucki, S. Karshenboim, and J. Sims for stimulating and helpful discussions, and J. Urban for carefully reading the manuscript. P.J.M. acknowledges the Alexander von Humboldt Foundation for continued support. We also wish to acknowledge support from BMBF and from the Gesellschaft für Schwerionenforschung.

[1] U. D. Jentschura and K. Pachucki, Phys. Rev. A **54**, 1853 (1996).
[2] P. J. Mohr and Y. K. Kim, Phys. Rev. A **45**, 2727 (1992).
[3] J. Sapirstein and D. R. Yennie, in *Quantum Electrodynamics*, edited by T. Kinoshita (World Scientific, Singapore, 1990), p. 560.
[4] G. W. Erickson and D. R. Yennie, Ann. Phys. (N.Y.) **35**, 271 (1965); **35**, 447 (1965).
[5] S. Klarsfeld and A. Maquet, Phys. Lett. **43B**, 201 (1973).
[6] G. W. F. Drake and R. A. Swainson, Phys. Rev. A **41**, 1243 (1990).
[7] K. Pachucki, Phys. Rev. A **46**, 648 (1992); Ann. Phys. (N.Y.) **226**, 1 (1993).
[8] H. A. Bethe and E. E. Salpeter, *Quantum Mechanics of One- and Two-Electron Atoms* (Plenum, New York, 1957).
[9] P. J. Mohr, Ann. Phys. (N.Y.) **88**, 26 (1974).
[10] P. J. Mohr, Ann. Phys. (N.Y.) **88**, 52 (1974).
[11] P. J. Mohr, Phys. Rev. A **26**, 2338 (1982).
[12] P. J. Mohr, Phys. Rev. A **46**, 4421 (1992).
[13] C. Itzykson and J. Zuber, *Quantum Field Theory* (McGraw-Hill, New York, 1980).
[14] S. Wolfram, *Mathematica-A System for Doing Mathematics by Computer* (Addison-Wesley, Reading, MA, 1988) (endorsement by NIST is not implied).
[15] R. A. Swainson and G. W. F. Drake, J. Phys. A **24**, 79 (1991).
[16] H. Buchholz, *The Confluent Hypergeometric Function* (Springer-Verlag, New York, 1969).
[17] H. Bateman, *Higher Transcendental Functions* (McGraw-Hill, New York, 1953).
[18] M. Gavrila and A. Costescu, Phys. Rev. A **2**, 1752 (1970).
[19] M. Lieber, in *Relativistic, Quantum Electrodynamic, and Weak Interaction Effects in Atoms*, edited by W. R. Johnson, P. J. Mohr, and J. Sucher (AIP, New York, 1989), p. 445.
[20] S. Karshenboim, Zh. Éksp. Teor. Fiz. **106**, 414 (1994) [Sov. Phys. JETP **79**, 230 (1994)].
[21] F. Pipkin in *Quantum Electrodynamics* (Ref. [3]), p. 696.
[22] W. A. Barker and F. N. Glover, Phys. Rev. **99**, 317 (1955).
[23] E. Salpeter, Phys. Rev. **87**, 328 (1952).
[24] E. Golosov, A. S. Elkhovskii, A. I. Milshtein, and B. Khriplovich, Zh. Éksp. Teor. Fiz. **107**, 393 (1995) [Sov. Phys. JETP **80**, 208 (1995)].
[25] S. Karshenboim, J. Phys. B **29**, L29 (1996).
[26] N. L. Manakov, A. A. Nekipedov, and A. G. Fainshtein, Zh. Éksp. Teor. Fiz. **95**, 1167 (1989) [Sov. Phys. JETP **68**, 673 (1989)].
[27] E. R. Cohen and B. N. Taylor, Rev. Mod. Phys. **59**, 1121 (1987).
[28] T. Kinoshita, Rep. Prog. Phys. **59**, 1459 (1996).