Higher-order binding corrections to the Lamb shift of $2P$ states

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We present an improved calculation of higher order corrections to the one-loop self energy of $2P$ states in hydrogen-like systems with small nuclear charge Z. The method is based on a division of the integration with respect to the photon energy into a high and a low energy part. The high energy part is calculated by an expansion of the electron propagator in powers of the Coulomb field. The low energy part is simplified by the application of a Foldy-Wouthuysen transformation. This transformation leads to a clear separation of the leading contribution from the relativistic corrections and removes higher order terms. The method is applied to the $2P_{1/2}$ and $2P_{3/2}$ states in atomic hydrogen. The results lead to new theoretical values for the Lamb shifts and the fine structure splitting.

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I. INTRODUCTION

The evaluation of the one-loop self-energy of a bound electron is a long standing problem in Quantum Electrodynamics. There are mainly two approaches. The first, developed by P. Mohr [1], relies on a multidimensional numerical integral involving a partial wave expansion of the electron propagator in the Coulomb field. This approach is particularly useful for heavy hydrogen-like ions. The second approach is based on an expansion of the electron self-energy in powers of $Z\,\alpha$,

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

where

$$\begin{aligned} F = {} & A_{40} + A_{41}\,\ln\left[(Z\alpha)^{-2}\right] + (Z\alpha)\,A_{50} + \\ & (Z\alpha)^2\left(A_{60} + A_{61}\,\ln\left[(Z\alpha)^{-2}\right] + A_{62}\,\ln^2\left[(Z\alpha)^{-2}\right] + o(Z\alpha)\right). \end{aligned} \tag{2}$$

The leading contribution as given by A_{41} has been originally calculated by Bethe in [2]. Many others have contributed to the evaluation of higher orders corrections, for details see an excellent review by Sapirstein and Yennie in [3]. A very general analytical method has been introduced by Erickson and Yennie in [4]. Erickson and Yennie were able to calculate all the coefficients in (2) except for A_{60}. The calculation of corrections of $(Z\,\alpha)^2$ relative order is a highly nontrivial task because the binding Coulomb field enters in a nonperturbative way, and there is no closed form expression for the Dirac-Coulomb propagator. Additionally, one-loop electron self-energy contributes to all orders in $Z\,\alpha$, and the separation of the $(Z\,\alpha)^2$ relative contribution involves hundreds of terms. A very efficient scheme of the calculation has been introduced in [5]. It was calculated there the A_{60} coefficient for the $1S$ and $2S$ states in hydrogen atom. The method was based on the division of the whole expression into two parts, E_L and E_H, by introducing an artificial parameter ϵ which is a cutoff in the photon frequency. In the high energy part E_H one expands the electron propagator in powers of the Coulomb field and uses Feynman gauge. In the low energy part one uses Coulomb gauge and applies a multipole expansion. The most important ingredient of this method is the expansion in the parameter ϵ after the expansion in $Z\,\alpha$ is performed (for details see the next section).

The calculation presented in this paper is a further development of this original method. In the low energy part we use a Foldy-Wouthuysen transformation. The transformation clearly identifies the leading order contribution and separates out all higher order terms. An additional advantage is that the nonrelativistic Schrödinger-Coulomb propagator can be used here. A closed-form expression of this propagator is known in coordinate and in momentum space (for details see [6]). This method is applied to the $2P_{1/2}$ and $2P_{3/2}$ states. All coefficients including A_{60} are obtained. We recover all the previously known results, and the new results for A_{60} are in agreement with those obtained from the extrapolation of P. Mohr's data. Our results are relevant for single electron, small Z systems (for example atomic hydrogen and He^+), which are currently investigated with very high precision. New theoretical values for the Lamb shift of the $2P_{1/2}$ and $2P_{3/2}$ states and the fine structure summarize our calculations.

II. THE ϵfw-METHOD

The self-interaction of the electron leads to a shift of the hydrogen energy levels. This shift at the one-loop level is given by

$$\delta E_{\rm SE} = ie^2 \int \frac{d^4k}{(2\pi)^4} D_{\mu\nu}(k) \langle\bar{\psi}|\gamma^\mu \frac{1}{\not{p} - \not{k} - m - \gamma^0 V}\gamma_\nu|\psi\rangle - \langle\bar{\psi}|\delta m|\psi\rangle, \tag{3}$$

where δm refers to the mass counter term, and it is understood that the photon propagator $D_{\mu\nu}$ has to be regularized to prevent ultraviolet divergences. $\bar{\psi}$ is the Dirac adjoint $\bar{\psi} = \psi^+\gamma^0$.

For the ω-integration ($k_0 \equiv \omega$), the lower part of the Feynman integration contour C_F is bent into the "right" half plane with $\Re(\omega) > 0$ and divided into two parts, the low energy contour C_L and the high energy contour C_H, see Fig. 1. The ϵ parameter corresponds to the cut-off K which was introduced by H. Bethe in his original evaluation of the low energy part of the electromagnetic shift of energy levels [2] (specifically, $K = \epsilon\, m$). The two contours are separated along the line $\Re(\omega) = \epsilon\, m$, where ϵ is some arbitrary dimensionless parameter, which we assume to be smaller than unity. This method of ω-integration has been described in detail in [5]. The two integrations lead to the high and low energy parts E_L and E_H, which are functions of the fine structure constant α and of the free parameter ϵ. Their sum, however,

$$\delta E_{\rm SE}(\alpha) = E_L(\alpha,\epsilon) + E_H(\alpha,\epsilon), \tag{4}$$

does not depend on ϵ. The most important step is the expansion in ϵ after the expansion in α. It eliminates, without actual calculations, many terms that vanish in the limit $\epsilon \to 0$. To be more specific, in expanding E_L and E_H in ϵ we keep only finite terms (the ϵ^0-coefficients) and the terms which diverge as $\epsilon \to 0$. The divergent terms cancel out in the sum, the finite terms contribute to the Lamb shift. This cancelation of the divergent terms is an important cross-check of the calculation. One may use different gauges of the photon propagator for the two parts, because the gauge-dependent term vanishes in the limit $\epsilon \to 0$. For convenience, we use the Feynman gauge for the high and the Coulomb gauge for the low energy part.

In this work, the treatment of the low energy part is largely simplified by the introduction of a Foldy-Wouthuysen (fw) transformation. It enables one to clearly separate out the leading (nonrelativistic dipole) term, which gives the $\alpha(Z\alpha)^4$-contribution, from the relativistic corrections, which give terms in $\alpha(Z\alpha)^6$. An additional advantage is the fact that all contributions to the low energy part can be evaluated using the nonrelativistic Schrödinger-Coulomb-Green's function, whose closed-form solution is well known [6]. Terms which contribute to the Lamb shift up to $\alpha(Z\alpha)^6$ can be readily identified, and each of these can be calculated independently. In the low energy part we may expand in the photon momentum k. The terms which contribute to the Lamb shift in the order of $\alpha(Z\alpha)^6$ correspond to the "non-relativistic dipole" term (involving the non-relativistic propagator and wave function), the "non-relativistic quadrupole" term and the "relativistic dipole" term (which involves the relativistic corrections to the wave function and the Dirac-Coulomb propagator). The terms of higher order in k vanishes in the limit $\epsilon \to 0$.

Calculations of the high-energy part are performed almost entirely with the computer algebra system *Mathematica* [7]. Because of the presence of an infrared cut-off, one can expand the Dirac-Coulomb propagator in powers of the Coulomb potential. A subsequent expansion of the propagator in electron momenta is also performed. This leads finally to the calculation of matrix elements of operators containing V and $\mathbf{p}$ on the P-states. Because P-wave functions vanish at the origin, all of the relevant matrix elements are finite up to the order of $(Z\alpha)^6$.

III. THE HIGH-ENERGY PART

In this part we use the Feynman gauge ($D_{\mu\nu}(k) = -g_{\mu\nu}/k^2$). and the Pauli-Villars regularization for the photon propagator

$$\frac{1}{k^2} \to \frac{1}{k^2} - \frac{1}{k^2 - M^2}, \tag{5}$$

so that the following expression remains to be evaluated:

$$E_H = -ie^2 \int_{C_H} \frac{d^4k}{(2\pi)^4} \left[\frac{1}{k^2} - \frac{1}{k^2 - M^2}\right] \langle\bar{\psi}|\gamma^\mu \frac{1}{\not{p} - \not{k} - m - \gamma^0 V}\gamma_\mu|\psi\rangle - \langle\bar{\psi}|\delta m|\psi\rangle \tag{6}$$

We start by calculating the matrix element

$$\tilde{P} = \langle \bar{\psi} | \gamma^\mu \frac{1}{\not p - \not k - m - \gamma^0 V} \gamma_\mu | \psi \rangle \tag{7}$$

up to the order of $(Z\alpha)^6$. The first step in the evaluation of $\tilde{P}$ is the expansion of the matrix

$$M = \gamma^\mu \frac{1}{\not p - \not k - m - \gamma^0 V} \gamma_\mu$$

in powers of the binding field. We denote the denominator of the free electron propagator by D ($D = \not p - \not k - m$). Realizing that the binding field $V = -(Z\alpha)^2\, m/\rho$ carries two powers of $(Z\alpha)$ (with $\rho = r/a_{\rm Bohr}$), we expand the matrix M up to V^3, which leads in turn to four matrices, denoted M_i,

$$\begin{aligned} M_0 &= \gamma^\mu \frac{1}{D} \gamma_\mu, \quad M_1 = \gamma^\mu \frac{1}{D} \gamma^0 V \frac{1}{D} \gamma_\mu, \quad M_2 = \gamma^\mu \frac{1}{D} \gamma^0 V \frac{1}{D} \gamma^0 V \frac{1}{D} \gamma_\mu, \\ M_3 &= \gamma^\mu \frac{1}{D} \gamma^0 V \frac{1}{D} \gamma^0 V \frac{1}{D} \gamma^0 V \frac{1}{D} \gamma_\mu. \end{aligned} \tag{8}$$

with $M = M_0 + M_1 + M_2 + M_3 + O((Z\alpha)^7)$. Defining $\tilde{P}_i = \langle \bar{\psi} | M_i | \psi \rangle$, we write the element $\tilde{P}$ as the sum

$$\tilde{P} = \tilde{P}_0 + \tilde{P}_1 + \tilde{P}_2 + \tilde{P}_3 + O((Z\alpha)^7). \tag{9}$$

This expansion corresponds to a division of the initial expression into 0-,1-,2- and 3-vertex parts. We then expand each of the matrices M_i into the standard 16 Γ matrices, which form a basis set of 4×4 matrices.

$$M_i = \sum_{\beta=0}^{15} c_{i,\beta}\, \Gamma^\beta \quad \text{where} \quad c_{i,\beta} = \frac{1}{4}\, \mathrm{Tr}(\Gamma_\beta M_i). \tag{10}$$

The expansion coefficients $c_{i,\beta}$ are rational functions of the binding field, the electron and photon energy and momenta. They can therefore be expanded in powers of α, leaving none of the electron momentum operators in the denominator. Next, we evaluate the matrix elements of these operators with the relativistic (Dirac) wave function ψ. It is a property of P states, which vanish at the origin, that up to order $(Z\alpha)^6$, all of the desired matrix elements are finite.

As an example, we describe here the evaluation of the three-vertex matrix element $\tilde{P}_3 = \langle \bar{\psi} | M_3 | \psi \rangle$. It takes on the same values for both $2P$ states. Expanding M_3 into the 16 Γ-matrices, we find that up to order $(Z\alpha)^6$, all expansion coefficients vanish except for the identity Id and γ^0-matrices. The expansion coefficients are explicitly

$$c_{3,\mathrm{Id}} = 16 V^3 \frac{k^2 - k^2\,\omega - 4\,\omega + 3\,\omega^2 + 2}{\left(k^2 + 2\,\omega - \omega^2\right)^4} \equiv b_{3,\mathrm{Id}} V^3, \tag{11}$$

where $k = |\mathbf{k}|$ and for simplicity $m = 1$, and

$$c_{3,\gamma^0} = 2\, V^3 \frac{k^4 - 8\,k^2 + 12\,k^2\,\omega + 16\,\omega - 6\,k^2\omega^2 - 12\,\omega^2 + 4\,\omega^3 - \omega^4 - 8}{\left(k^2 + 2\,\omega - \omega^2\right)^4} \equiv b_{3,\gamma^0} V^3. \tag{12}$$

So up to order $(Z\alpha)^6$, the two c-expansion coefficients are (except for their dependence on k and ω) functions of the binding field only. Thus, the matrix element $\tilde{P}_3$ is given by

$$\tilde{P}_3 = b_{3,\mathrm{Id}} \langle \bar{\psi} | V^3 | \psi \rangle + b_{3,\gamma^0} \langle \bar{\psi} | \gamma^0 V^3 | \psi \rangle. \tag{13}$$

The relevant matrix element of the wave function is

$$\langle \bar{\psi} | V^3 | \psi \rangle = \langle \bar{\psi} | \gamma^0 V^3 | \psi \rangle = -\frac{1}{24} (Z\alpha)^6\, m^3 + O((Z\alpha)^7). \tag{14}$$

where the first equality holds only in the order of $(Z\,\alpha)^6$. The above matrix elements take on the same values for the $2P_{1/2}$ and $2P_{3/2}$ states because the radial parts of both $2P$ states are the same in the non-relativistic limit.

For the other vertex parts, many more terms appear, and the matrix elements contribute in the lower order also. We give one example here, to be evaluated for the 1-vertex part,

$$\langle \bar{\psi} | \gamma^0 \mathbf{p} \cdot (V\, \mathbf{p})\, | \psi \rangle = -\frac{5}{48} (Z\alpha)^4\, m^3 - \frac{283}{1152}\, (Z\alpha)^6\, m^3 \quad \text{for } 2P_{1/2}. \tag{15}$$

and

$$\langle \bar{\psi} | \gamma^0 \mathbf{p} \cdot (V\,\mathbf{p})\,|\psi\rangle = -\frac{5}{48}\,(Z\alpha)^4\,m^3 - \frac{71}{1152}\,(Z\alpha)^6\;m^3 \quad \text{for } 2P_{3/2}. \tag{16}$$

For a more detailed review of the calculations see [8]. Having calculated $\tilde{P}$, we subtract the mass-counter-term before integrating with respect to k and ω. The final k and ω integration is performed in the following way. Those terms which appear to be ultraviolet divergent are regularized and integrated covariantly using Feynman parameter approach. The remaining terms are integrated with respect to k by residual integration and with respect to ω by changing the integration variable to

$$u = \frac{\sqrt{2\,m\,\omega - \omega^2} + i\omega}{\sqrt{2\,m\,\omega - \omega^2} - i\omega}. \tag{17}$$

This integration procedure is described in details in [5]. The final results for the high-energy-part are (for the definition of F see Eq. (1))

$$F_H(2P_{1/2}) = -\frac{1}{6} + (Z\alpha)^2\left[\frac{4177}{21600} - \frac{103}{180}\ln(2) - \frac{103}{180}\ln(\epsilon) - \frac{2}{9\epsilon}\right] \tag{18}$$

and

$$F_H(2P_{3/2}) = \frac{1}{12} + (Z\alpha)^2\left[\frac{6577}{21600} - \frac{29}{90}\ln(2) - \frac{29}{90}\ln(\epsilon) - \frac{2}{9\epsilon}\right]. \tag{19}$$

IV. THE LOW ENERGY PART

In this part we are dealing with low energy virtual photons, therefore we treat the binding field non-pertubatively. Choosing the Coulomb gauge for the photon propagator, one finds that only the spatial elements of this propagator contribute. The ω-integration along C_L is performed first, which leads to the following expression for E_L,

$$E_L = -e^2 \int_{|\mathbf{k}|<\epsilon} \frac{d^3k}{(2\pi)^3\,2|\mathbf{k}|}\,\delta^{T,ij}\langle\psi|\alpha^i e^{i\,\mathbf{k}\cdot\mathbf{r}}\frac{1}{H_D - (E_\psi - \omega)}\alpha^j e^{-i\,\mathbf{k}\cdot\mathbf{r}}|\psi\rangle \quad (\omega \equiv |\mathbf{k}|). \tag{20}$$

H_D denotes the Dirac-Coulomb-Hamiltonian, δ^T is the transverse delta function, and α^i refers to the Dirac α-matrices. In the matrix element

$$P^{ij} = \langle\psi|\alpha^i e^{i\,\mathbf{k}\cdot\mathbf{r}}\frac{1}{H_D - (E_\psi - \omega)}\alpha^j e^{-i\,\mathbf{k}\cdot\mathbf{r}}|\psi\rangle \tag{21}$$

we introduce a unitary Foldy-Wouthuysen transformation U,

$$P^{ij} = \langle U\psi|(U\,\alpha^i e^{i\,\mathbf{k}\cdot\mathbf{r}}\,U^+)\frac{1}{U\,(H_D - (E_\psi - \omega))\,U^+}(U\,\alpha^j e^{-i\,\mathbf{k}\cdot\mathbf{r}}\,U^+)|U\psi\rangle. \tag{22}$$

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

$$|U\psi\rangle = |\phi\rangle + |\delta\phi\rangle \quad \text{with} \quad \langle\phi|\delta\phi\rangle = 0, \tag{23}$$

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 Hamiltonian consists of even operators only. For the upper left 2×2 submatrix of this Hamiltonian, we have the result [9]

$$H_{\text{FW}} = U\,(H_D - (E_\psi - \omega))\,U^+ = m + H_S + \delta H, \tag{24}$$

where H_S refers to the Schrödinger Hamiltonian, and δH is is the relativistic correction,

$$\delta H = -\frac{(\mathbf{p})^4}{8\,m^3} + \frac{\pi\alpha}{2\,m^2}\,\delta(\mathbf{r}) + \frac{\alpha}{4\,m^2\,r^3}\,\boldsymbol{\sigma}\cdot\mathbf{L} \tag{25}$$

Now we turn to the calculation of the Foldy-Wouhuysen 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 $U\,\alpha^i\,e^{i\mathbf{k}\cdot\mathbf{r}}\,U^+$ in powers of $(Z\alpha)$. The result of the calculation is

$$\begin{aligned} U\,\alpha^i e^{i\mathbf{k}\cdot\mathbf{r}}\,U^+ = {} & \alpha^i\left(1 + i\,(\mathbf{k}\cdot\mathbf{r}) - \frac{1}{2}\,(\mathbf{k}\cdot\mathbf{r})^2\right) - \frac{1}{2\,m^2}p^i\,(\boldsymbol{\alpha}\cdot\boldsymbol{p}) \\ & +\gamma^0\,\frac{p^i}{m}\left(1 + i\,(\mathbf{k}\cdot\mathbf{r}) - \frac{1}{2}\,(\mathbf{k}\cdot\mathbf{r})^2\right) \\ & -\gamma^0\,\frac{1}{2\,m^3}p^i\mathbf{p}^2 - \frac{1}{2\,m^2}\,\frac{\alpha}{r^3}\,(\mathbf{r}\times\boldsymbol{\Sigma})^i \\ & +\frac{1}{2\,m}\gamma^0\,(\mathbf{k}\cdot\mathbf{r})\,(\mathbf{k}\times\boldsymbol{\Sigma})^i - \frac{i}{2\,m}\gamma^0\,(\mathbf{k}\times\boldsymbol{\Sigma})^i\,. \end{aligned} \tag{26}$$

In the limit $\epsilon \longrightarrow 0$ the odd operators in the above expression do not contribute to the self energy in $(Z\,\alpha)^2$ relative order, so one can neglect the odd operators. It can be shown easily that also the last term in the above expression (proportional to $\mathbf{k}\times\boldsymbol{\Sigma}$) does not contribute to the Lamb shift in $(Z\alpha)^2$ relative order for $\epsilon \longrightarrow 0$.

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 2×2 submatrix of Eq. (26), and we write $U\,\alpha^i\,e^{i\mathbf{k}\cdot\mathbf{r}}U^+$ as

$$\begin{aligned} U\,\alpha^i e^{i\mathbf{k}\cdot\mathbf{r}}\,U^+ \simeq {} & \frac{p^i}{m}\left(1 + i\,(\mathbf{k}\cdot\mathbf{r}) - \frac{1}{2}\,(\mathbf{k}\cdot\mathbf{r})^2\right) \\ & -\frac{1}{2\,m^3}p^i\mathbf{p}^2 - \frac{1}{2\,m^2}\,\frac{\alpha}{r^3}\,(\mathbf{r}\times\boldsymbol{\sigma})^i \\ & +\frac{1}{2\,m}\,(\mathbf{k}\cdot\mathbf{r})\,(\mathbf{k}\times\boldsymbol{\sigma})^i\,, \end{aligned} \tag{27}$$

This can be rewritten as

$$U\,\alpha^i\,e^{i\mathbf{k}\cdot\mathbf{r}}\,U^+ = \frac{p^i}{m}\,e^{i\mathbf{k}\cdot\mathbf{r}} + \delta y^i, \tag{28}$$

where δy^i is of order $(Z\alpha)^3$. It is understood that the term $\frac{p^i}{m}\,e^{i\mathbf{k}\cdot\mathbf{r}}$ is also expanded up to the order $(Z\alpha)^3$. Denoting by E the Schrödinger energy ($E = -(Z\alpha)^2\,m/8$ for 2P states) and by δE the first relativistic correction to E, we can thus write the matrix element P^{ij} as

$$P^{ij} = \langle\phi + \delta\phi|\left[\frac{p^i}{m}\,e^{i\mathbf{k}\cdot\mathbf{r}} + \delta y^i\right]\,\frac{1}{H_S - (E-\omega) + \delta H - \delta E}\,\left[\frac{p^j}{m}\,e^{-i\mathbf{k}\cdot\mathbf{r}} + \delta y^j\right]|\phi + \delta\phi\rangle. \tag{29}$$

In this expression, the leading term and the (first) relativistic corrections can be readily identified. Spurious lower order terms are not present in Eq. (29). By expansion of the denominator $H_S - (E-\omega) + \delta H - \delta E$ in powers of α, the whole expression can be written in a form which involves only the Schrödinger-Coulomb-Green's function

$$G(E-\omega) = \frac{1}{H_S - (E-\omega)}, \tag{30}$$

whose closed-form expression in coordinate space is given in Eq. (33). We now define the dimensionless quantity

$$P = \frac{m}{2}\,\delta^{T,ij}\,P^{ij}. \tag{31}$$

Using the symmetry of the P-wave functions and Eq. (29), we easily see that P can be written, up to $(Z\alpha)^2$, as the sum of the contributions (32, 39, 40, 41, 42, 43). The leading contribution (the "non-relativistic dipole") is given by

$$P_{\rm nd} = \frac{1}{3m}\,\langle\phi|p^i\,\frac{1}{H_S - (E-\omega)}\,p^i|\phi\rangle. \tag{32}$$

The evaluation of this matrix element is described here as an example. For the Schrödinger-Coulomb propagator, we use the following coordinate-space representation [6],

$$G(\mathbf{r}_1, \mathbf{r}_2, E-\omega) = \sum_{l,m} g_l(\mathbf{r}_1, \mathbf{r}_2, \nu)\, Y_{l,m}\,(\hat{\mathbf{r}}_1)\; Y^*_{l,m}\,(\hat{\mathbf{r}}_2)\,, \tag{33}$$

with $E - \omega \equiv -\alpha^2\, m/(2\nu^2)$.

$$g_l(r_1, r_2, \nu) = \frac{4m}{a\nu}\left(\frac{2r_1}{a\nu}\right)^l \left(\frac{2r_1}{a\nu}\right)^l e^{-(r_1+r_2)/(a\nu)} \sum_{k=0}^{\infty} \frac{L_k^{2l+1}\left(\frac{2r_1}{a\nu}\right)\, L_k^{2l+1}\left(\frac{2r_2}{a\nu}\right)}{(k+1)_{2l+1}\,(l+1+k-\nu)}, \tag{34}$$

where $a = a_{\rm Bohr} = 1/(\alpha m)$, and $(k)_c$ is the Pochhammer symbol. The evaluation of eq. (32) proceeds in the following steps: The angular integration is performed first. Secondly, the remaining integrals over r_1 and r_2 are evaluated using the formula (see e.g. [10]),

$$\int_0^\infty dt\, e^{-st}\, t^{\gamma-1}\, L_n^\mu(t) = \frac{\Gamma(\gamma)\Gamma(n+\mu+1)}{n!\,\Gamma(\mu+1)} s^{-\gamma}\; {}_2F_1\Big(-n, \gamma, 1+\mu; \frac{1}{s}\Big)\,. \tag{35}$$

The following formula is useful for carrying out the summation with respect to k [11],

$$\sum_{n=0}^{\infty} \frac{\Gamma(n+\lambda)}{n!}\, s^n\; {}_2F_1(-n, b; c; z) = \Gamma(\lambda)\,(1-s)^{-\lambda}\; {}_2F_1\Big(\lambda, b; c; -\frac{s\,z}{1-s}\Big). \tag{36}$$

The summations lead to hypergeometric functions in the result,

$$\begin{aligned} P_{\rm nd}(t) = {} & \frac{2t^2\left(3 - 6\,t - 3\,t^2 + 12\,t^3 + 29\,t^4 + 122\,t^5 - 413\,t^6\right)}{9\,(1-t)^5\,(1+t)^3} + \\ & \frac{256\,t^7\,(-3 + 11\,t^2)}{9\,(1-t)^5\,(1+t)^5}\; {}_2F_1\left(1, -2t; 1-2t; \left(\frac{1-t}{1+t}\right)^2\right) \end{aligned} \tag{37}$$

where

$$t \equiv \frac{\sqrt{-2\,m\,E}}{\sqrt{-2\,m\,(E-\omega)}} = \frac{1}{2}\nu. \tag{38}$$

In this expression the terms that gives divergent in ϵ terms are separated out of the hypergeometric function, so the could be easily integrated out. The other contributions to P (for definition fo P see eq. (31)) are

- the non-relativistic quadrupole,

$$P_{\rm nq} = \frac{1}{3m}\,\langle\phi|p^i\, e^{i\mathbf{k}\cdot\mathbf{r}}\, \frac{1}{H_S - (E-\omega)}\, p^i\, e^{-i\mathbf{k}\cdot\mathbf{r}}|\phi\rangle - P_{\rm nd}\,, \tag{39}$$

- the corrections to the current α^i from the Foldy-Wouthuysen transformation,

$$P_{\delta y} = \delta^{T,ij}\,\langle\phi|\delta y^i\, \frac{1}{H_S - (E-\omega)}\, p^j\, e^{-i\mathbf{k}\cdot\mathbf{r}}|\phi\rangle, \tag{40}$$

- the contribution due to the relativistic Hamiltonian,

$$P_{\delta H} = -\frac{1}{3m}\,\langle\phi|p^i\, \frac{1}{H_S - (E-\omega)}\, \delta H\, \frac{1}{H_S - (E-\omega)}\, p^i|\phi\rangle, \tag{41}$$

- the contribution due to the relativistic correction to the energy,

$$P_{\delta E} = \frac{1}{3m}\,\langle\phi|p^i\, \frac{1}{H_S - (E-\omega)}\, \delta E\, \frac{1}{H_S - (E-\omega)}\, p^i|\phi\rangle, \tag{42}$$

- and due to the relativistic correction to the wave function,

$$P_{\delta\phi} = \frac{2}{3m}\,\langle\delta\phi|p^i\,\frac{1}{H_S-(E-\omega)}\,p^i|\phi\rangle. \tag{43}$$

For almost all of the matrix elements we use the coordinate-space representation of the Schrödinger-Coulomb propagator given in Eq. (33). There are two exceptions: For the non-relativististic quadrupole, we use Schwinger's momentum space representation and carry out the calculation in momentum space. A rather involved contribution is

$$P_{\delta H} = -\frac{1}{3m}\,\langle\phi|p^i\,G(E-\omega)\,\left[-\frac{(\mathbf{p})^4}{8\,m^3}+\frac{\pi\alpha}{2\,m^2}\,\delta(\mathbf{r})+\frac{\alpha}{4\,m^2\,r^3}\,\boldsymbol{\sigma}\cdot\mathbf{L}\right]\,G(E-\omega)\,p^i|\phi\rangle. \tag{44}$$

where $G(E-\omega)=1/(H_S-(E-\omega))$. The form of δH implies a natural separation of $P_{\delta H}$ into three terms,

$$P_{\delta H} = P_{p^4} + P_\delta + P_{L\cdot S}. \tag{45}$$

For P_δ,

$$P_\delta = -\frac{1}{3m}\,\langle\phi|p^i\,G(E-\omega)\,\left[\frac{\pi\alpha}{2\,m^2}\,\delta(\mathbf{r})\right]\,G(E-\omega)\,p^i|\phi\rangle, \tag{46}$$

which involves the zitterbewegungs-term (proportional to the δ-function), we use a coordinate-space representation of the Schrödinger-Coulomb propagator involving Whittaker functions (this representation is also to be found in [6]). The result for $P_\delta(t)$ is

$$P_\delta(t) = -\frac{\alpha^2}{27}\,\frac{t^4\,\left(-3+4\,t+7\,t^2-8\,t\,F_2(t)\right)^2}{(t^2-1)^4} \tag{47}$$

where

$$F_2(t) = {}_2F_1\left(1,-2\,t,1-2\,t,\frac{t-1}{t+1}\right). \tag{48}$$

Both terms P_{p^4} and $P_{L\cdot S}$,

$$P_{p^4} = -\frac{1}{3m}\,\langle\phi|p^i\,G(E-\omega)\,\left[-\frac{(\mathbf{p})^4}{8\,m^3}\right]\,G(E-\omega)\,p^i|\phi\rangle \tag{49}$$

$$P_{L\cdot S} = -\frac{1}{3m}\,\langle\phi|p^i\,G(E-\omega)\,\left[\frac{\alpha}{4\,m^2\,r^3}\,\boldsymbol{\sigma}\cdot\mathbf{L}\right]\,G(E-\omega)\,p^i|\phi\rangle, \tag{50}$$

involve two propagators $G(E-\omega)$. We use the Schrödinger equation and the identity

$$[H_S-(E-\omega),\,\frac{1}{r}\,\frac{\partial}{\partial r}\,r] = \frac{\mathbf{L}^2}{m\,r^3}-\frac{Z\alpha}{r^2}. \tag{51}$$

to rewrite them to the form that contain only one propagator with modified parameters. Namely, to the desired order in $(Z\alpha)$, the expression with two propagators can be replaced by an expression with just one propagator, in which an $(Z\alpha)^2$-correction is added to the angular momentum parameter l or to the fine structure constant α in the radial part of the Schrödinger-Coulomb propagator as given in Eq. (33). For the P_{p^4} and $P_{L\cdot S}$ contributions, many more terms appear in the calculation, and derivatives of the hypergeometric functions with respect to parameters have to be evaluated. The result consists of terms involving elementary functions and hypergeometric functions only, and other terms which involve slightly more complex functions. Some of the summations give rise to the Lerch transcendent Φ. Summations of the form

$$\sum_{k=0}^{\infty} k^n\,\xi^k\,\frac{\partial}{\partial b}\,{}_2F_1(-k,b,c,z). \tag{52}$$

can be evaluated with the help of Eq. (36), for more details see [8]. Although we do not describe the calculations in detail, we stress that the summation with respect to the k-index is the decisive point in the calculation. In general, a sensible use of contiguous relations is necessary to simplify the result of any of the summations. Symbolic procedures were written to accomplish this. Through the compartmentalization of the calculation achieved by the Foldy-Wouthuysen transformation, it has been possible to keep the average length of intermediate expressions below 1000 terms.

The contribution to E_L due to the $\delta E_{\rm SE}$ is given by

$$E_L = -\frac{2\,\alpha}{\pi\, m} \int_0^\epsilon d\omega\, \omega\, P(\omega). \tag{53}$$

Changing the integration variable to t, we have

$$F = -\frac{1}{2} \int_{t_\epsilon}^1 dt\, \frac{1-t^2}{t^5}\, P(t). \tag{54}$$

The P-terms are integrated with respect to t by the following procedure. Terms which give a divergence for $\epsilon \to 0$ are extracted from the integrand. The extraction can be achieved by a suitable expansion in the argument of the hypergeometric function(s) which appear in $P(t)$. The extracted terms consist of elementary functions of t only, so they can be integrated analytically. After integration, the terms are first expanded in $(Z\alpha)$ up to $(Z\alpha)^2$, then in ϵ up to ϵ^0. The remaining part, which involves hypergeometric functions, is integrated numerically with respect to t by the Gaussian method.

The t-integration leads to F-terms which we name according to the P-terms $F_{\rm nd}$, $F_{\rm nq}$, $F_{\delta y}$, $F_{\delta H}$, $F_{\delta E}$ and $F_{\delta\phi}$. The $F_{\rm nd}$-term, which is the same for both $2P$-states, is given by

$$F_{\rm nd} = -\frac{4}{3} \ln k_0(2P) + \frac{2}{9}\, \frac{(Z\alpha)^2}{\epsilon}. \tag{55}$$

We have recovered the first 9 digits of the Bethe logarithm with our (Gaussian) integration procedure (the value for the Bethe logarithm given in [3] is $\ln k_0(2P) = -0.0300167089(3)$). The $F_{\rm nd}$-term has, for $\epsilon \to 0$, a divergence of $+2/9 (Z\alpha)^2/\epsilon$, which cancels the corresponding divergence in the high energy part. All other F-terms produce logarithmic divergences in $(Z\alpha)^2 \ln(\epsilon)$ (see Table I). The results for the low-energy parts of the $2P$-states are

$$F_L(2P_{1/2}) = -\frac{4}{3}\, \ln k_0(2P) + (Z\alpha)^2 \left[-0.79565(1) + \frac{103}{180} \ln\left((Z\alpha)^{-2}\right) + \frac{103}{180} \ln(\epsilon) + \frac{2}{9\,\epsilon} \right] \tag{56}$$

and

$$F_L(2P_{3/2}) = -\frac{4}{3}\, \ln k_0(2P) + (Z\alpha)^2 \left[-0.58452(1) + \frac{29}{90} \ln\left((Z\alpha)^{-2}\right) + \frac{29}{90} \ln(\epsilon) + \frac{2}{9\,\epsilon} \right]. \tag{57}$$

The divergence in $1/\epsilon$ and in $\ln(\epsilon)$ cancels out when the low- and high-energy-parts are added. The results for the F-factors (sum of low-energy-part and high-energy-part) are:

$$F(2P_{1/2}) = -\frac{1}{12} - \frac{4}{3}\, \ln k_0(2P) + (Z\alpha)^2 \left[-0.99891(1) + \frac{103}{180} \ln\left((Z\alpha)^{-2}\right) \right] \tag{58}$$

for the $2P_{1/2}$-state and

$$F(2P_{3/2}) = \frac{1}{6} - \frac{4}{3}\, \ln k_0(2P) + (Z\alpha)^2 \left[-0.50337(1) + \frac{29}{90} \ln\left((Z\alpha)^{-2}\right) \right] \tag{59}$$

for the $2P_{3/2}$-state. The A_{60} coefficients are given by

$$A_{60}(2P_{1/2}) = -0.99891(1) \tag{60}$$

and

$$A_{60}(2P_{3/2}) = -0.50337(1). \tag{61}$$

The last digit is the cumulated inaccuracy of the numerical integrations. The values for the A_{40} and A_{61} coefficients are in agreement with known results [3].

These results can be compared to those obtained by P. Mohr [13] by extrapolation of his numerical data for higher Z,

$$G_{SE}(2) = -0.96(4), \quad G_{SE}(1) = -0.98(4) \quad \text{for } 2P_{1/2}, \tag{62}$$

and

$$G_{SE}(2) = -0.46(2), \quad G_{SE}(1) = -0.48(2) \quad \text{for } 2P_{3/2}, \tag{63}$$

where the function $G_{\rm SE}(Z)$ for $2P$-states is defined by

$$F = A_{40} + (Z\alpha)^2 \left[A_{61} \ln\left((Z\alpha)^{-2}\right) + G_{\rm SE}(Z)\right] . \tag{64}$$

Because $G_{\rm SE}(Z = 0) = A_{60}$, these values are clearly in very good agreement with the results of our analytical calculation. Using P. Mohr's numerical data [12], we have obtained the following estimates for higher order terms summarized by $G_{\rm SE,7}$

$$F = A_{40} + (Z\alpha)^2 \left[A_{60} + A_{61} \ln\left((Z\alpha)^{-2}\right) + (Z\alpha)\, G_{\rm SE,7}(Z)\right] , \tag{65}$$

$$G_{\rm SE,7}(2P_{1/2}, Z=1) = 3.1(5) \quad \text{and} \quad G_{\rm SE,7}(2P_{3/2}, Z=1) = 2.3(5). \tag{66}$$

One of the most important aspects of rather lengthy calculations such as those presented here is to avoid errors. The result has been checked in many ways. Except for checking the values of the terms divergent in ϵ, it was also checked the value of each P-contribution as $\omega \longrightarrow 0$. It can be shown easily that the sum of all contributions to the matrix element P in the low-energy part must vanish in the limit $\omega \longrightarrow 0$. Care must be taken when checking the sum, because after the Foldy-Wouthuysen transformation, hidden terms are introduced which do not contribute to the Lamb shift, but contribute in the limit $\omega \longrightarrow 0$. The hidden terms originate from the odd operators in Eq. (26). Taking into account these terms, the sum vanishes for both states.

V. OTHER CONTRIBUTIONS TO THE LAMB SHIFT

For the Lamb shift $\mathcal{L}$, we use the implicit definition

$$E = m_r\,[f(n,j) - 1] - \frac{m_r^2}{2(m + m_N)}\,[f(n,j) - 1]^2 + \mathcal{L} + E_{\rm hfs}, \tag{67}$$

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.

For the final evaluation of the Lamb shift the following contributions are added:

1. One-loop self energy. The coefficients are presented in this work. For the determination of the Lamb shift the reduced mass dependence of the terms has to be restored. The relevant formulae are given in [3]. For example, the A_{60} have a reduced mass dependence of $(m_r/m)^3$. We use Eq. (66) to estimate the theoretical uncertainty from the one–loop contribution.

2. Vacuum polarization correction. It enters for P-states in higher order (for the formulae see [3], p. 570).

3. Two-loop contributions due to the anomalous magnetic moment [15]. It is given in analogy to the one-loop contribution as

$$\delta E_{2-\rm loop} = \left(\frac{\alpha}{\pi}\right)^2 m\,\frac{(Z\alpha)^4}{n^3}\,[B_{40} + \ldots] \tag{68}$$

   where the B-coefficients are labeled in analogy to the A-coefficients for the one-loop self energy. The B_{40} coefficient is due to the anomalous magnetic moment of the electron. It is given as

$$B_{40} = \frac{C_{jl}}{2(2l+1)}\left[\frac{197}{72} + \frac{\pi^2}{6} - \pi^2 \ln 2 + \frac{3}{2}\zeta(3)\right]\left(\frac{m_r}{m}\right)^2, \tag{69}$$

   where $C_{jl} = 2(j - l)/(j + 1/2)$.

4. Two loop contributions in higher order. Recently, the logarithmic term

$$B_{62} = \left[\frac{4}{27}\,\frac{n^2-1}{n^2}\,\ln^2\left((Z\alpha)^{-2}\right)\right]\left(\frac{m_r}{m}\right)^3, \tag{70}$$

has been calculated in [14]. The B_{62} term, which is enlarged by the logarithm, probably dominates the contributions to the two-loop self energy in higher order. So the result may also be used to estimate the theoretical uncertainty of the two–loop contribution, coming mainly from the unknown B_{61} coefficient. It is taken to be half the contribution from B_{62}.

5. Three-loop self energy as given by the anomalous magnetic moment [15].

$$\delta E_{3-\mathrm{loop}} = \left(\frac{\alpha}{\pi}\right)^3 m\,\frac{(Z\alpha)^4}{n^3}\left[C_{40}+\ldots\right] \tag{71}$$

where

$$C_{40} = \left[2\,\frac{C_{jl}}{2(2\,l+1)}\,1.17611(1)\right]\left(\frac{m_r}{m}\right)^2. \tag{72}$$

6. The additional reduced mass dependence of order $(m_r/m_N)^2\,(Z\alpha)^4$ [3], which we will refer to as the $(Z\alpha)^4$ recoil contribution,

$$\delta E_{\mathrm{rec},4} = \frac{(Z\alpha)^4}{2\,n^3}\,\frac{m_r^3}{m_N^2}\left(\frac{1}{j+1/2}-\frac{1}{l+1/2}\right)(1-\delta_{l0})\,, \tag{73}$$

7. The Salpeter correction (relativistic recoil) in order $(Z\alpha)^5$ as given in [3]. The formula is for P-states

$$\delta E_{\mathrm{rec},5} = \frac{m_r^3}{m\,m_N}\,\frac{(Z\alpha)^5}{\pi\,n^3}\left(-\frac{8}{3}\ln k_0(n)-\frac{7}{3}\,\frac{1}{l(l+1)(2\,l+1)}\right). \tag{74}$$

8. Relativistic recoil corrections in the order of $(Z\alpha)^6\,m_r/m_N$,

$$\delta E_{\mathrm{rec},6} = \frac{m^2}{m_N}\,(Z\alpha)^6\left[\frac{1}{2}\langle\phi|\frac{\mathbf{L}^2}{r^4}|\phi\rangle\right]. \tag{75}$$

The formula for P-states has been first calculated in [16]. This general form has been obtained by us.

The above contributions are listed in table II for the $2P$ states.

VI. RESULTS AND CONCLUSIONS

The new theoretical values for the Lamb shifts of the $2P_{1/2}$ and $2P_{3/2}$ states are

$$\mathcal{L}(2P_{1/2}) = -12835.99(8)\,\mathrm{kHz} \tag{76}$$

and

$$\mathcal{L}(2P_{3/2}) = 12517.46(8)\,\mathrm{kHz}. \tag{77}$$

¿From the values of the $2P$ Lamb shifts, the fine structure can be determined. It turns out that the limiting factor in the uncertatinty is the experimental value of the fine structure constant α. Using a value of [17] (1987)

$$\alpha^{-1} = 137.0359895(61) \quad (44\ \mathrm{ppb}), \tag{78}$$

the fine structure can be determined as

$$E(2P_{3/2}) - E(2P_{1/2}) = 10969043(1)\,\mathrm{kHz}. \tag{79}$$

With the most recent and most precise value of α available [18] (1995),

$$\alpha^{-1} = 137.03599944(57) \quad (4.2\ \mathrm{ppb}), \tag{80}$$

we obtain a value of

$$E(2P_{3/2}) - E(2P_{1/2}) = 10969041.52(9)(8)\,\mathrm{kHz}, \tag{81}$$

where the first error originates from the uncertainty in α and the second from the uncertainty in the Lamb shift difference. Our result for the fine structure disagrees with that used by Hagley and Pipkin in [19] for the determination of $L(2S - 2P_{1/2})$. Therefore their result of $L(2S - 2P_{1/2}) = 1057839(12)$ is to be modified and according to our calculation it should be

$$L(2S - 2P_{1/2}) = 1057842(12)\,\mathrm{kHz}. \tag{82}$$

Precise theoretical predictions for P-states could be used to compare two different kind of measurements of Lamb shifts in the hydrogen. One is the classic $2S_{1/2}$-$2P_{1/2}$ Lamb shift measured by several groups [20], [21], [19], and the second is the combined Lamb shift $\mathcal{L}(4S - 2S) - \frac{1}{4}\mathcal{L}(2S - 1S)$ as measured by the Hänsch group (for a review see [22]). The experimental value of 2S Lamb shift can be extracted from E($2S$-$2P_{1/2}$) having the precise value for $2P_{1/2}$ Lamb shift, and can also be determined from the combined Lamb shift through the formula

$$\mathcal{L}(2S) = \frac{8}{7}\left[\left(\mathcal{L}(4S) - \frac{5}{4}\mathcal{L}(2S) + \mathcal{L}(1S)\right)_{\mathrm{exp}} - \left(\mathcal{L}(4S) - \frac{17}{8}\mathcal{L}(2S) + \mathcal{L}(1S)\right)_{\mathrm{theo}}\right], \tag{83}$$

where the subscript *exp* denotes experimental, and the subscript *theo* denotes theoretical values. This *theo* combination has the property that terms scaling $1/n^3$ cancel out, which means that almost all QED effects do not contribute, and therefore the quantity can be precisely determined. Such a comparison of completely different experimental techniques is an interesting and valuable test of high precision experiments.

The method of calculation presented in this paper could be directly applied for the evaluation of Lamb shifts and the fine structure in two electron systems, for example in helium or positronium. It was a purpose of this method to use only a Schrödinger-Coulomb propagator, and relativistic effects are incorporated through the Foldy-Wouthuysen transformation. This method clearly separates out the lower and the higher order terms, and expresses the energy shift through the matrix elements of nonrelativistic operators.

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contribution	$2P_{1/2}$	$2P_{3/2}$
$F_{\rm nq}$	$-1.201150(1) + 49/90\ln\left(\epsilon/(Z\alpha)^2\right)$	$-1.201150(1) + 49/90\ln\left(\epsilon/(Z\alpha)^2\right)$
$F_{\delta y}$	$0.791493(1) - 2/9\ln\left(\epsilon/(Z\alpha)^2\right)$	$0.531475(1) - 2/9\ln\left(\epsilon/(Z\alpha)^2\right)$
$F_{\delta H}$	$0.322389(1) - 47/288\ln\left(\epsilon/(Z\alpha)^2\right)$	$0.293749(1) - 35/288\ln\left(\epsilon/(Z\alpha)^2\right)$
$F_{\delta E}$	$0.040095(1) + 5/96\ln\left(\epsilon/(Z\alpha)^2\right)$	$0.008019(1) + 1/96\ln\left(\epsilon/(Z\alpha)^2\right)$
$F_{\delta\phi}$	$-0.748478(1) + 13/36\ln\left(\epsilon/(Z\alpha)^2\right)$	$-0.216612(1) + 1/96\ln\left(\epsilon/(Z\alpha)^2\right)$
sum	$-0.79565(1) + 103/180\ln\left(\epsilon/(Z\alpha)^2\right)$	$-0.58452(1) + 29/90\ln\left(\epsilon/(Z\alpha)^2\right)$

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

contribution	$2P_{1/2}$ in kHz	$2P_{3/2}$ in kHz
one-loop self-energy	$-12846.92(2)$	$12547.95(2)$
two-loop self-energy	$25.98(7)$	$-12.79(7)$
three-loop self-energy	-0.21	0.10
vacuum polarization	-0.35	-0.08
$(Z\alpha)^4$ recoil	2.16	-1.08
$(Z\alpha)^5$ recoil	-17.08	-17.08
$(Z\alpha)^6$ recoil	0.42	0.42
sum for $2P_{1/2}$	$-12835.99(8)$	$12517.46(8)$

TABLE II. Contributions to the Lamb shift in kHz for the $2P_{1/2}$ and $2P_{3/2}$ states. Estimates of the contributions of uncalculated higher order terms are given in the text. Where no uncertainties are specified, they are negligible at the current level of precision.

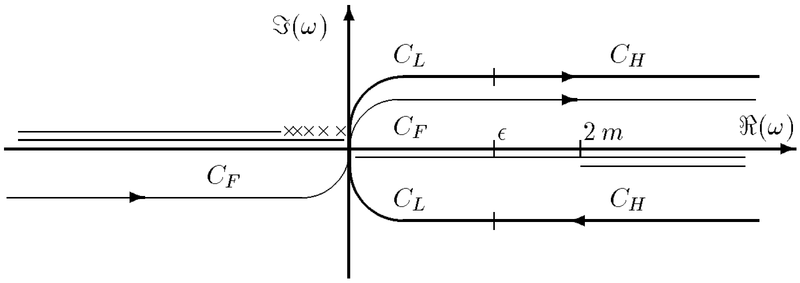

FIG. 1. The ω-integration contour used in the calculation. Bending the Feynman contour C_F in the specified way leads to the high and low energy parts C_H and C_L. Lines directly below and above the real axis denote branch cuts from the photon and electron propagator. Crosses denote poles originating from the discrete spectrum of the electron propagator.