Computationally efficient analytic representation of relativistic transition matrix elements in the Lamb shift calculations for hydrogenic atoms

J. SEKE
Institut für Theoretische Physik, Technische Universität Wien
Wiedner Hauptstrasse 8-10/136, A-1040 Wien, Austria
jseke@tph.tuwien.ac.at

A.V. SOLDATOV
Department of Mechanics, V.A. Steklov Mathematical Institute of the Russian Academy of Sciences,
8, Gubkina str., Moscow, 119991, Russia
soldatov@mi.ras.ru

M. POLAK
Institut für Theoretische Physik, Technische Universität Wien
Wiedner Hauptstrasse 8-10/136, A-1040 Wien, Austria
mpolak@tph.tuwien.ac.at

G. ADAM
Institut für Theoretische Physik, Technische Universität Wien
Wiedner Hauptstrasse 8-10/136, A-1040 Wien, Austria
gadam@tph.tuwien.ac.at

By using the plane-wave expansion for the electromagnetic-field vector potential, transition matrix elements between the relativistic bound and unbound states of hydrogenic atoms were expressed explicitly in terms of finite series made of hypergeometric functions of the type $2F_1$. This general formulae representation for the above mentioned matrix elements in terms of hypergeometric functions proved very convenient for direct numerical calculation of their contributions to the Lamb shift in hydrogenic atoms. All integrations over the angular variables of the wave vector $\mathbf{k}$ can be carried out analytically with the exception of only one principal-value integration over the absolute value $|\mathbf{k}|$ is left to be carried out numerically. Conciseness and reliance on functions already built-in to the standard computational packages like Mathematica renders this approach highly favorable for programming of computationally efficient algorithms.

PACS: 32.90.+a; 11.10.St; 03.70.+k; 31.30.Jv

Keywords: hydrogenic atom; transition matrix element; Fourier transform; Dirac relativistic wave functions; relativistic eigenfunctions; Lamb shift; hypergeometric function; renormalization
1. Introduction

The primary aim of the ongoing research is to develop a numerical calculation technique allowing for practical calculation of renormalized expression for the Lamb shift in hydrogenic atoms obtained by consistent renormalization in QED developed by Seke. Employing this method, the usage of the plane vector expansion for the vector potential is a preferable choice. In the context of this ultimate goal, plain-style Lamb-shift calculation undertaken in the present study, besides being of value in itself, also provides a good testing ground for the techniques of analytical and numerical evaluation of transition matrix elements between bound-bound and bound-unbound eigenstates of hydrogenic atoms elaborated so far just for the case of the plane-wave expansion for the electromagnetic-field vector potential.

In the second quantization, the relativistic Dirac Hamiltonian for the interaction between the atom and the radiation field reads as

\[
H_I = \int d^3r H_I(r) = -e \int d^3r j^\mu(r) A_\mu(r)
\]

(1)

\[
j^\mu(r) = \frac{1}{2} [\bar{\psi}(r), \gamma^\mu \psi(r)]
\]

(2)

with the vector potential \( A_\mu(r) \) in the covariant quantization (Feynman gauge):

\[
A_\mu(r) = \frac{1}{\sqrt{2(2\pi)^3}} \sum_{\lambda=0}^{3} \int d^3k(k)^{-1/2} [a^\lambda_{\mu}^-(k) \gamma^\lambda \psi(k) e^{-ikr} + a^\lambda_{\mu}^+(k) \gamma^\lambda \psi(k) e^{ikr}].
\]

(3)

Here, \( \gamma^\mu \) are the gamma matrices, \( a^\lambda_{\mu}^\pm(k) \), \( \lambda = 0, 1, 2, 3 \) are the photon creation and annihilation operators for the mode \( k, \lambda \), and \( \psi^\eta(x) \) and \( \overline{\psi}^\eta(x) = [\psi^\eta(x)]^+ \gamma_0 \) are the fermion field and its Dirac adjoint:

\[
\psi(x) = \sum_s c^-_s \psi_s(x) + \sum_{s'} d^+_s \psi_{s'}(x).
\]

(4)

Here, \( s \) stands for both the set of quantum numbers of the discrete and that of the continuous spectrum, while \( s' \) stands for the set of quantum numbers of the continuous spectrum only, \( c^-_s \) and \( d^+_s \) are the electron and positron creation and annihilation operators with the corresponding Dirac eigenfunctions \( \psi_s \) and \( \psi_{s'} \). This yields the following transition matrix elements

\[
M_{s_1,s_2}(k,\lambda) = M(s_1,s_2,k,\lambda) = \langle s_1; vac | H_I | s_2, k, \lambda \rangle = -e \int d^3r \langle s_1 | j^\mu(r) | s_2 \rangle \langle vac | A_\mu(r) | k, \lambda \rangle.
\]

(5)

Here, for the discrete spectrum, the discrete-spectrum eigenstates \( |s_1\rangle \) and \( |s_2\rangle \) of the hydrogen-like atom are denoted by the quantum numbers \( s_i = \{n'_i, \kappa_i, m_i\}; i = 1, 2, \) where \( n'_i \) is the radial quantum number and \( m_i \) is the magnetic quantum number. The eigenstates belonging to the continuous spectrum are denoted by the quantum...
numbers \( s_i = \{p_i, \kappa_i, m_i\}; \ i = 1, 2 \), where \( n'_i \) is the momentum quantum number. The inner quantum number \( j \) and orbital quantum number \( l \) are determined by strictly negative (for the eigenstates of the first type) or positive (for the eigenstates of the second type) integer quantum number \( \kappa \) through the relations: \( j = |\kappa| - 1/2 \) and \( l = \text{sign}(\kappa)(\kappa + 1/2) - 1/2 \), respectively. The notation \( |\text{vac}\rangle \) stands for photonic vacuum state.

Since the case of the bound-bound transition matrix elements has been thoroughly investigated in \(^5\), here we will concentrate mostly on the explicit calculation of contributions to the Lamb-shift stemming from relativistic transition matrix elements between bound and unbound eigenstates. The one-electron relativistic four-component spinor for the bound eigenstates of hydrogen-like atoms will be used in the form given by Bethe and Salpeter \(^7\) and by Rose \(^8\) for the unbound eigenstates. For reader’s convenience, we will also follow notations of these works \(^7\), \(^8\). From here on the natural units with Gaussian units will be used: \( \hbar = c = 1 \), \( e^2 = \alpha \).

2. Transition matrix element contribution to the Lamb shift

The starting point of the present study is the conventional expression for the hydrogenic atom Lamb shift in the second order, resulting from Eqs.\( (2-3) \),

\[
\Delta E_{s_1} = -\text{Re} \left[ \frac{i\alpha}{4\pi^3} \int d^4k \frac{1}{k_0^2 - k^2 + i\varepsilon} \langle s_1| e^{ikr}\alpha^\mu \frac{1}{E_{s_1} - \hat{H}_D - k^0 + i\eta} \alpha_\mu e^{-ikr}|s_1\rangle (6) \right]
\]

Here \( \hat{H}_D \) is the Dirac Hamiltonian of the hydrogenic atom, \( E_{s_1} \) is an eigenvalue belonging to the bound hydrogenic eigenstate \( |s_1\rangle \), \( \langle \bar{s}_1| \) is the corresponding Dirac conjugate eigenstate and the \( \alpha \)-matrices are defined as \( \alpha^\mu = \gamma^0\gamma^\mu, \alpha^0 = I \). Inserting a complete base of hydrogenic atom eigenstates \( \hat{I} = \sum s_2 |s_2\rangle\langle s_2| \) wherever necessary, further simplification of Eq.\( (6) \), better suited for numerical calculations to follow, is straightforward

\[
\Delta E_{s_1} = -\text{Re} \left[ \frac{i\alpha}{4\pi^3} \sum_{s_2} \int d^4k \frac{1}{k_0^2 - k^2 + i\varepsilon} \langle s_1| e^{ikr}\alpha^\mu|s_2\rangle \langle s_2| \alpha_\mu e^{-ikr}|s_1\rangle \right] (7)
\]

with \( E_{s_2} \) being the eigenvalue belonging to the eigenstate \( |s_2\rangle \), be it bound or unbound as well.

As readily seen from \( (7) \), the major problem in direct evaluation of the Lamb shift, as it stands, is posed by the necessity to calculate the transition matrix elements \( \langle s_1| e^{ikr}\alpha^\mu|s_2\rangle \) in the plane wave representation. A host of various efficient techniques for calculation of the transition matrix elements of all types possible, i.e. the elements corresponding to transitions between the bound-bound, bound-unbound and unbound-unbound hydrogenic atom eigenstates, has already been developed in our previous papers \(^3\), \(^4\), \(^5\), \(^6\). In particular, it was shown that any transition matrix element between hydrogenic atom bound eigenstates can be expressed
explicitly in terms of analytic formulae containing hypergeometric functions, which functions depend only on the absolute value of the wave vector $k$ and the quantum numbers of the two states building up the matrix element in question. The purpose of the present research is to show that there is no conceptual difference neither in the way one could handle contributions from two distinct types of matrix elements, the bound-bound and the bound-unbound ones, nor in the structure of the corresponding computational algorithms dedicated to this purpose.

3. Transition matrix elements

An elementary building block for any matrix element - bound-bound, bound-unbound and unbound-unbound - is a Fourier transform of the kind

$$U_{ij}(s_1, s_2) = \int d\mathbf{r} e^{i\mathbf{k}\cdot\mathbf{r}} \phi_{s_1,i}^*(\mathbf{r}) \phi_{s_2,j}(\mathbf{r}), \quad i, j = 1, ..., 4,$$

(8)

where $\phi_{s_1,i}^*(\mathbf{r})$ and $\phi_{s_2,j}(\mathbf{r})$ may stand for the $i$-th or $j$-th spinor component of relativistic eigenfunctions corresponding to the bound or unbound eigenstates $|s_1\rangle$ and $|s_2\rangle$ of hydrogenic atom. Any transition matrix element is a linear combination of four terms of the kind of (8) with proper coefficients provided by corresponding matrix $\alpha^\mu$, $\mu = 0, 1, 2, 3$. Due to expansion

$$e^{ikr} = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{l} i^l j_l(kr) Y^*_{l,m}(\mathbf{r}) Y_{l,m}(k),$$

(9)

where $j_l(kr)$ is a spherical Bessel function

$$j_l(z) = \sqrt{\frac{\pi}{2z}} J_{l+1/2}(z)$$

(10)

with $J_\nu(z)$ being a Bessel function of the first kind defined as

$$J_{n+1/2}(z) = \sqrt{\frac{1}{2\pi z}} \left\{ e^{iz} \sum_{k=0}^{n} \frac{(i)^{-n+k-1}(n+k)!}{k!(n-k)!(2z)^k} + e^{-iz} \sum_{k=0}^{n} \frac{(-i)^{-n+k-1}(n+k)!}{k!(n-k)!(2z)^k} \right\}, \quad n = 0, 1, 2, ...$$

(11)

the expression (8) can be rewritten as
\[ U_{ij}(s_1, s_2) = \]
\[ = C(l_1, m_1, t_1; l_2, m_2, t_2) \cdot 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{l} i^l Y_{l,m}(k) \times \]
\[ \times \int_{0}^{2\pi} d\phi \int_{0}^{\pi} d\theta \sin(\theta) Y_{l,m}^{*}(r) Y_{l_1,m_1}(r) Y_{l_2,m_2}(r) \times \]
\[ \times \int_{0}^{\infty} dr r^2 j_l(kr) F^1_l(x_1, l_1, r) F^2_l(x_2, l_2, r). \quad (12) \]

Here \( s_1 = \{x_1, l_1, m_1, t_1\} \), \( s_2 = \{x_2, l_2, m_2, t_2\} \) are the corresponding quantum numbers, and \( \tilde{m}_1, \tilde{m}_2 \) stand for \( m_1 \pm 1/2 \), \( m_2 \pm 1/2 \), where \( m_1 \), \( m_2 \) are casual magnetic quantum numbers, \( t = 1, 2 \) indicate the type of the state – the first or the second one, \( x_i = n_i' \) or \( p_i \) for the bound and unbound eigenstates correspondingly. The coefficient function \( C(l_1, m_1, t_1, l_2, m_2, t_2) \) is a proper product of coefficients being found at the corresponding spinor components given in \([7] \) and \([8] \). The functions \( F^1_l(n_1' \text{(or } p_1 \text{)}, l_1, r) \), \( F^2_l(n_2' \text{(or } p_2 \text{)}, l_2, r) \) stand for the corresponding radial parts in expressions outlined in \([7] \) for the bound eigenstates and in \([8] \) for the unbound ones. The integrals over three spherical harmonics in (12) are known as the Gaunt coefficients. \([9] \) Gaunt coefficients are closely related to the Clebsch-Gordon coefficients. \([10] \) They can be either evaluated directly by some fast computer algebra algorithm \([11] \) or, alternatively, the expression (12) can be transformed into

\[ U_{ij}(s_1, s_2) = C(l_1, m_1, t_1; l_2, m_2, t_2) \cdot 4\pi \times \]
\[ \times \sum_{l=|m_2-m_1|}^{l_1+l_2} \left( \frac{2^{l+1} (l-m)!}{(l+m)!} \right) \times \]
\[ \times \int_{0}^{\pi} d\theta \sin(\theta) P^m_l(\cos(\theta)) P^{m_1}_{l_1}(\cos(\theta)) P^{m_2}_{l_2}(\cos(\theta)) \Big|_{m=m_2-m_1} \times \]
\[ \times \int_{0}^{\infty} dr r^{2} j_l(kr) F^1_l(n_1' \text{(or } p_1 \text{)}, l_1, r) F^2_l(n_2' \text{(or } p_2 \text{)}, l_2, r). \quad (13) \]

written in terms of the Gaunt integrals over three associated Legendre functions \( P^m_l(x) \):

\[ \int_{-1}^{1} dx P^m_{l_1}(x) P^m_{l_2}(x) P^m_{l_3}(x). \quad (14) \]

Formulas for evaluating the definite integral (14) for \( m_1 = m_2 + m_3 \) were derived by Gaunt \([9] \) and later confirmed by Infeld and Hull \([11] \). In particular, it has been shown that in order for the integral (14) to be nonvanishing the triangular conditions

\[ l_1 + l_2 + l_3 = \text{even integer} \quad (15) \]
J. Seke, A.V. Soldatov, M. Polak, G. Adam,

\[ l_2 - l_1 \leq l_3 \leq l_2 + l_1 \]  \hspace{1cm} (16)

must be satisfied. However, these conditions are not exhaustive and the integral (14) may in some cases vanish even if these conditions are satisfied\[13\]. For the sake of simplicity and convenience, we would prefer to take recourse to the standard computer algebra algorithms built in Mathematica software package to integrate over the angular variable $\theta$ analytically, so that the only integration left in (13) will be that one over $r$.

### 3.1. Radial part integration for bound-bound matrix elements

If both functions in the integrand, $F_i^1$ and $F_j^2$, belong to the bound eigenstates and, being such, are expressed each in terms of Laguerre polynomials after\[14\], then the resulting term-by-term evaluation deals with a sum of integrals of the type

\[
\int_0^\infty dr r^2 \sqrt{\frac{\pi}{2kr}} J_{l+\frac{1}{2}}(kr)e^{-\frac{kr}{N(n'_1,l_1,t_1)\alpha}} e^{-\frac{kr}{N(n'_2,l_2,t_2)\alpha}} r^{\gamma_1(l_1)-1+q_1} r^{\gamma_2(l_2)-1+q_2}, \hspace{1cm} (17)
\]

\[
\gamma(l) = \sqrt{\kappa(l)} - (Z\alpha)^2, \hspace{1cm} q_1, q_2 = 0, 1, 2, ..., \hspace{1cm} (18)
\]

each of which can be expressed explicitly in terms of hypergeometric functions as

\[
\int_0^\infty dr e^{-\alpha r} r^{\mu - 1} J_\nu(\beta r) = \frac{\left(\frac{\beta}{2a}\right)^\nu \Gamma(\nu + \mu)}{\alpha^\mu \Gamma(\nu + 1)} e^{2F_1\left(\frac{\nu + \mu}{2}, \frac{1 + \mu + \nu}{2}; \nu + 1; -\frac{\beta^2}{\alpha^2}\right)}, \hspace{1cm} (19)
\]

where

\[ [\text{Re}(\nu + \mu) > 0, \text{Re}(\alpha + i\beta) > 0, \text{Re}(\alpha - i\beta) > 0]. \hspace{1cm} (20) \]

### 3.2. Radial part integration for bound-unbound matrix elements

In the case when one of the states belongs to the discrete and the other to the continuous spectrum, a typical integral to be evaluated is

\[
\int_0^\infty dr r^2 \sqrt{\frac{\pi}{2kr}} J_{l+1/2}(kr) e^{\gamma(l_1,t_1)-1+q_1} e^{-\frac{kr}{N(n'_1,l_1,t_1)\alpha}} \times \\
\times r^{\gamma(l_2,t_2)-1} e^{-ipr} F_1(\gamma(l_2,t_2) + 1 + i\alphaZW(p)/p, 2\gamma(l_2,t_2) + 1; 2ipr), \hspace{1cm} (21)
\]

\[ q_1 = 0, 1, 2, ...; \hspace{1cm} |\tilde{m}_2 - \tilde{m}_1| \leq l \leq l_1 + l_2, \]
where \( _1F_1 \) is a confluent hypergeometric function, \( W(p) = \sqrt{m^2 + p^2} \). After substituting expansion (11) for the Bessel function in (21), any such integration can be carried out analytically with the results expressed in terms of hypergeometric functions \( _2F_1 \) with the help of two general integration rules

\[
\int_0^\infty dt e^{-st} t^{b-1} _1F_1(a; c; pt) = \frac{\Gamma(b)}{s^b} _2F_1(a, b; c; p/s),
\]

and

\[
\int_0^\infty dre^{-sr} r^{b-1} _1F_1(a; c; pr) \frac{\sin(kr)}{kr} = \\
= \frac{\Gamma(c)}{\Gamma(a)} \sqrt{\frac{2\pi}{k}} \left( \frac{k}{2} \right)^{1/2} \frac{\Gamma(1/2 + b)}{s^b \Gamma(1/2 + 1)} \left[ _2F_1\left(\frac{1/2 + b}{2}, \frac{1 + b + 1/2}{2}, 1/2 + 1; -\frac{k^2}{s^2}\right) + \left( \frac{k}{s} \right)^b - 1 \right] \frac{\Gamma(b - 1)}{2ik} \frac{\Gamma(a) (s - ik)^{b-1}}{\Gamma(a)} \left( \frac{p}{s - ik} \right) - 1.
\]

Here, in both cases,

\[\text{Re}[b] > 0, \quad \text{Re}[s] > 0.\]

The rules can be readily derived by taking into account the basic definitions and general properties of the hypergeometric functions (see, e.g., [15]).

### 4. Integration over the wave-vector \( k \)

The following simplified formulae for the Lamb shift

\[
\Delta E_{s1} = -\frac{\alpha}{4\pi^2} \sum_{s_2} \mathcal{P} \int_0^\infty dk \int d\Omega_k \frac{\langle s_1 | e^{ikr} \alpha^\mu | s_2 \rangle \langle s_2 | \alpha_\mu e^{-ikr} | s_1 \rangle}{E_{s_1} - E_{s_2} - k + i\eta},
\]

which results immediately from the original expression (7) after conventional integration over \( k^0 \) in the complex plane, must be employed in the plain-style numerical calculation of the contributions from various transition matrix elements between hydrogenic atom bound eigenstates. Due to universal analytic representation for all transition matrix elements given by expressions of the type (13), the integration over the angular polar coordinates \( \int d\Omega_k \) can be carried out analytically resulting in selection rules of the kind

\[
\int d\Omega_k Y_{l,m}^*(k) Y_{l,m}(k) = \delta_{ll'} \delta_{mm'},
\]
and only the remaining one-dimensional principal value integration over $k$ is to be done numerically. Another performance-enhancing distinctive feature of the numerical technique introduced in this study is that, unlike to the numerical approach undertaken in [16], a complete matrix element is actually never calculated at once but rather is broken down into a sum of very simple easy-to-handle terms of similar structure. Then, the numerator in Eq. (25) for each intermediate quantum eigenstate $|s_2\rangle$ involved and each $k$ would be a sum of four structurally similar terms

$$|\langle s_1|e^{ikr}|s_2\rangle|^2 - |\langle s_1|e^{ikr}\alpha^1|s_2\rangle|^2 - |\langle s_1|e^{ikr}\alpha^2|s_2\rangle|^2 - |\langle s_1|e^{ikr}\alpha^3|s_2\rangle|^2,$$

(27)
each of which is, in its turn, an absolute value of the sum of four elementary terms of the kind of (8). Of course, for the sake of convenience, the terms inside these sums are broken down even further by means of the expansion (11) for the Bessel function and polynomial expansion after Davis [14] for the confluent hypergeometric functions featured in radial parts of all bound eigenstates. Afterwards, each thus built smallest partial term in the numerator is integrated over $k$ with subsequent summation of all such partial outcomes of this integration, which makes inherently complicated numerical calculations feasible even on a modest desktop computer.

5. Complete renormalization

Our approach to renormalization, developed by J. Seke [12], originates from the concept postulating that the free electron, by its very definition, may not experience any energy shift by the interaction with the vacuum radiation field. This means that all corrections coming from the interaction with the vacuum radiation field for a freely propagating electron have to be removed by renormalization. This should be applied for the renormalization of the bound electron by identifying the free electron contributions and removing them.

5.1. Renormalization of the bound electron to the second order

The expression for the second order self energy of the bound electron can be written as

$$\langle n|\Sigma^{(2)}_{\text{bnd}}(E_n)|n\rangle = i\epsilon^2\langle n|\int \frac{d^4k}{(2\pi)^4k^2}\gamma^\mu \frac{1}{P_n - k - m}\gamma_\mu|n\rangle,$$

(28)where

$$P_n = \gamma_0 E_n - \gamma_i P^i - e\gamma_0 A^0,$$

the on-shell momentum operator of an electron in the potential $A^0$ and $n$ stands for all quantum numbers characterizing the corresponding state. In order to identify the part belonging to the free electron, it seems to be self-evident to perform a potential expansion and identify the first (zero potential) term with the contribution of the free electron. However, it turns out that parts of this term cancel out against those of all the multipotential terms. Therefore, we perform a "shifted" potential expansion which automatically cancels
all these terms. This expansion can be performed by inserting the complete basis

\[ 1 = \int d^3p' \sum_{s'} \gamma_0 u_{s'}(p') u_{s'}^\dagger(p)|p\rangle|\gamma_0 = \int d^3p' \sum_{s'} |p's'angle|\Pi_{s'}|, \]

in the expression below

\[ \frac{1}{\Pi_n - \hat{k} - m} = \frac{1}{\hat{p}_{p's'} - \hat{k} - m} - \frac{1}{\hat{p}_{p's'} - \hat{k} - m} \gamma_0(E_n - E_{p's'} - eA^0) \frac{1}{\Pi_n - \hat{k} - m}, \]

which results in

\[ \frac{1}{\Pi_n - \hat{k} - m} = \frac{1}{\hat{p}_{p's'} - \hat{k} - m} - \frac{1}{\hat{p}_{p's'} - \hat{k} - m} \gamma_0(E_n - E_{p's'} - eA^0) \frac{1}{\Pi_n - \hat{k} - m}, \]

Here, the first term can immediately be recognized as

\[ \frac{1}{\Pi_n - \hat{k} - m} = \frac{1}{\hat{p}_{p's'} - \hat{k} - m} - \frac{1}{\hat{p}_{p's'} - \hat{k} - m} \gamma_0(E_n - E_{p's'} - eA^0) \frac{1}{\Pi_n - \hat{k} - m}, \]

i.e. the so-called mass-renormalization term of the free electron which, consequently, has to be removed by renormalization.

The second term, however, has to be treated further by commuting the expression \( E_n - E_{p's'} - eA^0 \) to the left, giving rise to a commutator of the denominator with the potential \( A^0 \) and letting it act on the states, where the advantage of the relation

\[ \langle n|E_n - E_{p's'} - eA^0|p's'\rangle = \langle n|\gamma_0(E_n - E_{p's'} - eA^0)|p's'\rangle, \]

\[ - \gamma_0 E_{p's'}|p's'\rangle = - (\gamma_i p^i + m)|p's'\rangle = - (\gamma_i p^i + m)|p's'\rangle \]

is taken. Therefore,

\[ \langle n|E_n - E_{p's'} - eA^0|p's'\rangle = \langle n|\Pi_n - m|p's'\rangle = 0, \]

which means that only the commutator involving the potential \( A^0 \) remains, and, being so, cannot be attributed to the free electron.

Hence, we may conclude that there are no other free-electron contributions besides the free-electron mass-renormalization term (\( \delta m \)) in the case of the second-order self-energy. In other words, this is the only term that has to be removed by
the renormalization, in both cases - the complete and the conventional renormalization. As a consequence, the renormalized second-order bound-electron self-energy reads as

$$\langle n | \Sigma^{(2)}_{\text{ren}}(E_n) | n \rangle = \langle n | (\Sigma^{(2)}_{\text{bnd}}(E_n) - \delta m) | n \rangle =$$

$$= ie^2 \langle n | \int \frac{d^4 k}{(2\pi)^4} k^2 \left( \frac{1}{k_n - \not k - m} \gamma_\mu - \right.$$

$$- \left. \frac{1}{k_n - \not k - m} \gamma_\mu \right) | n \rangle,$$

$$(37)$$

5.2. Numerical renormalization

As a result of the presented matrix element calculation analytic technique, only one improper integration over $|k|$ is to be carried out numerically with an infinite upper limit, when calculating contributions of the bound-bound and bound-unbound matrix elements to the unrenormalized Lamb shift at the second order of the conventional perturbational QED approach. It is worth noticing, that all the techniques developed above can be applied unchanged to the case when all calculations are carried out with the regularized photon propagator

$$D^{\text{reg}}_{\mu\nu} = -g_{\mu\nu} \left[ \frac{1}{k_0^2 - k^2 + i\epsilon} - \frac{1}{k_0^2 - k^2 + i\epsilon - \Lambda^2} \right],$$

$$(38)$$

with $\Lambda$ being the regularization parameter. In this case the renormalized shift is

$$\Delta E_{s_1}^{\text{ren,reg}} = \Delta E_{s_1}^{\text{reg}} - \delta m \langle s_1 | s_1 \rangle,$$

$$(39)$$

where $\delta m$ can be defined through one-dimensional integration of the kind

$$\delta m = \int_0^\infty dk f(k, \Lambda^2),$$

$$(40)$$

convergent for finite $\Lambda^2$, where $f(k, \Lambda^2)$ is a well-known, albeit cumbersome, function (see, e.g., [17]). Therefore, the renormalization procedure can be accomplished numerically by including the subtraction of the integrand in Eq. (40) directly in the numerical one-dimensional integration over $|k|$ in the regularized expression (25) for the unrenormalized Lamb shift.

6. Summary

Our objective so far has been and is to carry out the plain-style calculations of the second-order renormalized expression (6) without making any approximations concerning the transition matrix elements. The next goal would be to carry out higher-order Lamb shift calculations by using the shifted potential expansion and complete renormalization method - both developed by Seke. It was demonstrated
that the technique of the transition-matrix element calculation developed so far
and rectified further, especially in the present work, fits these purposes quite well. It is possible now to represent all matrix elements in a form suitable for extensive numerical calculations with arbitrary precision. In our approach, all bound-bound as well as bound-unbound matrix elements are derived analytically. The same technique of the matrix-element evaluation is applicable for all possible values of discrete and continuous quantum numbers of hydrogenic eigenstates and photon wave-vector \( k \). Only one improper integration over \( |k| \) is to be carried out numerically with an infinite upper limit, when calculating contributions of the bound-bound and bound-unbound matrix elements to the Lamb shift. Matrix elements of both types are represented now in a closed analytic form suitable for subsequent numerical calculations of the renormalized Lamb shift as well as for other possible applications in QED and related fields of research whatever they might be. Numerical computations, based on our analytic matrix-element representations, can rely totally on functions already built into the standard computational packages like \textit{Mathematica}, which feature renders this approach highly favorable for programming of computationally efficient and numerically precise algorithms.

\textbf{Acknowledgements}

This work was supported by the \textit{Dr. Anton Oelzelt-Newinsche Stiftung} of the Austrian Academy of Sciences. A.V.S. acknowledges support from the Ausseninstitut of the Technische Universität Wien, the RFBR grant No.09-01-00086-a and the RAS research program “Mathematical Methods in Nonlinear Dynamics”.

\textbf{References}

1. J.Seke, \textit{Physica}, A \textbf{312}, 392 (2002).
2. J.Seke, \textit{Physica}, A \textbf{278}, 222 (2000).
3. A.V. Soldatov, J.Seke, G. Adam and M. Polak, \textit{Mod. Phys. Lett. B} \textbf{23}, (n.2), 111 (2009).
4. A.V. Soldatov, J.Seke, G. Adam and M. Polak, \textit{Int. J. Mod. Phys. B} \textbf{22}, (n.21), 1 (2008).
5. A.V. Soldatov, J.Seke, G. Adam, \textit{Int. J. Mod. Phys. B} \textbf{21}, 3825 (2007).
6. A.V. Soldatov, J.Seke, G. Adam, \textit{Int. J. Mod. Phys. B} \textbf{20}, 1123 (2006).
7. H.A. Bethe and E.E. Salpeter, ”Quantum Mechanics of One- and Two-Electron Systems” (Springer - Verlag, Berlin, Göttingen, Heidelberg, 1957).
8. M.E. Rose, \textit{Phys. Rev.}, \textbf{51}, 484 (1937).
9. J.A. Gaunt, \textit{Phil. Trans. R. Soc. Lond.}, A \textbf{228}, 151 (1929).
10. A. Messiah, ”Quantum mechanics”, Volume II, North-Holland Publishing Company, Amsterdam, 1962, p.1057.
11. L. Infeld and T.E. Hull, Rev. Mod. Phys., \textbf{23}, 21 (1951).
12. Yu-Lin Xu, Math. of Comput., \textbf{65}, n.16, 1601 (1996).
13. G. Gjellestad, Proc. Nat. Acad. Sci., \textbf{41}(11), 954-956 (1955).
14. L. Davis, \textit{Phys. Rev.}, \textbf{56}, 186 (1939).
15. I.S. Gradshtein and I.M. Ryzhik, ”Tables of Integrals, Series and Products” (Academic Press, New York and London), Eq.( 3.381 (4)), p.317
12 J. Seke, A.V. Soldatov, M. Polak, G. Adam,

16. J. Seke, Physica, A 233, 469 (1996).
17. S.S. Schweber, ”An Introduction to Relativistic Quantum Field Theory” (Harper & Row, Publishers, Inc., Sec. Print., 1962).