Perturbed Orbital Contribution to the Two-Loop Lamb Shift in Hydrogen

S. Mallampalli and J. Sapirstein
Department of Physics, University of Notre Dame, Notre Dame, Indiana 46556
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A part of the two-loop Lamb shift called the perturbed orbital term is evaluated with exact Dirac-Coulomb propagators. It is shown to be the most nonperturbative function of $Z\alpha$ yet encountered in QED, so much so that even at $Z = 1$ the leading term in its $Z\alpha$ expansion is of the opposite sign from the complete answer. The higher order contributions are $-71(1)$ kHz to the ground state Lamb shift in hydrogen and $-8.9(1)$ and $-346(1)$ kHz to the $n = 2$ Lamb shift in hydrogen and He^+, respectively. [S0031-9007(98)06394-7]

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In the evaluation of radiative corrections in bound state QED in the nonrecoil limit, two types of expansion can be carried out. The first expansion, in the number of loops present, is governed by powers of α/π. In the bound state problem each order of α/π multiplies a function of $Z\alpha$, where Z is the nuclear charge. For example, the Lamb shift through two loops of a state n of a hydrogenic ion can be written as

$$\Delta E_n = m\frac{\alpha}{\pi}\frac{(Z\alpha)^4}{n^3}F_n(Z\alpha) + m\left(\frac{\alpha}{\pi}\right)^2\frac{(Z\alpha)^4}{n^3}G_n(Z\alpha), \tag{1}$$

where F_n is associated with the one-loop Lamb shift and G_n with the two-loop Lamb shift. For low Z it is standard to take advantage of the smallness of $Z\alpha$, and to further expand F_n and G_n in powers of $Z\alpha$. [The expansion is actually a double expansion, as each order of $Z\alpha$ can be accompanied by various powers of $\ln(Z\alpha)$]. However, at higher values of Z, the expansion in $Z\alpha$ no longer converges, and in that case F_n and G_n must be evaluated exactly, which can be done by using numerical representations of the exact Dirac-Coulomb propagators in terms of which they are expressed. The most accurate calculations have been carried out for the one-loop Lamb shift by Mohr and collaborators [1]. Similar calculations for the two-loop Lamb are incomplete: the purpose of this Letter is to present an exact calculation for a part of G_n called the perturbed orbital term.

Recently three calculations have been carried out that raise the question of whether the perturbative approach is valid for the self-energy part of the two-loop Lamb shift even at low Z. The leading term in the series expansion of $G_n^{\rm SE}(Z\alpha)$ has been known for some time [2]. More recently two independent calculations [3,4] determined an unusually large coefficient for the second term in the expansion:

$$G_n^{\rm SE}(Z\alpha) = 1.409\,251 - 24.266(3)\,(Z\alpha). \tag{2}$$

Because the second term contributes -41.8 kHz to the $n = 2$ Lamb shift in hydrogen, which is known with an accuracy of 9 kHz [5], in the absence of a complete calculation of the $(Z\alpha)^2$ corrections it is not clear whether a perturbative expansion is adequate even for hydrogen. A first indication that this is not, in fact, the case is the calculation of a contribution of order $(Z\alpha)^2\ln^3(Z\alpha)^{-2}$ by Karshenboim [6] associated with the perturbed orbital term, which is part of Fig. 1a. The leading order of the perturbed orbital (PO) term is $Z\alpha$, being part of the coefficient -24.266 in Eq. (2).

Including Karshenboim's logarithmic term, its series expansion is

$$G_n^{\rm PO}(Z\alpha) = Z\alpha\,[\,2.299\,53 - \frac{8}{27}(Z\alpha)\ln^3(Z\alpha)^{-2}\,]. \tag{3}$$

The origin of the high power of $\ln Z\alpha$ is the presence of a factor of $\ln Z\alpha$ in each one-loop self-energy subdiagram in Fig. 1a along with an additional factor arising from the integration over the central propagator. The large size of this correction leads to the remarkable result for the $n = 2$ Lamb shift that, even at $Z = 1$, the first term is essentially canceled by the second term, even though that term is of the next order in α: specifically, a 4 kHz contribution is reduced to 0.4 kHz. We will show in this paper that the full answer changes even further, to -5.0 kHz. However, as will be explained in more detail below, the bulk of this additional change will not be attributed to higher order terms, but rather a coefficient of the logarithmic term larger than, and in significant disagreement with, the $-8/27$ found in Ref. [6]. While it is important to resolve this discrepancy, in either case the large size of the logarithmic term clearly makes it desirable to carry out an exact calculation that avoids expansion in $Z\alpha$ altogether.

We now describe such a calculation for the ground state of low-Z hydrogenlike ions. As discussed in Ref. [7],

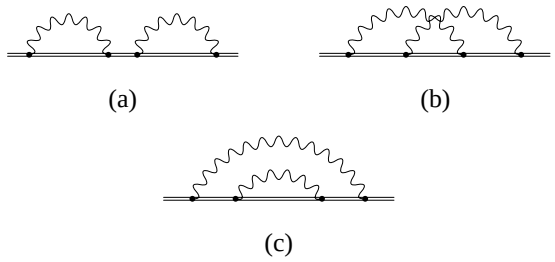

FIG. 1. Fourth-order self-energy diagrams.

part of Fig. 1a leads to a derivative term, and part to the PO term. If a spectral representation of the central propagator is used, the derivative term is associated with $n = v$, where v represents the ground state, and the PO term is given by

$$\Sigma_{\mathrm{PO}} = \sum_{n \neq v} \frac{\Sigma_{vn}(\epsilon_v)\Sigma_{nv}(\epsilon_v)}{\epsilon_v - \epsilon_n}. \quad (4)$$

Here we have introduced a generalization of the self-energy, with the self-mass counterterm understood to be added in,

$$\Sigma_{mn}(E) \equiv -ie^2 \int d^3x d^3y \int \frac{d^n k}{(2\pi)^n} \frac{e^{i\vec{k}\cdot(\vec{x}-\vec{y})}}{k^2 + i\delta} \times \bar{\psi} m(\vec{x}) \gamma_\mu S_F(\vec{x}, \vec{y}; E - k_0) \gamma^\mu \psi_n(\vec{y}). \quad (5)$$

The usual self-energy is, of course, $\Sigma_{vv}(\epsilon_v)$. Ultraviolet divergences have been regulated by working in $n = 4 - \epsilon$ dimensions, where the ϵ is taken to zero after renormalization.

We choose to use two methods to represent the electron propagator without expansion in $Z\alpha$. The first method is applied to the reduced Green's function associated with the central propagator in Fig. 1a. While various representations of the reduced Dirac-Coulomb propagator are known [8,9] they involve an infinite sum over analytic functions. We instead choose to use finite basis set techniques [10] to replace the infinite summation in the spectral representation with a finite sum over basis set functions. This eliminates the need for methods to deal with an infinite summation, and allows the trivial implementation of the restriction $n \neq v$. A basis set with 50 positive energy and 50 negative energy states leads to sufficient accuracy for our purposes. A different method is used for the evaluation of Σ_{vn}. In this case we use differential equation techniques, the use of which in closely related calculations is described in Refs. [11] and [12]. The evaluation of Σ_{vn} involves a partial wave summation that must be extended to high values of l, which is much easier in the differential equation approach than with basis sets.

At this point, the calculation is straightforward but computationally intensive. Three numerical issues have to be treated with particular care. The first involves taking the Fourier transform of the basis set states n, which is required because part of the calculation of Σ_{vn} is carried out in momentum space. The techniques that work for Σ_{vv}, which involves bound state wave functions with, at most, a few oscillations in momentum space, are of insufficient accuracy when extended to continuum states. While it is possible to create basis sets entirely in momentum space [13], except for a few low lying states, the basis functions are not Fourier transforms of corresponding functions in the coordinate space basis set. This precludes the use of momentum space basis sets as we require the intermediate state n to be the same in both the coordinate and momentum space parts of the calculation. Hence, working with basis sets created in coordinate space, we simply use extremely fine grids in both coordinate and momentum space to carry out a sufficiently accurate Fourier transform.

The second numerical issue involves the partial wave expansion, which is associated with the part of the calculation carried out in coordinate space. As was also found in recent work on radiative corrections in the presence of external potentials [12], at the lowest values of Z keeping only the first 12 or so partial waves leads to misleading answers. While at high Z, the series has become asymptotic by $l = 12$, at low Z the series usually changes sign at a somewhat higher value of l, increases in magnitude for the next few l values, and only then becomes asymptotic. To control this behavior requires going to very high values, typically $l_{\max} = 40$.

Finally, when the intermediate states correspond to positive energies, the use of the Feynman gauge leads to terms of spurious order in $Z\alpha$ from different parts of Σ_{vn}. For example, in the calculation of the one-loop self-energy, Σ_{vv}, these spurious terms enter at order Z a.u. and cancel down to $Z^4\alpha^3$ a.u. This cancellation is severe at low Z and leads to a loss of several significant digits. While the parts evaluated in coordinate space could be obtained with sufficient numerical precision, the momentum space part, which is a four dimensional integral and is evaluated with the adaptive Monte Carlo integration program VEGAS [14], is more difficult to determine precisely. To treat it, we devised a subtraction term that contains the leading spurious order, but which could be recast into a one dimensional integral and then obtained with negligible error. Nevertheless, the remaining statistical error from the subtracted term forms the largest part of the quoted numerical uncertainty in the calculation.

Several checks were made of the calculation. In one, the accuracy of the Fourier transforms was tested by replacing the operator Σ with the simpler object $1/r$, and checking that the same result was found in both coordinate and momentum space. The assumption that the partial wave expansion was asymptotic was checked by fitting it to a formula for a given range of high l, and then comparing the predicted values at even higher l with actual runs. We also checked that the one-loop Lamb shift calculated for $n = v$ agreed with Mohr's results [1] to within numerical error. Dependencies on basis sets were tested at $Z = 1$ by employing a basis set consisting of 60 positive and 60 negative energy states and checking that the results were in agreement within the quoted numerical error. Finally, the PO term at high values of Z, specifically $Z = 70, 80, 90$, and 92, was evaluated with the same methods applied to the low Z case, and found to agree with an independent calculation [15].

While our interest is primarily in the cases $Z = 1$ and $Z = 2$, we also calculated the PO term for a range of Z

TABLE I. Perturbed orbital contributions to the ground state Lamb shift. All energies are in a.u. $[-x]$ denotes a multiplicative factor of 10^{-x}.

Z	$\Delta E_{1s}^{\mathrm{PO}}$		G_{1s}^{PO}	Z	$\Delta E_{1s}^{\mathrm{PO}}$		G_{1s}^{PO}
0.50	−9.9(5)	[−14]	−1.5(1)	7	−1.767(1)	[−07]	−5.016(3)
0.75	−1.11(2)	[−12]	−2.23(4)	10	−1.0277(3)	[−06]	−4.9016(14)
1	−6.0(1)	[−12]	−2.87(5)	15	−7.199(1)	[−06]	−4.5218(6)
1.50	−5.53(3)	[−11]	−3.47(2)	20	−2.7653(2)	[−05]	−4.1217(3)
2	−2.66(1)	[−10]	−3.965(15)	70	−8.388(1)	[−03]	−2.3804(3)
3	−2.292(5)	[−09]	−4.50(1)	80	−1.6436(1)	[−02]	−2.3923(2)
4	−1.024(2)	[−08]	−4.77(1)	90	−3.1357(3)	[−02]	−2.5328(3)
5	−3.231(3)	[−08]	−4.931(5)	92	−3.567(1)	[−02]	−2.581(1)

values for fitting purposes. Our results are tabulated in Table I, and plotted in Fig. 2, where they are compared with the first term in the series expansion.

The most remarkable feature of our results is the fact that while at $Z = 0$ the PO term is 2.3, at $Z = 1$ it has become $-2.87(5)$. This is the most nonperturbative behavior exhibited by any of the functions of $Z\alpha$ yet encountered in bound state QED, and indicates the need for exact methods when dealing with the two-loop Lamb shift. While a clear trend towards a positive result can be seen at low Z, numerical difficulties described earlier prevented a direct calculation at values of Z smaller than 0.5, where the function is still negative. However, we were able to find the following fit to the data, assuming the correctness of the first term:

$$G_{1S}^{\mathrm{PO}}(Z\alpha) = Z\alpha[2.3 - 0.9(Z\alpha)\ln^3(Z\alpha)^{-2} + 1.9(Z\alpha)\ln^2(Z\alpha)^{-2} - 2.9(Z\alpha)\ln(Z\alpha)^{-2}]. \quad (6)$$

If we instead also fit the first term, we find the result 2.3(2) when the data point at $Z = 0.5$ is excluded, and 2.8(2) when it is included. We interpret the slight discrepancy in the latter case as an indication that systematic errors are beginning to affect our numerical methods. A more precise determination of the constant will require the development of techniques that work at values of Z less than 0.5; however, satisfactory control of the calculation at physical values of Z has been obtained, so we have not pursued this issue further.

While we confirm the conclusion of Ref. [6] of the presence of a cubed logarithm, the coefficient we obtain is significantly larger. The reason for this is not known at present.

We now turn to the experimental consequences of our results. The present calculation is for the ground state, so to obtain predictions for the $n = 2$ Lamb shift we assume $1/n^3$ scaling. The status of the Lamb shift in hydrogen and He^+ has recently been reviewed by Pachucki [16], keeping terms up to order $m\alpha^2(Z\alpha)^5$ in the two-loop Lamb shift, but not including the Karshenboim correction. We reproduce these results, which use the Mainz proton radius [17] for the determination of the finite nuclear size effect, in Table II with the new corrections calculated in this paper added in, which we stress are not the only corrections starting in order $m\alpha^2(Z\alpha)^6$ present. In both cases, the extra part of the PO term acts to make experiment and theory more discrepant. The discrepancy is increased if a newer analysis of the Mainz proton size is used [18], and increased even further if the Stanford proton radius [19] is used. The new contributions calculated in this paper, that is, the exact PO term with the contributions from the leading coefficient in the $Z\alpha$ expansion subtracted out, are shown in the last row of Table II.

While experiment and theory now disagree for both hydrogen and He^+, this simply indicates the need for an exact calculation of all parts of the two-loop Lamb shift: the new results that lead to the discrepancy come only from the PO term. It is useful to note that this term forms only about 10% of the $m\alpha(Z\alpha)^5$ self-energy correction, with the remainder coming from the graphs of Figs. 1b and 1c. (There is also a set of vacuum-polarization graphs that contribute to the two-loop Lamb shift, but an exact treatment of one of them at low Z [22] suggests that

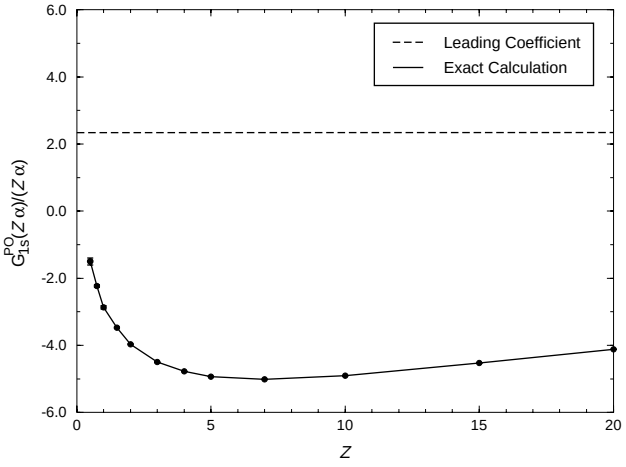

FIG. 2. Plot of $G_{1S}^{\mathrm{PO}}(Z\alpha)$ and the leading coefficient in its $Z\alpha$ expansion at low Z.

TABLE II. Comparison of experiment with theory of the Lamb shift including the results of this calculation.

	$L(1S)$ in H	$L(2S\text{-}2P)$ in H	$L(2S\text{-}2P)$ in He^+
Experiment	8172.876(29) MHz [20]	1057.845(9) MHz [5]	14 042.52(16) MHz [21]
Theory[a]	8172.731(40) MHz	1057.830(6) MHz	
Theory[b]	8172.691(40) MHz	1057.825(6) MHz	
Theory[c]	8172.582(40) MHz	1057.812(6) MHz	
Theory			14 040.98(18) MHz
New contributions	−0.071(1) MHz	−0.0089(1) MHz	−0.346(1) MHz

[a]Uses the Mainz proton radius [17].
[b]Uses the new Mainz proton radius [18].
[c]Uses the Stanford proton radius [19].

the higher order terms are very small when a vacuum polarization loop is present.)

In summary, the main point of this Letter is that unexpectedly large contributions starting in order $m\alpha^2(Z\alpha)^6$ have been shown to arise from one part of the two-loop Lamb shift. Because of this, it is clearly necessary to at least calculate all terms of that order, and preferably to carry out exact calculations of the remaining parts of the two-loop Lamb shift, which must also have strikingly nonperturbative behavior if the present discrepancy between theory and experiment is to be removed. Only when this is done can one begin to draw conclusions about the size of the proton from the Lamb shift in hydrogen, or reliably use He^+ as a test of QED.

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