Fourth-order vacuum-polarization contribution to the Lamb shift

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The vacuum-polarization contribution to the two-loop ground-state self-energy of hydrogenic ions is calculated with an exact Dirac-Coulomb propagator. Agreement at low Z with previous calculations is found and predictions for the effect at high Z are presented. [S1050-2947(96)02610-8]

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Theoretical treatments of the two-loop Lamb shift have been given almost since the introduction of the modern form of quantum electrodynamics (QED), starting with the classic calculation of Karplus and Kroll [1]. While the lowest-order result, first correctly calculated by Appelquist and Brodsky [2], enters in order $(Z\alpha)^4$ atomic units (a.u.), there are two reasons for interest in corrections of higher order in $Z\alpha$, known as binding corrections. The first is their relevance to the Lamb shift in hydrogen. Two recent calculations [3,4] have found rather large contributions in order $(Z\alpha)^5$ a.u. that significantly affect the interpretation of experiment. Because the lowest-order effect is 101 kHz, and the next-order result −37.1 kHz for the $2S$ state of hydrogen, the convergence of the $Z\alpha$ expansion is called into question. The second is recent progress in high-precision spectroscopy of highly charged ions, where QED effects are being measured with a precision that is beginning to require inclusion of the two-loop Lamb shift. However, it is well known from studies of the one-loop Lamb shift that at high Z, the expansion in $Z\alpha$ breaks down completely. This may be expected to be even more the case for the two-loop Lamb shift, given the large coefficient mentioned above. For both these reasons, an exact approach, in which no expansion in $Z\alpha$ is made, is clearly desirable.

As a first step in the exact evaluation of two-loop corrections, we calculate in this paper the vacuum-polarization contribution to the ground-state Lamb shift, given by Fig. 1(a), where the double lines indicate Dirac-Coulomb propagators. However, in the calculation reported here, we use free propagators in the vacuum-polarization loop. We make this approximation because when free propagators are used, the diagram becomes an integral over a modified form of the one-loop electron self-energy. This latter function has been intensively studied [5], and accurate numerical methods have been developed that allow it to be evaluated to all orders in $Z\alpha$. We will in the next section describe how this two-loop contribution is evaluated. By studying its behavior at low Z we will be able to confirm the $Z\alpha$ corrections calculated independently by Pachucki [6] and Eides and Grotch [7], and by studying its behavior at high Z, make predictions for the size of the effect for highly charged ions. We conclude with a short discussion of the issues involved in undoing the approximation of treating the electrons in the vacuum-polarization loop as free and evaluating the remaining graphs contributing to the two-loop Lamb shift.

DESCRIPTION OF THE CALCULATION

As noted above, we wish to evaluate the electron self-energy graph with the photon line modified to include a photon self-energy subgraph. We use the method of dimensional regularization to regulate the infinities with the number of space-time dimensions $n=4-\epsilon$. This corresponds to modifying the photon propagator to [8]

$$\frac{1}{k^2+i\delta}\rightarrow -\frac{\alpha C}{4\pi}\int_0^1 dz\,\frac{z^2(1-\frac{1}{3}z^2)}{[m^2-\frac{1}{4}k^2(1-z^2)-i\delta]^{1+(\epsilon/2)}}, \tag{1}$$

where $C=(4\pi)^{\epsilon/2}\Gamma(1+\epsilon/2)$. The energy shift of a state v is then given by

$$\begin{aligned}\Delta E_v = i\alpha^2 C\int d^3r\; d^3r'\int_0^1 dz\; z^2 &\\ \times\left(1-\frac{1}{3}z^2\right)\int\frac{d^nk}{(2\pi)^n}&\frac{e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}}{\left[m^2-\dfrac{k^2(1-z^2)}{4}-i\delta\right]^{1+(\epsilon/2)}}\\ \times\overline{\psi_v}(\mathbf{r})\,\gamma_\mu S_F(\mathbf{r},\mathbf{r}';\epsilon_v-k_0)\,\gamma^\mu\psi_v(\mathbf{r}')&\\ -\delta m^{4VP}\int d^3r\;\overline{\psi_v}(\mathbf{r})\,\psi_v(\mathbf{r}),&\end{aligned} \tag{2}$$

where

$$\delta m^{4VP}=\frac{m\alpha^2}{\pi^2}\,(4\pi e^{-\gamma_E})^{\epsilon}\left(\frac{1}{2\epsilon^2}-\frac{5}{24\epsilon}+\frac{9}{8}\,\zeta(2)-\frac{143}{96}\right), \tag{3}$$

in agreement with Ref. [8]. Here γ_E is Euler's constant.

The bound electron propagator S_F is expanded in terms of the free electron propagator S_F^0 as

$$\begin{aligned}S_F(\mathbf{r},\mathbf{r}';E)=S_F^0(\mathbf{r},\mathbf{r}';E)&\\ +\int d^3x\; S_F^0(\mathbf{r},\mathbf{x};E)\,\gamma_0 V(\mathbf{x})S_F^0(\mathbf{x},\mathbf{r}';E)&\\ +\int d^3x\; d^3y S_F^0(\mathbf{r},\mathbf{x};E)\,\gamma_0 V(\mathbf{x})S_F(\mathbf{x},\mathbf{y};E)&\\ \times\gamma_0 V(\mathbf{y})S_F^0(\mathbf{y},\mathbf{r}';E),&\end{aligned} \tag{4}$$

where for this calculation $V(\mathbf{x})$ is taken to be the Coulomb potential. The three terms in the right-hand side are known as the zero-potential, one-potential, and many-potential terms,

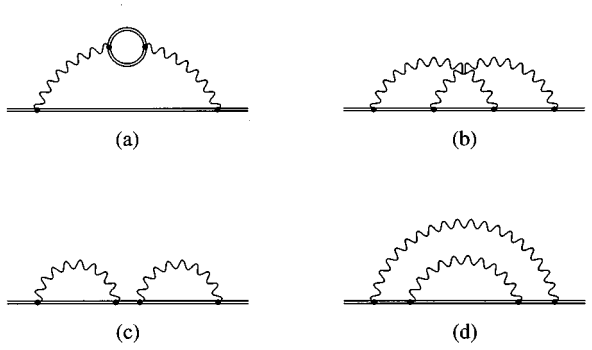

FIG. 1. Two-loop self-energy Feynman diagrams.

referred to in the following as 0P, 1P, and MP, respectively. We evaluate the MP term by using the above equation to express it as

$$S_F^{\rm MP}(\mathbf{r},\mathbf{r}';E)=S_F(\mathbf{r},\mathbf{r}';E)-S_F^0(\mathbf{r},\mathbf{r}';E) - \int d^3x\; S_F^0(\mathbf{r},\mathbf{x};E)\,\gamma_0 V(\mathbf{x}) S_F^0(\mathbf{x},\mathbf{r}';E). \tag{5}$$

As in Ref. [5], the first two terms are evaluated in momentum space. The 0P term is given by

$$\Delta E_v^{\rm 0P}=\delta m^{4VP}\int d^3p\;\overline{\psi_v}(\mathbf{p})\psi_v(\mathbf{p})-\frac{\alpha^2}{\pi^2}\,(4\pi e^{-\gamma_E})^{\epsilon} \times\left(\frac{1}{6\epsilon^2}-\frac{13}{72\epsilon}-\frac{7}{24}\,\zeta(2)+\frac{599}{864}\right)\int d^3p\;\overline{\psi_v}(\mathbf{p}) \times(\not p-m)\psi_v(\mathbf{p})-\frac{\alpha^2}{2\pi^2}\int d^3p\int_0^1 dx\;dz \times\frac{z^2(1-\frac{1}{3}z^2)}{1-z^2}\;\overline{\psi_v}(\mathbf{p})[2m-\not p x]\psi_v(\mathbf{p}) \times\ln\left[\frac{4x+(1-z^2)(1-x)\left(1-\dfrac{p^2}{m^2}\,x\right)}{4x+(1-z^2)(1-x)^2}\right] \tag{6}$$

and the 1P term is given by

$$\Delta E_v^{\rm 1P}=\frac{\alpha^2}{\pi^2}\,(4\pi e^{-\gamma_E})^{\epsilon}\left(\frac{1}{6\epsilon^2}-\frac{13}{72\epsilon}+\frac{1}{24}\,\zeta(2)+\frac{133}{864}\right) \times\int d^3p\;\overline{\psi_v}(\mathbf{p})(\not p-m)\psi_v(\mathbf{p})+\frac{\alpha^2(Z\alpha)}{4\pi^4} \times\int\frac{d^3p\,d^3p'}{|\mathbf{p}-\mathbf{p}'|^2}\;\overline{\psi_v}(\mathbf{p})\gamma_0\psi_v(\mathbf{p}')\int_0^1 dz\;\frac{z^2(1-\frac{1}{3}z^2)}{1-z^2} \times\int_0^1\rho d\rho\;dx\;\ln\left(\frac{\Delta}{m^2}\right)+\frac{\alpha^2(Z\alpha)}{4\pi^4} \times\int_0^1 dz\;\frac{z^2(1-\frac{1}{3}z^2)}{1-z^2}\int_0^1 d\rho\;dx\int\frac{d^3p\;d^3p'}{|\mathbf{p}-\mathbf{p}'|^2}\,\frac{N}{\Delta}. \tag{7}$$

Here Δ and N are defined by

$$\Delta=1+\frac{1-z^2}{4(1-\rho)}\,[\rho m^2-\rho(1-\rho)\epsilon_v^2+\rho x\mathbf{p}^2 +\rho(1-x)\mathbf{p}'^2-\mathbf{Q}^2] \tag{8}$$

and

$$N=\psi_v^{\dagger}(\mathbf{p})\{4m\epsilon_v(1-\rho)\gamma_0+\epsilon_v(1-\rho)(\mathbf{p}+\mathbf{p}'-2\mathbf{Q})\cdot\boldsymbol{\alpha} -[\epsilon_v^2(1-\rho)^2+m^2]-(\mathbf{p}'-\mathbf{Q})\cdot\boldsymbol{\alpha}(\mathbf{p}-\mathbf{Q})\cdot\boldsymbol{\alpha}\}\psi_v(\mathbf{p}'), \tag{9}$$

with $\mathbf{Q}=\rho x\mathbf{p}+\rho(1-x)\mathbf{p}'$.

The $1/\epsilon^2$ and $1/\epsilon$ divergences in the 1P term are cancelled by similar ones in the 0P term as required by the Ward identity [9]. The finite integrals are evaluated using adaptive Monte Carlo methods [10]. Both terms enter first in order $(Z\alpha)^2$ a.u., but this spurious term cancels in the sum. To increase accuracy at low Z, subtraction terms that manifested the cancellation which could be evaluated analytically were included in the numerical integrations. The combined result is tabulated in the first column of Table I.

The MP term is evaluated in coordinate space. This term is ultraviolet finite, and we set $n=4$ at the beginning of the calculation. While doing the integration over the photon 4-momentum, we perform a Wick rotation $k_0\rightarrow i\omega$. In carrying out this rotation full or half poles are picked up in the first quadrant corresponding to bound states with energy $\epsilon_n\leqslant\epsilon_v$. These pole terms are then given by

$$\Delta E_v^{\rm pole}=\frac{\alpha^2}{\pi}\int_0^1 dz\;\frac{z^2(1-\frac{1}{3}z^2)}{1-z^2}\sum_{\epsilon_n\leqslant\epsilon_v}\left(1-\frac{1}{2}\,\delta_{nv}\right) \times\int\frac{d^3x d^3y}{|\mathbf{x}-\mathbf{y}|}\;\overline{\psi_v}(\mathbf{x})\gamma_\mu\psi_n(\mathbf{x})\overline{\psi_n}(\mathbf{y}) \times\gamma^\mu\psi_v(\mathbf{y})e^{-\omega_n|\mathbf{x}-\mathbf{y}|}, \tag{10}$$

where $\omega_n^2=4m^2/(1-z^2)-(\epsilon_v-\epsilon_n)^2$.

The remaining part of the MP term after the Wick rotation is

$$\Delta E_v^{\rm MP}=-\frac{\alpha^2}{2\pi^2}\int_0^1 dz\;\frac{z^2(1-\frac{1}{3}z^2)}{1-z^2}\int d\omega\int\frac{d^3x\;d^3y}{|\mathbf{x}-\mathbf{y}|} \times e^{-\omega'|\mathbf{x}-\mathbf{y}|}\overline{\psi_v}(\mathbf{x})\gamma^\mu S_F^{\rm MP}(\mathbf{x},\mathbf{y};E_v-i\omega)\gamma_\mu\psi_v(\mathbf{y}), \tag{11}$$

where $\omega'^2=4m^2/(1-z^2)+\omega^2$.

The integration over x and y was done over an exponential grid for the radial coordinates while the integral over z was done using Gaussian integration. It was found necessary to use a rather fine grid, with several thousand points, to be able to control the numerics of the calculation. The MP term

TABLE I. Breakdown of the fourth-order vacuum-polarization result. $[-x]$ denotes multiplication by 10^{-x}, and the units are a.u.

Z	0P+1P	MP	Total	Lowest plus first order	Inferred higher order
5	2.039[−8]	0.353(18)[−8]	2.392(18)[−8]	2.401[−8]	−0.009(18)[−8]
7	7.762[−8]	1.401(23)[−8]	9.163(23)[−8]	8.992[−8]	0.171(23)[−8]
10	3.200[−7]	0.566(17)[−7]	3.766(17)[−7]	3.601[−7]	0.165(17)[−7]
12	6.599[−7]	1.162(22)[−7]	7.761(22)[−7]	7.268[−7]	0.493(22)[−7]
15	1.602[−6]	0.263(03)[−6]	1.865(03)[−6]	1.701[−6]	0.164(03)[−6]
17	2.637[−6]	0.414(05)[−6]	3.051(05)[−6]	2.727[−6]	0.324(05)[−6]
20	5.047[−6]	0.740(28)[−6]	5.787(28)[−6]	4.993[−6]	0.794(28)[−6]
22	7.392[−6]	1.032(46)[−6]	8.424(46)[−6]	7.085[−6]	1.339(46)[−6]
25	1.236[−5]	0.161(06)[−5]	1.397(06)[−5]	1.125[−5]	0.272(06)[−5]
27	1.687[−5]	0.210(08)[−5]	1.897(09)[−5]	1.480[−5]	0.417(09)[−5]
30	2.589[−5]	0.302(12)[−5]	2.891(12)[−5]	2.139[−5]	0.752(12)[−5]
40	8.501[−5]	0.802(36)[−5]	9.303(36)[−5]	5.530[−5]	3.773(36)[−5]
50	2.210[−4]	0.173(06)[−4]	2.383(06)[−4]	1.050[−4]	1.333(06)[−4]
60	5.006[−4]	0.349(17)[−4]	5.355(17)[−4]	1.555[−4]	3.800(17)[−4]
70	1.042[−3]	0.069(04)[−3]	1.111(04)[−3]	0.173[−3]	0.938(04)[−3]
80	2.065[−3]	0.146(04)[−3]	2.211(04)[−3]	0.098[−3]	2.113(04)[−3]
90	4.005[−3]	0.330(05)[−3]	4.335(05)[−3]	−0.158[−3]	4.493(05)[−3]
92	4.572[−3]	0.367(05)[−3]	4.939(05)[−3]	−0.242[−3]	5.181(05)[−3]
100	7.830[−3]	0.809(06)[−3]	8.639(06)[−3]	−0.721[−3]	9.360(06)[−3]

turns into a sum over partial waves. As with the 0P and 1P terms, spurious terms of order $(Z\alpha)^2$ appear in the pole and Wick rotated parts of the MP term. In the latter they are associated with the first partial wave $(l=0)$. For this reason that wave was separated out and evaluated with high accuracy, and combined with the pole term. The sum is then added to the remaining partial waves, which contribute in the correct order, and the result presented in the second column of Table I. The numerical difficulties of the problem as compared to the self-energy calculation have to do with the higher-energy scales characteristic of the vacuum-polarization loop. Particularly at low Z, the asymptotic region in the one-loop self-energy calculation is reached well below an electron mass, but because the energy scale of the vacuum-polarization loop is two electron masses, much higher values of ω are needed to reach the asymptotic limit. This requires significant modification of the routines to solve for the Green's functions, and also leads to slower convergence of the partial wave expansion. The observed fall off at high partial waves (the calculation went to $l=16$) is only $1/l^2$ as opposed to the $1/l^3$ behavior of the one-loop self-energy. While a fit to a power series $a/l^2+b/l^3+c/l^4$ allows the sum to be continued to infinity, the uncertainties in the fit lead to the numerical errors quoted for the MP term, which are the largest errors in the problem.

While the present calculation is valid to all orders in $(Z\alpha)$, it is of interest to compare it with the known expansion,

$$E=[0.014\,392-0.023\,208(Z\alpha)](Z\alpha)^4 \text{ a.u.}, \qquad (12)$$

where the first number is known analytically [11] to be $5/216-7/(81\pi^2)$. This result is tabulated in the fourth column of Table I. As expected, at low Z the difference between the calculations is relatively small. However, even by $Z=30$, a 30% difference is seen, and beyond that point the expansion in $Z\alpha$ breaks down dramatically, as happens also with the one-loop self-energy. Of particular note is the 20-fold enhancement at $Z=92$, which arises from the almost exact cancellation of the first two terms of the power series.

As a check on the calculation, this procedure was reversed at low Z in the following way. Rather than assume the above behavior, we instead made a fit to

$$E=[A+B(Z\alpha)+C(Z\alpha)^2\ln(Z\alpha)](Z\alpha)^4 \text{ a.u.} \qquad (13)$$

We found $A=0.0143(2)$, $B=-0.022(3)$, and $C=-0.04(1)$, consistent within the errors with the lower-order results, and incidentally indicating the presence of the higher-order logarithmic term, which is expected on power counting grounds. We also attempted to include a constant term in order $(Z\alpha)^6$, but the numerical errors in our calculation prohibited a meaningful determination of this coefficient.

The next step in this calculation is the exact calculation of Fig. 1(a). What we have calculated is the analog of the Uehling potential term [12], and there remains the calculation of the analog of the Wichmann-Kroll terms [13]. The first corrections to the result presented here are the four-photon graphs, which enter in order $(Z\alpha)^5$ a.u., and have already been evaluated in Refs. [6, 7]. We intend to follow the approach of Soff and Mohr [14] in this calculation, which will pick up all higher-order terms in $Z\alpha$ in addition to the four-photon contribution.

The heart of the calculation is the evaluation of the remaining diagrams of Fig. 1. There are two difficulties that we wish to note in connection with them. The first arises from our using Green's functions to represent the propagators, as opposed to using a spectral representation. After separating out angular dependence, these functions break

into two parts, as they depend on the magnitude of two radial coordinates in different ways depending on which is larger. Because there are two photon propagators and three fermion propagators, there are 32 different regions to be considered. While symmetries reduce the actual number to be coded, this makes the problem significantly more complex than the one-loop self-energy. The second difficulty has to do with renormalization. In the one-loop Lamb shift, breaking the propagator into three parts, 0P, 1P, and MP, allows isolation of all ultraviolet divergences in the first two parts. If the same procedure is followed in the two-loop case, breaking the three electron propagators up in this way leads again to a large number of terms, as was found in the recent treatment of Ref. [15]. We are presently attempting to devise a more compact treatment of the ultraviolet divergences that will allow the numerical evaluation of these remaining diagrams. We are particularly interested in the higher-order terms in $Z\alpha$ that are automatically contained in calculations that use exact Dirac-Coulomb propagators: the large size of the first-order corrections found in Refs. [3, 4] makes it possible that these terms could play a role in the interpretation of the Lamb shift in hydrogen. At high Z, we would also expect to see the behavior already demonstrated in this paper for the vacuum-polarization part of the calculation, a complete departure of the exact result from the calculation carried out to first order in $Z\alpha$.

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