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Calculation of the Electron Self-Energy for Low Nuclear Charge

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We present a nonperturbative numerical evaluation of the one-photon electron self-energy for hydrogenlike ions with low nuclear charge numbers $Z = 1$ to 5. Our calculation for the $1S$ state has a numerical uncertainty of 0.8 Hz for hydrogen and 13 Hz for singly ionized helium. Resummation and convergence acceleration techniques that reduce the computer time by about 3 orders of magnitude were employed in the calculation. The numerical results are compared to results based on known terms in the expansion of the self-energy in powers of $Z\alpha$. [S0031-9007(98)08043-0]

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Recently, there has been a dramatic increase in the accuracy of experiments that measure the transition frequencies in hydrogen and deuterium [1,2]. This progress is due in part to the use of frequency chains that bridge the range between optical frequencies and the microwave cesium time standard. The most accurately measured transition is the $1S$-$2S$ frequency in hydrogen; it has been measured with a relative uncertainty of 3.4×10^{-13} or 840 Hz. With trapped hydrogen atoms, it should be feasible to observe the $1S$-$2S$ frequency with an experimental linewidth that approaches the 1.3 Hz natural width of the $2S$ level [3,4]. Indeed, it is likely that transitions in hydrogen will eventually be measured with an uncertainty below 1 Hz [5,6].

In order for the anticipated improvement in experimental accuracy to provide better values of the fundamental constants or better tests of QED, there must be a corresponding improvement in the accuracy of the theory of the energy levels in hydrogen and deuterium, particularly in the radiative corrections that constitute the Lamb shift. As a step toward a substantial improvement of the theory, we have carried out a numerical calculation of the one-photon self-energy of the $1S$ state in a Coulomb field for values of the nuclear charge $Z = 1$, 2, 3, 4, and 5. This is the first complete calculation of the self-energy at low Z and provides a result that contributes an uncertainty of about 0.8 Hz in hydrogen and deuterium. This is a decrease in uncertainty of more than 3 orders of magnitude over previous results.

Among all radiative corrections, the largest by several orders of magnitude are the one-photon self-energy and vacuum polarization corrections. Of these, the larger and historically most problematic is the self-energy. Analytic calculations of the electron self-energy at low nuclear charge Z have extended over 50 years. The expansion parameter in the analytic calculations is the strength of the external binding field $Z\alpha$. This expansion is semianalytic [i.e., it is an expansion in powers of $Z\alpha$ and $\ln(Z\alpha)^{-2}$]. The leading term was calculated in [7]. It is of the order of $\alpha\,(Z\alpha)^4\,\ln(Z\alpha)^{-2}$ in units of $m_e\,c^2$, where m_e is the mass of the electron. In subsequent work [7–25], higher-order coefficients were evaluated.

The analytic results are relevant to low-Z systems. For high Z, the complete one-photon self-energy has been calculated without expansion in $Z\alpha$ by numerical methods [26–37]. However, such numerical evaluations at low nuclear charge suffer from severe loss of numerical significance at intermediate stages of the calculation and slow convergence in the summation over angular momenta. As a consequence, the numerical calculations have been confined to higher Z.

Despite these difficulties, the numerical calculations at higher Z could be used together with the power-series results to extrapolate to low Z with an assumed functional form in order to improve the accuracy of the self-energy at low Z [30]; until now, this approach has provided the most accurate theoretical prediction for the one-photon self-energy of the $1S$ state in hydrogen [38].

However, this method is not completely satisfactory. The extrapolation procedure gives a result with an uncertainty of 1.7 kHz, but employs a necessarily incomplete analytic approximation to the higher-order terms. It therefore contains a component of uncertainty that is difficult to reliably assess. Termination of the power series at the order of $\alpha\,(Z\alpha)^6$ leads to an error of 27 kHz. After the inclusion of a result recently obtained in [25] for the logarithmic term of order $\alpha\,(Z\alpha)^7\,\ln(Z\alpha)^{-2}$ the error is still 13 kHz.

A detailed comparison between the analytic and numerical approaches has been inhibited by the lack of accurate numerical data for low nuclear charge. The one-photon problem is especially well suited for such a comparison because five terms in the $Z\alpha$ expansion have been checked in independent calculations. The known terms correspond to the coefficients A_{41}, A_{40}, A_{50}, A_{62}, and A_{61} listed below in Eq. (3).

The energy shift ΔE_{SE} due to the electron self-energy is given by

$$\Delta E_{\mathrm{SE}} = \frac{\alpha}{\pi}\,\frac{(Z\alpha)^4}{n^3}\,m_e c^2 F(Z\alpha)\,, \qquad (1)$$

where n is the principal quantum number. For a particular atomic state, the dimensionless function F depends only on one argument, the coupling $Z\alpha$. The semianalytic expansion of $F(Z\alpha)$ about $Z\alpha = 0$ gives rise to the following terms:

$$F(Z\alpha) = A_{41}\ln(Z\alpha)^{-2} + A_{40} + (Z\alpha)A_{50} + (Z\alpha)^2 \times [A_{62}\ln^2(Z\alpha)^{-2} + A_{61}\ln(Z\alpha)^{-2} + G_{\mathrm{SE}}(Z\alpha)], \quad (2)$$

where $G_{\mathrm{SE}}(Z\alpha)$ represents the nonperturbative self-energy remainder function. The first index of the A coefficients gives the power of $Z\alpha$ [including the $(Z\alpha)^4$ prefactor from Eq. (1)]; the second corresponds to the power of the logarithm. For the $1S$ ground state, which we investigate in this Letter, the terms A_{41} and A_{40} were obtained in [7–13]. The correction term A_{50} was found in [14–16]. The higher-order corrections A_{62} and A_{61} were evaluated and confirmed in [17–21]. The results are

$$A_{41} = \frac{4}{3}, \qquad A_{40} = \frac{10}{9} - \frac{4}{3}\ln k_0,$$
$$A_{50} = 2\pi\left(\frac{139}{64} - \ln 2\right), \qquad A_{62} = -1, \quad (3)$$
$$A_{61} = \frac{28}{3}\ln 2 - \frac{21}{20}.$$

The Bethe logarithm $\ln k_0$ has been evaluated, e.g., in [39,40] as $\ln k_0 = 2.984\,128\,555\,8(3)$.

For our high-accuracy, numerical calculation of $F(Z\alpha)$, we divide the calculation into a high- and a low-energy part (see Ref. [28]). Except for a further separation of the low-energy part into an infrared part and a middle-energy part, which is described in [41] and not discussed further here, we use the same integration contour for the virtual photon energy and basic formulation as in [28].

The numerical evaluation of the radial Green function of the bound electron (see Eq. (A.16) in [28]) requires the calculation of the Whittaker function $W_{\kappa,\mu}(x)$ (see [42], p. 296) over a very wide range of parameters κ, μ, and arguments x. Because of numerical cancellations in subsequent steps of the calculation, the function W has to be evaluated to one part in 10^{24}. In a problematic intermediate region, which is given approximately by the range $15 < x < 250$, we found that resummation techniques applied to the divergent asymptotic series of the function W provide a numerically stable and efficient evaluation scheme. These techniques follow ideas outlined in [43] and are described in detail in [41].

For the acceleration of the slowly convergent angular momentum sum in the high-energy part (see Eq. (4.3) in [29]), we use the combined nonlinear-condensation transformation [44]. This transformation consists of two steps: First, we apply the van Wijngaarden condensation transformation [45] to the original series to transform the slowly convergent monotone input series into an alternating series [46]. In the second step, the convergence of the alternating series is accelerated by the δ transformation (see Eq. (3.14) in [44]). The δ transformation acts on the alternating series much more effectively than on the original input series. The highest angular momentum, characterized by the Dirac quantum number κ, included in the present calculation is about 3 500 000. However, even in these extreme cases, evaluation of less than 1 000 terms of the original series is required. As a result, the computer time for the evaluation of the slowly convergent angular momentum expansion is reduced by roughly 3 orders of magnitude. The convergence acceleration techniques remove the principal numerical difficulties associated with the singularity of the relativistic propagators for nearly equal radial arguments. These singularities are present in all QED effects in bound systems, irrespective of the number of photons involved. It is expected that these techniques could lead to a similar decrease in computer time in the calculation of QED corrections involving more than one photon.

In the present calculation, numerical results are obtained for the scaled self-energy function $F(Z\alpha)$ for the nuclear charges $Z = 1$, 2, 3, 4, and 5 (see Table I). The value of α used in the calculation is $\alpha_0 = 1/137.036$. This is close to the current value from the anomalous magnetic moment of the electron [47]:

$$1/\alpha = 137.035\,999\,58(52).$$

The numerical data points are plotted in Fig. 1, together with a graph of the function determined by the analytically known lower-order coefficients listed in Eq. (3).

In order to allow for a variation of the fine-structure constant, we repeated the calculation with two more values of α, which are

$$1/\alpha_> = 137.035\,999\,5 \quad \text{and} \quad 1/\alpha_< = 137.036\,000\,5.$$

On the assumption that the main dependence of F on $Z\alpha$ is represented by the lower-order terms in (3), the change in $F(Z\alpha)$ due to the variation in α is

$$\frac{\partial F(Z\alpha)}{\partial\alpha}\,\delta\alpha = -2A_{41}\frac{\delta\alpha}{\alpha} + [ZA_{50} + \mathrm{O}(\alpha\ln^2\alpha)]\delta\alpha$$

for a given nuclear charge Z. Based on this analytic estimate, we expect a variation

$$F(Z\alpha_>) - F(Z\alpha_0) \approx F(Z\alpha_0) - F(Z\alpha_<) \approx -9\times 10^{-9}$$

TABLE I. Scaled self-energy function and nonperturbative self-energy remainder function for low-Z hydrogenlike systems.

	$F(Z\alpha_0)$ and $G_{\mathrm{SE}}(Z\alpha_0)$	
Z	$F(Z\alpha_0)$	$G_{\mathrm{SE}}(Z\alpha_0)$
1	10.316 793 650(1)	−30.290 24(2)
2	8.528 325 052(1)	−29.770 967(5)
3	7.504 503 422(1)	−29.299 170(2)
4	6.792 824 081(1)	−28.859 222(1)
5	6.251 627 078(1)	−28.443 472 3(8)

for the different values of α. This variation is in fact observed in our calculation. For example, for the case $Z = 2$ we find

$$F(2\alpha_<) = 8.528\,325\,061(1)\,,$$
$$F(2\alpha_0) = 8.528\,325\,052(1) \quad \text{and}$$
$$F(2\alpha_>) = 8.528\,325\,043(1)\,.$$

This constitutes an important stability check on the numerics, and it confirms that the main dependence of F on its argument is indeed given by the lowest-order analytic coefficients A_{41} and A_{50}.

In addition to the results for $F(Z\alpha_0)$, numerical results for the nonperturbative self-energy remainder function $G_{\rm SE}(Z\alpha_0)$ are also given in Table I. The results for the remainder function are obtained from the numerical data for $F(Z\alpha_0)$ by direct subtraction of the analytically known terms corresponding to the coefficients A_{41}, A_{40}, A_{50}, A_{62}, and A_{61} [see Eqs. (2) and (3)]. Note that because the dependence of F on $Z\alpha$ is dominated by the subtracted lower-order terms, we have at the current level of accuracy $G_{\rm SE}(Z\alpha_<) = G_{\rm SE}(Z\alpha_0) = G_{\rm SE}(Z\alpha_>)$. The numerical uncertainty of our calculation is $0.8 \times Z^4$ Hz in frequency units.

A sensitive comparison of numerical and analytic approaches to the self-energy can be made by extrapolating the nonperturbative self-energy remainder function $G_{\rm SE}(Z\alpha)$ to the point $Z\alpha = 0$. It is expected that the function $G_{\rm SE}(Z\alpha)$ approaches a constant in the limit $Z\alpha \to 0$. This constant is referred to as $G_{\rm SE}(0) \equiv A_{60}$. In the analytic approach, much attention has been devoted to the coefficient A_{60} [21–24]. The correction has proven to be difficult to evaluate, and analytic work on A_{60} has extended over three decades. A step-by-step comparison of the analytic calculations has not been feasible, because the approaches to the problem have differed widely. An additional difficulty is the isolation of terms which contribute in a given order in $Z\alpha$, i.e., the isolation of only those terms which contribute to A_{60} (and not to any higher-order coefficients).

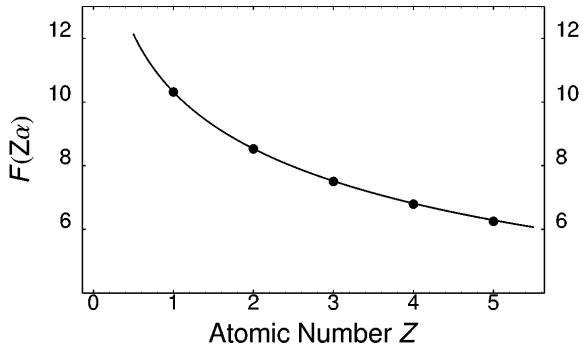

FIG. 1. The self-energy function $F(Z\alpha)$. The points are the numerical results of this work; the curve is given by the analytically known terms that correspond to the coefficients listed in Eq. (3).

In order to address the question of the consistency of A_{60} with our numerical results, we perform an extrapolation of our data to the point $Z\alpha = 0$. The extrapolation procedure is adapted to the problem at hand. We fit $G_{\rm SE}$ to an assumed functional form which corresponds to A_{60}, A_{71}, and A_{70} terms, with the coefficients to be determined by the fit. We find that our numerical data is consistent with the calculated value $A_{60} = -30.924\,15(1)$ [24,48]. It is difficult to assess the seventh-order logarithmic term A_{71}, because the extrapolated value for A_{71} is very sensitive to possible eighth-order triple and double logarithmic terms, which are unknown. We obtain as an approximate result $A_{71} = 5.5(1.0)$, and we therefore cannot conclusively confirm the result [25]

$$A_{71} = \pi\left(\frac{139}{64} - \ln 2\right) = 4.65\,.$$

Since our all-order numerical evaluation eliminates the uncertainty due to higher-order terms, we do not pursue this question any further.

The numerical data points of the function $G_{\rm SE}(Z\alpha)$ are plotted in Fig. 2 together with the value $G_{\rm SE}(0) = A_{60} = -30.924\,15(1)$. For a determination of the Lamb shift, the dependence of $G_{\rm SE}$ on the reduced mass $m_{\rm r}$ of the system has to be restored. In general, the coefficients in the analytic expansion (2) acquire a factor $(m_{\rm r}/m_{\rm e})^3$, because of the scaling of the wave function. Terms associated with the anomalous magnetic moment are proportional to $(m_{\rm r}/m_{\rm e})^2$ [49]. The nonperturbative remainder function $G_{\rm SE}$ is assumed to be approximately proportional to $(m_{\rm r}/m_{\rm e})^3$, but this has not been proved rigorously. Work is currently in progress to address this question [50].

We conclude with a brief summary of the results of this Letter. (i) We have obtained accurate numerical results for the self-energy at low nuclear charge. Previously, severe numerical cancellations have been a problem for these evaluations. (ii) For a particular example, we have addressed the question of how well semianalytic expansions represent all-order results at low nuclear charge. Our numerical data is consistent with the value $A_{60} = -30.924\,15(1)$ [24,48]. (iii) Numerical techniques

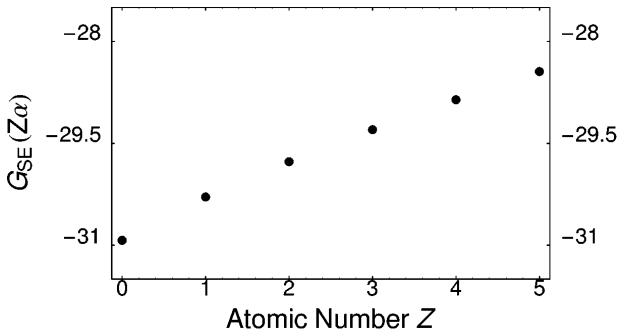

FIG. 2. Results for the scaled self-energy remainder function $G_{\rm SE}(Z\alpha)$ at low Z.

[44] have been developed that reduce the computer time for the problem by about 3 orders of magnitude.

The calculation presented here is of importance for the interpretation of measurements in hydrogen, deuterium and singly ionized helium and for the improvement of the Rydberg constant, because of recent and projected progress in accuracy. In the determination of the Rydberg constant, uncertainty due to the experimentally determined proton radius can be eliminated by comparing the frequencies of more than one transition [2]. We have shown that an all-order calculation can provide the required accuracy if suitable numerical methods are used.

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