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Electron self-energy for higher excited S levels

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A nonperturbative numerical evaluation of the one-photon electron self-energy for the $3S$ and $4S$ states with charge numbers $Z=1$ to 5 is described. The numerical results are in agreement with known terms in the expansion of the self-energy in powers of $Z\alpha$.

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In this Brief Report, we consider the one-loop self-energy shift which is the dominant radiative correction to the energy of hydrogenic bound states. For high-precision spectroscopy, S states are rather important because they can be excited from the ground state via Doppler-free two-photon spectroscopy. We calculate the self-energy numerically to high accuracy for $3S$ and $4S$ states (nuclear charge number $Z = 1, \dots, 5$). We follow the approach previously outlined for $1S$ (Ref. [1]) and $2S$ and $2P$ states (Ref. [2]).

The natural unit system with $\hbar=c=m_e=1$ and $e^2=4\pi\alpha$ is employed, as is customary in bound-state quantum electrodynamics. The (real part of the) energy shift ΔE_{SE} due to the electron self-energy radiative correction is usually written as [3]

$$\Delta E_{SE} = \frac{\alpha (Z\alpha)^4 m_e}{\pi n^3} F(nl_j, Z\alpha), \quad (1)$$

where F is a dimensionless quantity. In writing the expression $F(nl_j, Z\alpha)$, we follow the usual spectroscopic notation for an atomic state with principal quantum number n , orbital angular momentum l and total electron angular momentum j .

The leading terms in the semianalytic expansion of $F(nS_{1/2}, Z\alpha)$ about $Z\alpha=0$ read

$$\begin{aligned} F(nS_{1/2}, Z\alpha) &= A_{41}(nS_{1/2}) \ln(Z\alpha)^{-2} + A_{40}(nS_{1/2}) \\ &+ (Z\alpha) A_{50}(nS_{1/2}) + (Z\alpha)^2 [A_{62}(nS_{1/2}) \ln^2(Z\alpha)^{-2} \\ &+ A_{61}(nS_{1/2}) \ln(Z\alpha)^{-2} + G_{SE}(nS_{1/2}, Z\alpha)]. \end{aligned} \quad (2)$$

The A coefficients have two indices, the first of which denotes the power of $Z\alpha$ [including those powers explicitly contained in Eq. (1)], while the second index denotes the power of the logarithm $\ln(Z\alpha)^{-2}$.

We now list the analytic coefficients and the Bethe logarithms relevant to the atomic states under investigation [4–23],

$$A_{41}(nS_{1/2}) = \frac{4}{3}, \quad (3a)$$

$$A_{40}(nS_{1/2}) = \frac{10}{9} - \frac{4}{3} \ln k_0(nS), \quad (3b)$$

$$A_{50}(nS_{1/2}) = 4\pi \left[\frac{139}{128} - \frac{1}{2} \ln 2 \right], \quad (3c)$$

$$A_{62}(nS_{1/2}) = -1. \quad (3d)$$

A_{61} coefficients read

$$A_{61}(1S_{1/2}) = \frac{21}{20} + \frac{28}{3} \ln 2, \quad (4a)$$

$$A_{61}(2S_{1/2}) = \frac{67}{30} + \frac{16}{3} \ln 2, \quad (4b)$$

$$A_{61}(3S_{1/2}) = \frac{6163}{1620} + \frac{28}{3} \ln 2 - 4 \ln 3, \quad (4c)$$

$$A_{61}(4S_{1/2}) = \frac{4}{3} \ln 2 + \frac{391}{80}. \quad (4d)$$

The Bethe logarithms $\ln k_0(nS)$ are known [24–29], and we here present a reevaluation,

$$\ln k_0(1S) = 2.984\,128\,555\,765\,497\,611(1), \quad (5a)$$

$$\ln k_0(2S) = 2.811\,769\,893\,120\,563\,520(1), \quad (5b)$$

$$\ln k_0(3S) = 2.767\,663\,612\,491\,821\,190(1), \quad (5c)$$

$$\ln k_0(4S) = 2.749\,811\,840\,454\,057\,422(1). \quad (5d)$$

The evaluation of the coefficient

$$A_{60}(nS_{1/2}) \equiv \lim_{Z\alpha \rightarrow 0} G_{SE}(nS_{1/2}, Z\alpha) \quad (6)$$

has been historically problematic [19–23], and it has therefore been a considerable challenge to reliably estimate the self-energy remainder function G_{SE} , especially in the range of low nuclear charge number Z . Our calculation of the non-perturbative (in $Z\alpha$) electron self-energy for the $3S_{1/2}$ state (see Table I) has a numerical uncertainty of 2 Hz in atomic hydrogen. For the $4S_{1/2}$ state, the numerical uncertainty is $Z^4 \times 3$ Hz (see Table II). The value of the fine-structure constant α employed in the calculation is $\alpha^{-1} = 137.036$; this is close to the 1998 and 2002 CODATA recommended values

TABLE I. Numerical results for the scaled self-energy function F ($3S$ state) and the self-energy remainder function G_{SE} , in the regime of low nuclear charge numbers Z .

Z	$F(3S_{1/2}, Z\alpha)$	$G_{SE}(3S_{1/2}, Z\alpha)$
1	10.605 614 22(5)	-31.047 7(9)
2	8.817 615 14(5)	-30.512 6(2)
3	7.794 461 17(5)	-30.022 7(1)
4	7.083 612 42(5)	-29.564 53(6)
5	6.543 385 98(5)	-29.130 61(4)

[30,31]. The entries for the self-energy remainder function G_{SE} in Tables I and II are in agreement with those used in the latest adjustment of the fundamental physical constants [31] (the G_{SE} values used in [31] are based on an extrapolation of numerical data previously obtained [32] for higher nuclear charge numbers). Our all-order evaluation eliminates any uncertainty due to the unknown higher-order analytic terms that contribute to the bound electron self-energy of $3S$ and $4S$

TABLE II. Numerical results for the scaled self-energy function $F(4S_{1/2}, Z\alpha)$ and the self-energy remainder function G_{SE} .

Z	$F(4S_{1/2}, Z\alpha)$	$G_{SE}(4S_{1/2}, Z\alpha)$
1	10.629 388 4(2)	-30.912(4)
2	8.841 324 1(2)	-30.380 0(9)
3	7.818 078 5(2)	-29.892 4(4)
4	7.107 116 6(2)	-29.437 1(2)
5	6.566 758 8(2)	-29.006 0(2)

states [see Eq. (2)]. This improves our knowledge of the spectrum of hydrogenlike atoms (e.g., atomic hydrogen, He^+).

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