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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 3*S* and 4*S* 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 3*S* and 4*S* states (nuclear charge number $Z=1,\ldots,5$). We follow the approach previously outlined for 1*S* (Ref. [1]) and 2*S* and 2*P* 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 $\Delta E_{\rm SE}$ due to the electron self-energy radiative correction is usually written as [3]

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

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

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

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],

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

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

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

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

A_{61} coefficients read

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

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

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

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

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

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

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

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

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

The evaluation of the coefficient

$$A_{60}(nS_{1/2})\equiv\lim_{Z\alpha\to0}G_{\rm SE}(nS_{1/2},Z\alpha) \tag{6}$$

has been historically problematic [19–23], and it has therefore been a considerable challenge to reliably estimate the self-energy remainder function $G_{\rm SE}$, especially in the range of low nuclear charge number Z. Our calculation of the nonperturbative (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 $Z^4\times3$ 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	$F(3S_{1/2},Z\alpha)$	$G_{\mathrm{SE}}(3S_{1/2},Z\alpha)$
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)

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	$F(4S_{1/2},Z\alpha)$	$G_{\mathrm{SE}}(4S_{1/2},Z\alpha)$
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)

[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 $4S$ states [see Eq. (2)]. This improves our knowledge of the spectrum of hydrogenlike atoms (e.g., atomic hydrogen, He^{+}).

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