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Self-energy values for *P* states in hydrogen and low-*Z* hydrogenlike ions

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We describe a nonperturbative (in $Z\alpha$) numerical evaluation of the one-photon electron self-energy for $3P_{1/2}$, $3P_{3/2}$, $4P_{1/2}$, and $4P_{3/2}$ states in hydrogenlike atomic systems with charge numbers $Z=1$ to 5. The numerical results are found to be in agreement with known terms in the expansion of the self-energy in powers of $Z\alpha$ and lead to improved theoretical predictions for the self-energy shift of these states.

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In this Brief Report, we consider the one-loop self-energy shift for excited *P* states in hydrogenlike systems. High-accuracy numerical calculations of this effect are notoriously difficult, especially in the region of low nuclear charge numbers *Z*, because the renormalization entails a loss of up to nine decimal figures in the numerical calculation (the bound-electron self-energy is a residual effect that corresponds to the difference of the divergent self-energy of the bound electron, minus the corresponding, also divergent, shift for a free electron).

Furthermore, the calculations are needed for a self-consistent determination of fundamental constants, which relies on the experimental/theoretical analysis of a number of hydrogenic transitions.

One may obtain rather accurate values for the so-called self-energy remainder functions by an interpolation [1] of results for high and low nuclear charge numbers, which rely on two different approaches: (i) direct numerical calculations at high nuclear charge numbers (see, e.g., [2], no $Z\alpha$-expansion), and (ii) analytic calculations at low nuclear charge numbers, employing the $Z\alpha$ expansion (see, e.g., [3]). In this case, the values obtained for low nuclear charge depend on the interpolation method used, as well as (of course) on the reliability of both the numerical calculations at high *Z* and the analytic calculations for a low nuclear charge number.

Here, we follow a third approach and calculate the self-energy without $Z\alpha$ expansion, at low *Z*, using a method described previously in [4–6]. Essentially, this method relies on an adequate formulation of the physical problem, by which divergent terms are suitably identified and calculated separately using semianalytic approaches, and on the use of efficient numerical methods for the high-accuracy calculation of the Green's function of the relativistic electron and for the evaluation of slowly convergent sums of intermediate angular momenta (it might be useful to mention the keyword "convergence acceleration" in that context [7]). On modern computer processors, it is not even necessary to parallelize the calculation; that latter approach had previously been employed in [4,5].

All calculations reported here are carried out in the no-recoil limit, which corresponds to an infinitely heavy nucleus. It might be instructive to recall the following subtlety, which is well known, and to include a slight detour: At the current level of accuracy and especially at low *Z*, the reduced-mass dependence of the self-energy should be included for a comparison of the effect with experiment. This can be done *a posteriori* by considering the semianalytic expansion in Eq. (2) below, using the formulas given in Eq. (2.5b) of Ref. [8], which indicate the reduced-mass dependence of the coefficients, and then the self-energy remainder values given in Tables I–IV in this Brief Report.

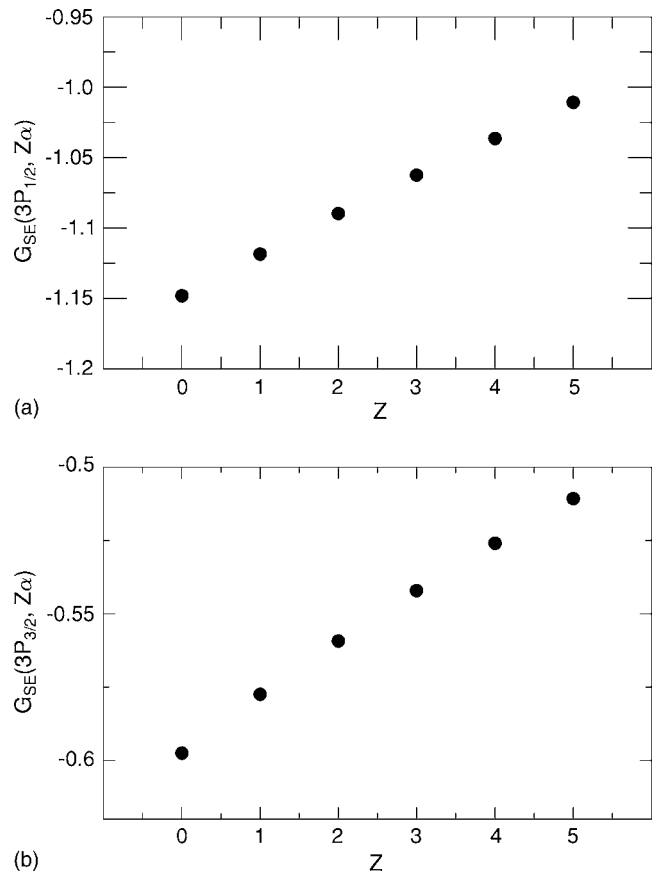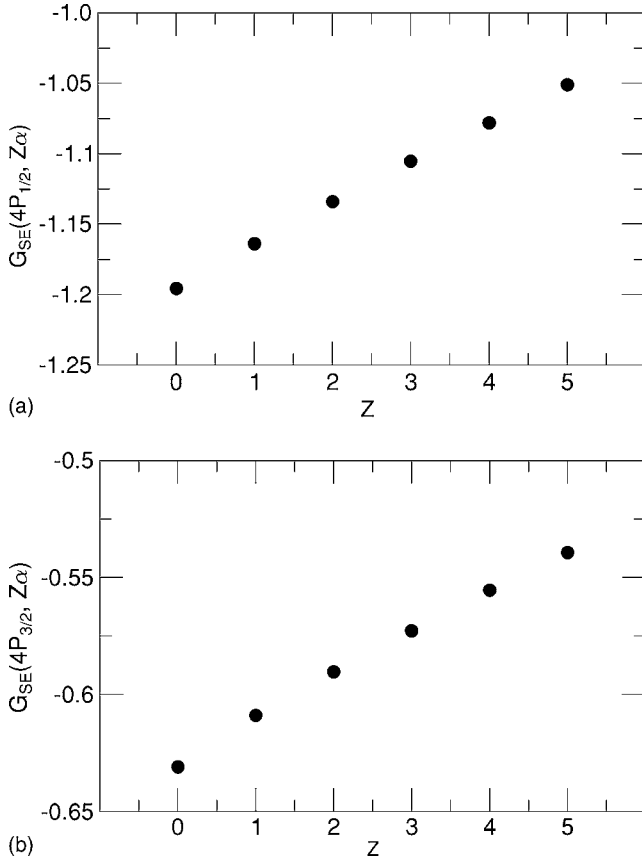Returning to the discussion of our calculation, we write

FIG. 1. A comparison of the self-energy remainder for $3P_{1/2}$ and $3P_{3/2}$ states, as listed in Tables I and II, to their low-*Z* limit, which is the A_{60} coefficient [see Eqs. (3) and (6)]. Here, *Z* is the nuclear charge, and the self-energy remainder G_{SE} is a dimensionless quantity. The nuclear charge number is denoted by *Z*.

FIG. 2. The analog of Fig. 1 for $4P_{1/2}$ and $4P_{3/2}$ states.

the (real part of the) energy shift ΔE_{SE} due to the electron self-energy radiative correction as [8]

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

where F is a dimensionless quantity (m_e is the electron mass, α is the fine-structure constant, and c is the speed of light in vacuum). In writing the expression $F(nL_j, Z\alpha)$, we follow the usual spectroscopic notation for the quantum numbers of the single electron in a hydrogenlike ion; namely, we denote the principal quantum number by n, the orbital angular momentum by L and the total electron angular momentum by j.

The leading terms in the semianalytic expansion of $F(nP_j, Z\alpha)$ about $Z\alpha = 0$ read as

TABLE I. Numerical results for the scaled self-energy function $F(3P_{1/2}, Z\alpha)$ and the self-energy remainder function G_{SE}, as defined in Eq. (1), in the regime of low nuclear charge numbers Z. See also Fig. 1(a).

Z	$F(3P_{1/2}, Z\alpha)$	$G_{SE}(3P_{1/2}, Z\alpha)$
1	−0.115 459 16(5)	−1.118 5(9)
2	−0.114 787 32(5)	−1.089 7(2)
3	−0.113 831 60(5)	−1.062 5(1)
4	−0.112 644 39(5)	−1.036 30(6)
5	−0.111 258 78(5)	−1.010 84(4)

TABLE II. The same as Table I, for the $3P_{3/2}$ state. See also Fig. 1(b).

Z	$F(3P_{3/2}, Z\alpha)$	$G_{SE}(3P_{3/2}, Z\alpha)$
1	0.134 414 38(5)	−0.577 5(9)
2	0.134 792 58(5)	−0.559 3(2)
3	0.135 332 45(5)	−0.542 1(1)
4	0.136 006 06(5)	−0.526 06(6)
5	0.136 795 05(5)	−0.510 76(4)

$$F(nP_j, Z\alpha) = A_{40}(nP_j) + (Z\alpha)^2 [A_{61}(nP_j)\ln(Z\alpha)^{-2}$$
$$+ G_{SE}(nP_j, Z\alpha)]. \qquad (2)$$

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

$$A_{60}(nS_{1/2}) \equiv \lim_{Z\alpha \to 0} G_{SE}(nS_{1/2}, Z\alpha), \qquad (3)$$

has been historically problematic.

We now list the analytic coefficients and the Bethe logarithms relevant to the atomic states under investigation, referring the reader to [9] for a more detailed discussion and further references,

$$A_{40}(nP_{1/2}) = -\frac{1}{6} - \frac{4}{3}\ln k_0(nP), \qquad (4a)$$

$$A_{40}(nP_{3/2}) = \frac{1}{12} - \frac{4}{3}\ln k_0(nP). \qquad (4b)$$

Numerical values for the Bethe logarithms $\ln k_0(nP)$ are well known [10,11].

The A_{61} coefficients for the states under investigation read as

$$A_{61}(3P_{1/2}) = \frac{268}{405}, \quad A_{61}(3P_{3/2}) = \frac{148}{405}, \qquad (5a)$$

$$A_{61}(4P_{1/2}) = \frac{499}{720}, \quad A_{61}(4P_{3/2}) = \frac{137}{360}. \qquad (5b)$$

The A_{60} coefficients have been evaluated in [9], and more recently in [3] to an increased accuracy,

$$A_{60}(3P_{1/2}) = -1.148\ 189\ 956(1), \qquad (6a)$$

TABLE III. The same as Tables I and II, for the $4P_{1/2}$ state. See also Fig. 2(a).

Z	$F(4P_{1/2}, Z\alpha)$	$G_{SE}(4P_{1/2}, Z\alpha)$
1	−0.110 425 6(1)	−1.164(2)
2	−0.109 720 3(1)	−1.134 1(5)
3	−0.108 717 9(1)	−1.105 5(2)
4	−0.107 471 8(1)	−1.078 1(1)
5	−0.106 016 8(1)	−1.051 20(8)

TABLE IV. Numerical results for the scaled self-energy function F and the self-energy remainder function G_{SE} for the $4P_{3/2}$ state. See also Fig. 2(b).

Z	$F(4P_{3/2}, Z\alpha)$	$G_{SE}(4P_{3/2}, Z\alpha)$
1	0.139 440 2(1)	−0.609(2)
2	0.139 832 7(1)	−0.590 4(5)
3	0.140 392 7(1)	−0.572 9(2)
4	0.141 091 6(1)	−0.555 5(1)
5	0.141 909 8(1)	−0.539 41(8)

$$A_{60}(3P_{3/2}) = -0.597\ 569\ 388(1), \qquad (6b)$$

$$A_{60}(4P_{1/2}) = -1.195\ 688\ 142(1), \qquad (6c)$$

$$A_{60}(4P_{3/2}) = -0.630\ 945\ 796(1). \qquad (6d)$$

Note that the result for $3P_{1/2}$ had been given inaccurately as −1.147 68(1) in [9].

Our calculation of the nonperturbative (in $Z\alpha$) electron self-energy for the $3P_j$ state (see Tables I and II) has a numerical uncertainty of 2 Hz in atomic hydrogen. For the $4P_j$ states, the numerical uncertainty is $1.3 \times Z^4$ Hz (see Tables III and IV). In the nonrecoil limit, our result for $4P_{1/2}$, $Z = 1$, corresponds to a self-energy shift of

$$\Delta E_{SE}(4P_{1/2}, Z = 1) = -1\ 404.239(1)\ \text{kHz}, \qquad (7)$$

which is in agreement with the result −1 404.240(2) kHz obtained in [12] via an interpolation of the low-Z analytic results and high-Z numerical data, confirming (in this particular case) the validity of the interpolation procedure used for various excited hydrogenic states in the latest adjustment of the fundamental physical constants [13]. Indeed, all entries for the self-energy remainder function G_{SE} in Tables I–IV are in agreement with those used in [13,14] for the determination of the fundamental constants, and for the precise calculation of hydrogenic energy levels using the method of least squares. Our all-order evaluation eliminates any uncertainty due to the unknown higher-order analytic terms that contribute to the bound electron self-energy of $3P$ and $4P$ states [see Eq. (2)] and improves our knowledge of the spectrum of hydrogenlike atoms (e.g. atomic hydrogen, He$^+$). Furthermore, the numerical data for the self-energy remainders *check* the validity of the highly involved analytic approach that led to the evaluation of the A_{60} coefficients, as listed in Eq. (6).

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