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Toward high-precision values of the self energy of non-S states in hydrogen and hydrogen-like ions

E.-O. Le Bigot, U.D. Jentschura, P. Indelicato, and P.J. Mohr

Abstract: The method and status of a study to provide numerical, high-precision values of the self-energy level shift in hydrogen and hydrogen-like ions is described. Graphs of the self energy in hydrogen-like ions with nuclear charge number between 20 and 110 are given for a large number of states. The self-energy is the largest contribution of Quantum Electrodynamics (QED) to the energy levels of these atomic systems. These results greatly expand the number of levels for which the self energy is known with a controlled and high precision. Applications include the adjustment of the Rydberg constant and atomic calculations that take into account QED effects.

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Résumé : Nous rapportons les derniers développements d'une étude destinée à fournir des valeurs numériques de grande précision du déplacement de self-énergie dans l'hydrogène et les ions hydrogénoïdes. Nous présentons des graphes de la self-énergie dans les ions hydrogénoïdes de nombre de charge compris entre 20 et 110, pour de nombreux niveaux. La self-énergie est la contribution la plus importante de l'électrodynamique quantique aux niveaux d'énergie de ces systèmes atomiques. Les résultats présentés étendent largement l'ensemble des niveaux atomiques dont on connaît le déplacement de self-énergie avec une précision importante et contrôlée. Les applications de ce travail incluent l'ajustement de la constante de Rydberg et les calculs atomiques qui prennent en compte les effets de l'électrodynamique quantique.

1. Introduction and outline

This paper presents graphs of new high-precision numerical values of the self energy shift in hydrogen-like ions, and describes work in progress on high-precision self energy values in hydrogen.

The self energy is the dominant contribution of quantum electrodynamics (QED) to the energy levels of these one-electron atomic systems (see, *e.g.*, Fig. 2 in Ref. [1]). The total energy of the orbiting electron can be expressed as the following sum (see, *e.g.*, Refs. [2, 3, 4]):

electron energy = Dirac (relativistic) energy + pure recoil + pure finite nuclear size

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E.-O. Le Bigot. Laboratoire Kastler Brossel, École Normale Supérieure et Université Pierre et Marie Curie, Case 74, 4 place Jussieu, 75005 Paris, France

U.D. Jentschura. Max-Planck-Institut für Kernphysik, Saupfercheckweg 1, 69117 Heidelberg, Germany

P. Indelicato. Laboratoire Kastler Brossel, École Normale Supérieure et Université Pierre et Marie Curie, Case 74, 4 place Jussieu, 75005 Paris, France

P.J. Mohr. National Institute of Standards and Technology, Mail Stop 8401, Gaithersburg, MD 20899-8401, USA

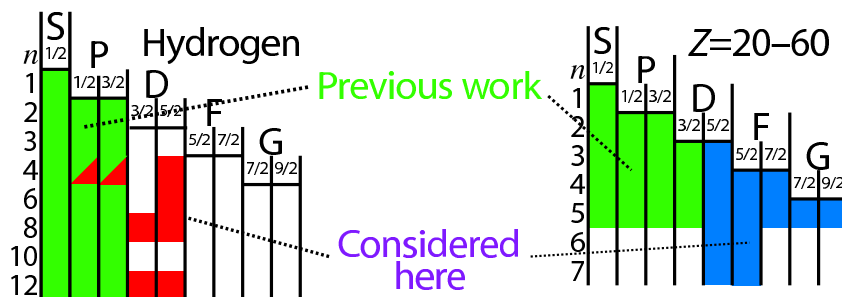
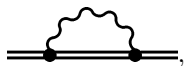


Fig. 1. Electron states for which a high-precision self-energy shift with known uncertainty has been obtained (through a method which does not treat the electron-nucleus interaction only *via* perturbation theory). n denotes the electron principal quantum number and Z is the nuclear charge number of the hydrogen-like ion. Previous studies have concentrated on lower- n and lower angular momentum states. The results presented here have applications in the adjustment of the Rydberg constant [13]: the new results for hydrogen were obtained for all the non-S levels of [7, p. 433], *i.e.*, for all the (non-S) levels that are implied in the principal spectroscopy experiments contributing to the Rydberg constant. The self energy of the states included in the figure can also be used for including QED effects in the energy levels of atoms and ions (possibly via extrapolations or interpolations).

+ pure QED + rest,

where the term denoted by “rest” encompasses other forces (strong and weak), as well as mixed effects (*e.g.*, the energy shift due to recoil in a QED process). The self energy is generally the largest contribution to the “pure QED” term, and in particular to the Lamb shift [5].

The self energy is the QED process in which the electron emits a photon and re-absorbs it, as is depicted in the corresponding Feynman diagram:



(1)

where the double line and the wavy line respectively represent the electron (bound to the nucleus) and a photon.

Calculating QED effects in atoms is of general interest. First, high-precision spectroscopy results can only be fully explained within QED; an example is the well-known Lamb shift [5] and its calculation by Bethe [6]. Second, precise atomic QED calculations, along with corresponding experiments, give some of the most precise determinations of some fundamental constants [7], notably the Rydberg constant [8] and the mass of the electron [9]; the fine structure constant α [10] and the proton charge radius [11] are also expected to be soon determined with very high accuracy from atomic studies. Last, highly-charged hydrogen-like ions allow for tests of QED in situations where an electron experiences a strong field. The electric field at the surface of a uranium nucleus is thus about $2 \cdot 10^{21}$ V/m [2, p. 230]; this value can for instance be compared to the characteristic field $2\pi m_e c^2 / (|e| \lambda_e)$ of about 10^{18} V/m that gives a non-negligible probability of spontaneous electron-positron pair creation in a volume λ_e^3 in a time λ_e/c [12, Eq. (6.41)]—here, c is the speed of light, and m_e , e and λ_e respectively denote the electron mass, charge and Compton wavelength (about $2 \cdot 10^{-12}$ m).

The purpose of this paper is to graphically present new self-energy shifts in hydrogen-like ions with nuclear charge number larger than 20. We also report the high-precision evaluation, for many states, of self energies in hydrogen, and briefly describe the method we used. All the self energies were calculated for a static, point nucleus (finite proton mass and non-zero proton radius effects can be treated as a perturbation). Hydrogen is a system in which precise numerical calculations that treat the electron-proton interaction without perturbation are recent and notoriously difficult [14, 15, 16]—numerical self-energy calculations were originally designed for highly-charged hydrogen-like ions [17,

18, 19, 20, 21]. The atomic states for which we calculated the self energy are depicted in Fig. 1, and extend the set of states considered in previous works.

The self-energy values considered here were obtained with a high precision, and a known uncertainty (which contrasts with perturbation calculations, in which omitted terms can be difficult to estimate [22]). In hydrogen, we take “high precision” to mean that energy shifts have an uncertainty of about 1 Hz: in fact, spectroscopy experiments are reaching the 1 Hz limit in the visible domain [23]. Having high-precision self-energy shifts available is also useful for obtaining precise extrapolations (see Sec. 4) and for performing comparisons between independent calculations.

2. Outline and notation

In this paper, the self-energy shifts \mathcal{E}_{SE} are expressed with the conventional “reduced” self energy F , which is defined by

$$\mathcal{E}_{\text{SE}}(nL_j, Z) = \frac{\alpha (Z\alpha)^4}{\pi n^3} F(nL_j, Z\alpha) m_e c^2, \quad (2)$$

where nL_j is the usual spectroscopic notation for an electron of principal quantum number n , orbital angular momentum L and total angular momentum j ; Z is the nuclear charge number, α is the fine structure constant, m_e the mass of the electron and c the speed of light. Much of the behavior of the self-energy shift \mathcal{E}_{SE} with n and Z is captured in this formula: F has the property of not varying much with these parameters (see, *e.g.*, Sec. 3)—the dependence of F on the angular momenta l and j can be estimated from the perturbation expansion of F (see, *e.g.*, App. A in Ref. [7]).

In the following, we present graphs of the self-energy values for middle- Z hydrogen-like ions (Sec. 3), and describe the way self energies were obtained in hydrogen (Sec. 4).

3. Self energy in middle- Z ions

This section presents graphs of self-energy values for hydrogen-like atoms of nuclear charge number Z comprised between 20 and 60. Figure 1 shows the states for which self-energy results are presented. The nucleus is approximated as a point-like charge of infinite mass. The main result of this part is displayed in Fig. 2, under the form of the reduced self energy F defined in Eq. (2). In the graphs of Fig. 2, each curve point took about two days of calculation time on a modern computer. The typical relative precision of these self-energy values is 10^{-5} (numerical values will be given elsewhere). As can be seen in the graphs, the reduced self energy of D, F and G states does not vary much with n and Z (changes of the order of 10 %). This implies that extrapolations of the self energy to states with other principal quantum numbers than those considered in Fig. 2 can be done to a good precision. We expect such a smooth behavior of F with n and Z to generally hold for electrons of higher angular momentum.

Calculating the self energy shift consists essentially in evaluating a multi-dimensional integral (see, *e.g.*, Ref. [2]):

$$\mathcal{E}_{\text{SE}}(nL_j, Z) = \int dz \int d^3x_2 \int d^3x_1 \phi^\dagger(\mathbf{x}_2) \mathcal{G}(\mathbf{x}_2, \mathbf{x}_1, z) \phi(\mathbf{x}_1), \quad (3)$$

where ϕ is the Dirac wave-function of the state for which the shift is calculated, and where \mathcal{G} contains the effect of both the photon and the electron propagating between the two interaction points in (1). In Eq. (3), the variable z represents the virtual energy of the photon, and the positions \mathbf{x}_1 and \mathbf{x}_2 are integrated over all the possible locations of the two interaction points in (1).

In order to compute (3), we used a method developed by one of us (P.J.M. [20, 21]), along with the corresponding code. Contrary to methods introduced before [17, 19], it allows for precise calculations of the electron self energy over a large range of nuclei ($Z = 5\text{--}110$ [25]); this was made possible

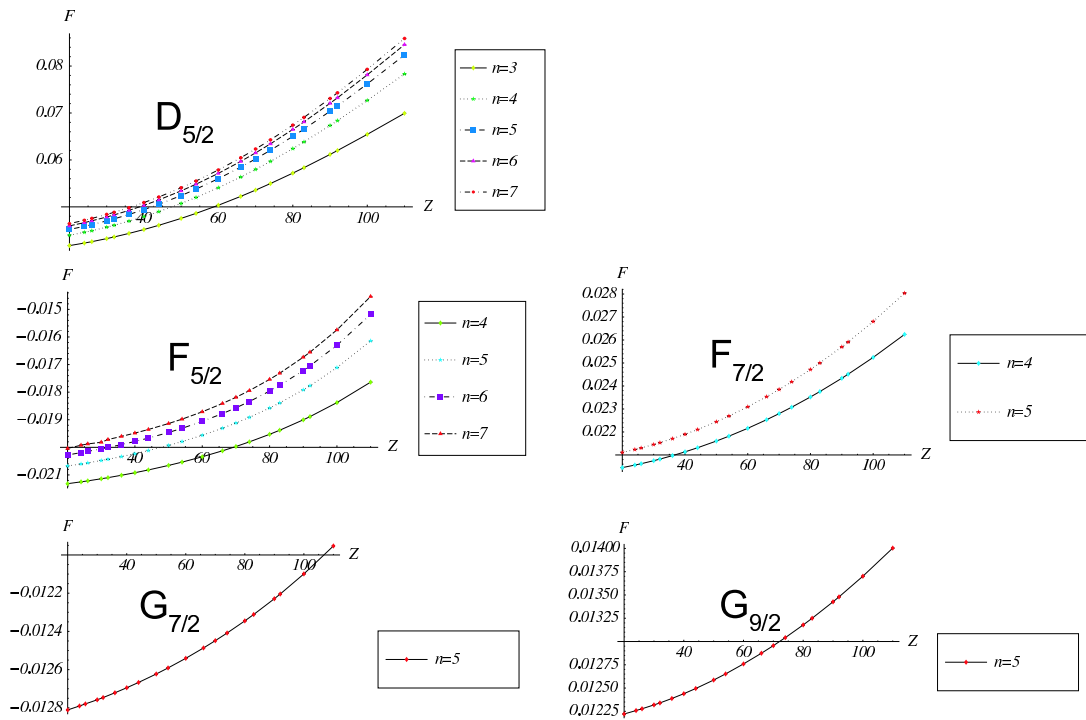


Fig. 2. Values of the reduced self energy F , for various D, F and G states of hydrogen-like ions, as a function of the nuclear charge number Z of the nucleus and of the principal quantum number n of the electron. The values for $Z < 60$ are new, while higher- Z results can be found in [24]. The weak dependence of F on n and Z indicates that the self energy shift \mathcal{E}_{SE} scales essentially as Z^4/n^3 , as can be seen from Eq. (2).

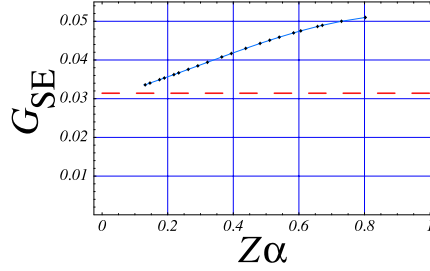


Fig. 3. Plot of the self-energy remainder $G_{\text{SE}}(Z\alpha)$ defined in Eq. (4), and calculated with the values displayed in Fig. 2, for the $4D_{5/2}$ level. The dashed line represents an independent calculation of $\lim_{Z \rightarrow 0} G_{\text{SE}}(Z\alpha)$. The curve is compatible with a convergence of the numerical values of G_{SE} toward the correct limit. Similar checks of the new self-energy values were performed for all the other levels considered in Fig. 2.

through the use of analytic expressions of the Dirac Green's function, and of an integration order in (3) that guarantees good convergence properties in numerical calculations. The code was incrementally improved along two directions: a more efficient handling of renormalization [26], and the possibility of calculating the self energy of states with “large” total angular momentum $j > 3/2$ [24]. The calculation of (3) requires high-precision evaluations of integrals and of hypergeometric functions (and in particular Whittaker functions).

The self-energy values in Fig. 2 were checked against perturbation theory results. In fact, the reduced self energy of non-S states can be expanded as (see, *e.g.*, App. A in Ref. [7]):

$$F(Z\alpha) = A_{40} + (Z\alpha)^2 \{A_{61} \ln[(Z\alpha)^{-2}] + G_{\text{SE}}(Z\alpha)\}, \quad (4)$$

where the dependence of the terms on the electron state nL_j is implicit; A_{40} is a coefficient which has been calculated for many states; A_{61} is known analytically; $G_{\text{SE}}(Z\alpha)$ is a remainder whose limit as $Z \rightarrow 0$ has recently been calculated for all the states considered here [27, 28]. In order to check our calculations of F , we made sure that the numerical values of $G_{\text{SE}}(Z\alpha)$ obtained from F and Eq. (4) were compatible with a convergence to the correct limit as $Z\alpha \rightarrow 0$. This procedure also implicitly checks the compatibility of the new numerical values of F with the values of A_{40} and A_{61} . An example of the curves that we plotted for verification purposes is given in Fig. 3.

The range of nuclear charges under consideration ($20 \leq Z < 60$) extends beyond the range of results of Ref. [24]. The orbital angular momentum of an $n = 5$ electron in the ground state of atoms can reach $l = 3$ (f states), and that of an $n = 6$ electron, $l = 2$ (d states); the self energy was thus calculated for both 5f and 6f states (see Fig. 2), so as to provide values that could be used in atomic calculations that incorporate QED corrections (see also Ref. [29]). The self energy was also calculated for higher- n d and f electrons, so as to cover some excited atomic states. Moreover, spectroscopy experiments with middle-charge hydrogen-like ions have been, and may be performed in the future: the self-energy values in Fig. 2, which represent the dominant QED shift, might be useful in interpreting coming experiments. Finally, these results, which do not treat the electron-nucleus interaction with perturbation theory, allow for checks of corresponding perturbation results [28].

4. Self energy in hydrogen

This section describes how we obtained self-energy shifts in hydrogen through interpolations and extrapolations, to a high precision (better than 2 Hz) for the hydrogen states included in Fig. 1. As for the middle- Z results, only the leading self-energy contribution \mathcal{E}_{SE} , obtained for a infinite-mass, point-like nucleus, is discussed here. With the extrapolation method described below, we obtained for

instance the self energy shift value

$$\mathcal{E}_{\text{SE}}(4\text{P}_{1/2}, Z = 1) = -1\,404.240(2) \text{ kHz.} \quad (5)$$

This value is consistent with previous estimates of the $4\text{P}_{1/2}$ self energy (see Ref. [30] and Ref. [7, p. 468]). Actual self energy values for the states included in Fig. 1 will be given elsewhere.

Value (5) can be compared to perturbation calculations. Thus, for non-S states, the reduced self energy in Eq. (2) is expanded as

$$F(Z\alpha) = A_{40} + (Z\alpha)^2\{A_{61} \ln[(Z\alpha)^{-2}] + A_{60}\} + (Z\alpha)^3 G_{\text{SE},7}(Z\alpha), \quad (6)$$

where A_{60} is a coefficient and $G_{\text{SE},7}(Z\alpha)$ a function which converges as $Z\alpha \rightarrow 0$ (see, *e.g.*, Eq. (7) in Ref. [28]). No other coefficient than the three present in (6) is currently known; references about the known coefficients can for instance be found in [28]. It is instructive to truncate expansion (6) to the first two terms, and estimate the self energy of a $4\text{P}_{1/2}$ electron as

$$\mathcal{E}_{\text{SE}}(4\text{P}_{1/2}, Z = 1) = -1\,403.5(7?) \text{ kHz,} \quad (7)$$

where the uncertainty is defined by letting $A_{60} + \alpha G_{\text{SE},7}(\alpha) = 0(1?)$, and where question marks indicate that the uncertainty is only an estimate. The crude estimate used here is intended to illustrate the usefulness of exact numerical calculations (as opposed to pure perturbation calculations) in situations where not much is known about the perturbation remainder. The numerical examples we use here are given for demonstration purposes only (in fact, in the particular case of the $4\text{P}_{1/2}$ level, the remainder has been previously evaluated to good accuracy [30]). Doing the same with the first three terms in (6)—*i.e.* with all the terms calculated with perturbation theory—yields

$$\mathcal{E}_{\text{SE}}(4\text{P}_{1/2}, Z = 1) = -1\,404.260(6?) \text{ kHz,} \quad (8)$$

where the value $G_{\text{SE},7}(\alpha) = 0(1?)$ was assigned. By comparing (7) and (8) with the exact result (5), we see that the exact result is more precise than the perturbation estimates. It also has the advantage of providing an error estimate which is more reliable than those of the perturbation results.

Our high-precision self-energy values were obtained by using middle- Z numerical self energies and performing interpolations and extrapolations to hydrogen, *i.e.*, to $Z = 1$. Similar methods were used in the past, and yielded very accurate self-energy values (see Refs. [31, 32, 30, 33, 34] and Ref. [7, p. 468]). With the recent application [16] of convergence acceleration techniques to the calculation method we use, a direct numerical computation of self-energy shifts in hydrogen could have been possible for any [24] of the states of hydrogen depicted in Fig. 1. However, the computation of the self-energy shift of one nL_j level takes a few weeks, on a modern processor, and a simpler method can yield values with an accuracy better than the experimental precision. We thus performed extrapolations of middle- Z self-energy shifts or interpolations between perturbation and exact results (middle- Z self energies were found in previously published works, or taken from the results presented in Sec. 3). In order to obtain high-precision shifts, two strategies were used. First, we employed the general interpolation/extrapolation method described in the appendix of Ref. [28], and which was first sketched in Ref. [31]. The principle of this method is given in Fig. 4. Second, the extrapolated (or interpolated) quantity was not F itself, but “remainders” of F : we extrapolated (or interpolated) to $Z = 1$ both $G_{\text{SE},7}(Z\alpha)$ and $A_{60} + (Z\alpha)G_{\text{SE},7}(Z\alpha)$ —we used Eq. (6) as a magnifying glass that can show small variations in F . Since no middle- Z self energies are available for the $n = 8$ and $n = 12$ states included in Fig. 1, we also performed extrapolations to these principal quantum numbers; such extrapolations can be performed with good accuracy because self-energy values do not vary much with n , as is depicted in Fig. 2. More details on the interpolation and extrapolation procedures that yielded the self energy for the other hydrogen states included in Fig. 1 will be given elsewhere.

The hydrogen states for which we calculated the self energy (see Fig. 1) represent all the non-S states used in the CODATA98 adjustment of the fundamental constants [7, p. 433]—these states are

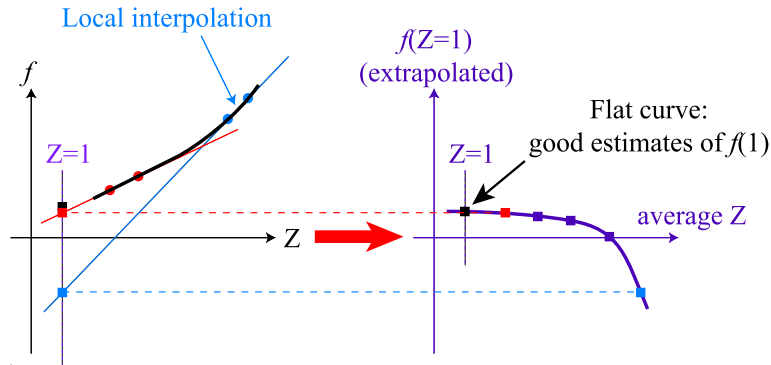


Fig. 4. Principle of the interpolation/extrapolation method [31, 28] used in obtaining self energies in hydrogen ($Z = 1$) from middle- Z self energies. In order to estimate the limit of a function $f(Z)$ as $Z \rightarrow 1$, it is possible to plot its curve and visually estimate the limit along with an uncertainty (left-hand graph). A more precise estimate can be obtained by performing a linear interpolation between two successive points of the curve, and plotting the ordinate of the line at its intersection with the $Z = 1$ axis, as a function of the average Z of the two points (right-hand graph). This process can be generalized to polynomial interpolations of each group of three (or more) successive data points of $f(Z)$: each interpolation has a value at $Z = 1$, which can be plotted as in the right-hand graph. Higher-order interpolations can yield more and more precise estimates of $\lim_{Z \rightarrow 1} f(Z)$.

all involved in some high-precision spectroscopy experiment. The self-energy values were used in the latest CODATA adjustment [13]. The precisions of our self energy values are below 2 Hz, which is smaller than the uncertainty in the best experimental frequency measurement ever achieved in the optical domain (about 50 Hz [23]).

5. Conclusion

We have discussed high-precision numerical evaluations of the self energy (1), which is the dominant QED contribution to the energy levels of hydrogen and of hydrogen-like ions. The atomic levels which were considered are depicted in Fig. 1. They greatly extend the set of states for which the self energy is known with a high precision and a controlled uncertainty. The results that are reported here for hydrogen were used in the latest CODATA adjustment of the fundamental constants [13]. The middle- Z results can find application in atomic calculations that include QED contributions. The high precision of all the results can also allow for comparisons with results obtained through independent methods, or for extrapolations (or interpolations) to other states or nuclear charge numbers than those considered in this paper.

The self-energy values in hydrogen considered here were obtained by taking advantage of the availability of both perturbation and exact numerical results (which permitted interpolations and precision extrapolations). Nonetheless, it is desirable to perform a direct numerical evaluation of these energy shifts, and check their consistency with the values presented here.

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