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Evaluation of the Two-Photon Self-Energy Correction for Hydrogenlike Ions

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Abstract. We report on the recent evaluation of the two-photon electron self energy to all orders in the interaction with the Coulomb field of the nucleus. With the present results at hand the major theoretical uncertainty is diminished, which provides predictions of the ground-state energy with a relative accuracy of about 10^{-6} for the hydrogenlike uranium and lead systems. This allows for high-precision tests of quantum electrodynamics (QED) in strong fields that are expected to be experimentally available in the near future.

Key words: atomic binding energy, highly charged ions, quantum electrodynamics.

An ideal scenario to test quantum electrodynamics (QED) in the strong field limit is provided by the strong electric field of the nucleus in highly charged ions, e.g., by measurements of the Lamb shift at utmost precision. Therefore, at the SIS/ESR facilities in Darmstadt one is aiming for an accuracy of about 1 eV in measurements of the ground-state Lamb shift for hydrogenlike uranium in the near future [1]. Theoretical evaluations on the same level of accuracy require calculations of the complete set of radiative corrections of order α^2 (α is the fine structure constant) but to all orders in the coupling constant $Z\alpha$ to the Coulomb field of the nucleus. The set of these second-order diagrams includes all various combinations of the first-order self-energy (SE) and vacuum-polarization (VP) graphs. The present status of the theoretical predictions for the Lamb shift in different one-electron ions is presented in [2]. Most of these diagrams have already been calculated in recent years. However, calculations of the most difficult set, the second-order self-energy correction (SESE) are yet incomplete. In this paper we report the present status of this challenging theoretical problem for the most interesting cases of the hydrogenlike uranium and lead systems.

The general renormalization scheme for the two-photon self energy was considered in more detail in [3]. The loop-after-loop diagram SESE (a) can be divided into an irreducible and a reducible part. For an elegant way deriving the corresponding energy shifts in reducible as well as irreducible diagrams of bound-state QED we refer to the two-times Green-function method [4]. The irreducible part

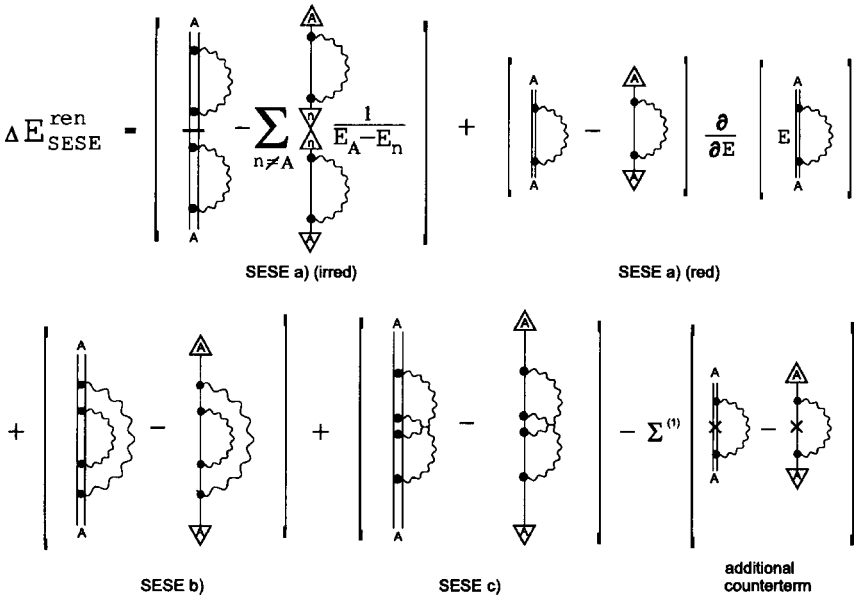

Figure 1. The graphical representation of the partial wave renormalization approach. The bar in the irreducible part denotes the exclusion of the state A in the sum over the intermediate states n. The double and ordinary solid lines with the cross denote the quadratic denominators in the bound and free electron propagators. The triangles represent Fourier expansion of the bound state A wavefunction into free electron states.

SESE (a) (irred) is invariant under covariant gauges [5] and therefore this part can be renormalized and calculated separetely. In [6] the corresponding energy shift of the SESE (a) (irred) diagram has already been evaluated for the nuclear charge numbers $Z = 70, 80, 90$ and 92, and in [7, 8] for arbitrary nuclear charge numbers in the range $3 \leqslant Z \leqslant 92$. In the high-$Z$ limit the results of [6, 7] and [8] are in coincidence with each other ($\Delta E_{1s}^{\mathrm{SESE(a)(irred)}} = -0.97$ eV for uranium). But in the low-Z limit a disagreement has been obtained. This discrepancy is a subject of several controversial statements made in a series of subsequent papers [8–12]. For more details on this point we refer also to [13]. We would like to emphasize that while the discrepancy between the different calculations of the SESE (a) (irred) contribution for low-Z values still needs to be resolved, for the high-Z region all the calculations [6–8] give identical results.

Now we shall consider the SESE (a) (red) as well as the SESE (b), (c) diagrams. The renormalized expression for the SESE-contribution is depicted in Figure 1. In the Feynman gauge only the sum of the graphs in the renormalized expression in Figure 1 is ultraviolet as well as infrared convergent. Therefore these diagrams should be calculated together. According to the partial wave renormalization method [14, 15] all single terms, including the mass counterterms, are decomposed in partial waves. Accordingly, the renormalized expression of the two-photon electron self energy can be expressed as a double sum over two partial

Table I. Partial wave contributions $\Delta E_{1s}^{(l_1,l_2)}$ to $\Delta E_{1s}^{\mathrm{SESE(a)(red),(b),(c)(ren)}}$ for H-like U and Pb (in eV)

U	$l_2=0$	$l_2=1$	$l_2=2$	$l_2=3$	Pb	$l_2=0$	$l_2=1$	$l_2=2$	$l_2=3$
$l_1=0$	0.699	0.384	0.106	−0.059	$l_1=0$	0.439	0.158	0.051	−0.04
$l_1=1$	0.384	−0.188	0.563		$l_1=1$	0.186	−0.092	0.228	
$l_1=2$	−0.427	−0.376			$l_1=2$	−0.135	−0.124		
$l_1=3$	0.501				$l_1=3$	0.172			

waves l_1 and l_2:

$$\Delta E_{\mathrm{A}}^{\mathrm{SESE(a)(red),(b),(c)(ren)}} = \sum_{l_1=0}^{\infty}\sum_{l_2=0}^{\infty} \Delta E_{\mathrm{A}}^{(l_1,l_2)}. \tag{1}$$

The decisive advantage of the PWR approach is that every single partial wave is already UV- as well as IR-finite.

For the ground state $|A\rangle = |1\mathrm{s}\rangle$ of uranium and lead we were able to compute 4 partial waves $l_1, l_2 = 0, 1, 2, 3$ with the limitation $l_1 + l_2 \leqslant 3$ for the sum. The individual terms $\Delta E_{1s}^{(l_1,l_2)}$ of the double partial–wave expansion for uranium ($Z = 92$) and lead ($Z = 82$) ions are listed in Table I.

The inaccuracy of our calculations is determined by the unstability of the numerical results with the change of the number of grid points within the B-spline approximation [16] for the solution of the radial Dirac equation from $N = 23$ to $N = 46$. We estimate this inaccuracy as 12%. The final value $\Delta E_{1s}^{\mathrm{SESE(a)(red),(b),(c)(ren)}}$ was obtained by an extrapolation from the numbers given in Table I. Accordingly, we evaluated the accumulated sums

$$S_l = \sum_{l_1,l_2}^{l_1+l_2=l} \Delta E_{1s}^{(l_1,l_2)} \tag{2}$$

for $l = 0$, 1, 2 and 3. Corresponding values in eV for U and Pb are

$$\begin{array}{lllll} \text{U:} & S_0 = 0.70, & S_1 = 1.47, & S_2 = 0.96, & S_3 = 1.59, \\ \text{Pb:} & S_0 = 0.439, & S_1 = 0.783, & S_2 = 0.607, & S_3 = 0.843. \end{array} \tag{3}$$

The values for S_l reflect again the behaviour of the corresponding accumulated sums for the first-order self-energy [8]. Therefore we performed the same kind of extrapolation as in [8] leading to the energy shift

$$\begin{aligned} \Delta E_{1s}^{\mathrm{SESE(a)(red),(b),(c)(ren)}}(Z=92) &= \frac{S_2+S_3}{2} = 1.28 \pm 0.15 \text{ eV}, \\ \Delta E_{1s}^{\mathrm{SESE(a)(red),(b),(c)(ren)}}(Z=82) &= \frac{S_2+S_3}{2} = 0.73 \pm 0.09 \text{ eV}. \end{aligned} \tag{4}$$

It is interesting to note that the so-called *sign approximation* [17] gives already ≈40% of the exact result. The limit of the number of partial waves was set by

the extremely large computer time required. The calculations were performed at the computer center of the Technical University of Dresden on the CRAY-T3E supercomputer with 32 parallel processors. The inclusion of 4 partial waves $l_1, l_2 = 0, 1, 2, 3$ in both partial wave expansions with the limitation $l_1 + l_2 \leqslant 3$ required more than 20 thousand single-processor CPU hours for each ion (U,Pb). The inaccuracy assigned to our results for SESE (a) (red) and SESE (b), (c) corrections remains the main source of the total error in the theoretical Lamb shift prediction. We expect that the inaccuracy can be substantially diminished within the framework of the method described above.

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