Estimate of the second-order electron self-energy corrections in highly charged heavy ions

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An estimate for the last unknown gauge-invariant set of QED corrections of order α^2, the second-order self-energy correction, is presented utilizing the so-called sign approximation. This is able to reduce the present uncertainties in Lamb-shift predictions considerably.

Highly charged ions provide an ideal scenario to demonstrate the validity of QED in strong fields, e.g., by measurements of the Lamb shift at utmost precision. In this respect the recent experimental progress made in measurements in hydrogen-like uranium [1] indicates that calculations of higher-order radiative corrections become relevant. The set of second-order QED diagrams includes all various combinations of the first-order self-energy (SE) and vacuum polarization (VP) effects. The present status of theoretical predictions for the Lamb shift in different one-electron ions is presented in [2]. However, the calculations of the most difficult set of diagrams (see figure 1), the second-order self-energy correction (SESE) are yet uncomplete [3–6], which remains as source for major theoretical uncertainties in present Lamb-shift predictions. To close this gap is a challenge for theory. As a step towards this, we present an estimate for the two-photon self-energy contribution.

The graph SESE (a) consists of the irreducible and the reducible contributions. Utilizing Feynman gauge the first part can be renormalized and calculated separately since it does not contain infrared divergencies. The irreducible part has been calculated in [3] for large nuclear charge numbers Z and in [4,6] for arbitrary values of Z. For high-Z systems all results obtained coincide, while for low- and intermediate-Z values a discrepancy between [4] and [6] has been found. In Feynman gauge, the remaining reducible part of the SESE (a) graph and the two diagrams SESE (b) and (c) have to be calculated simultaneously in order to cancel infrared and ultraviolet divergences arising from different diagrams [7].

The general renormalization scheme for all two-photon self-energy diagrams has been first presented in [7] and has been confirmed in [8]. For the calculation we employ an approach based on the multiple commutator expansion [9,10] in combination with the partial-wave renormalization (PWR) [11,12]. The renormalized two-loop self-

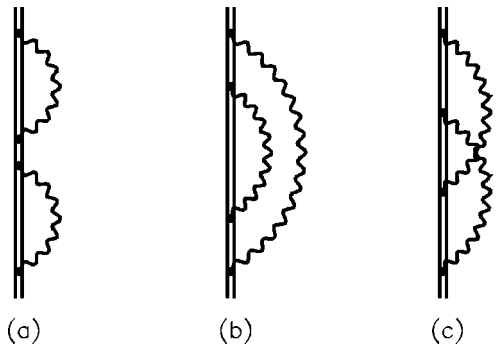

Figure 1. Feynman diagrams corresponding to the second-order electron self-energy corrections in hydrogen-like ions: the loop-after-loop (a), the loop-inside-loop (b), and the crossed-loops (c) contributions. The double solid line indicates the bound electron.

energy shift $\Delta E_n^{(2)\mathrm{ren}}$ for the bound electron state $|n\rangle$ excluding the irreducible SESE (a) term can be written as (see [7] for detailed explanations)

$$\begin{aligned}\Delta E_n^{(2)\mathrm{ren}} &= \Delta E_n^{(\mathrm{red})} + \Delta E_n^{(\mathrm{in})} + \Delta E_n^{(\mathrm{cr})} + \Delta E_n^{(\mathrm{ac})} \\ &= \Delta E_n^{(1)\mathrm{ren}} \left[\frac{\partial}{\partial E}\big\langle n\big|\gamma_0 \widehat{\Sigma}_b^{(1)}(E)\big|n\big\rangle\right]_{E=E_n} + \big[\Delta E_n^{(\mathrm{in})} - \delta m^{(\mathrm{in})}\langle n|\gamma_0|n\rangle\big] \\ &\quad + \big[\Delta E_n^{(\mathrm{cr})} - \delta m^{(\mathrm{cr})}\langle n|\gamma_0|n\rangle\big] - \delta m^{(1)}\big[\big\langle n\big|\gamma_0 \widehat{\widehat{\Sigma}}_b^{(1)}(E_n)\big|n\big\rangle - \delta \widetilde{m}^{(1)}\langle n|\gamma_0|n\rangle\big].\end{aligned} \tag{1}$$

As indicated by subscripts the various terms here denote the reducible loop-after-loop (red), the loop-inside-loop (in), the crossed-loops (cr) contributions, and an additional counter term (ac) of the SESE (b) graph, respectively, after partial renormalization. Each individual term in eq. (1) is still ultraviolet divergent, but the total sum is finite. The expression $\langle n|\gamma_0 \widehat{\Sigma}_b^{(1)}(E)|n\rangle$ evaluated at $E = E_n$ corresponds to unrenormalized one-loop self-energy shift $\Delta E_n^{(1)}$ of the bound-electron state $|n\rangle$. The additional counterterm $\Delta E_n^{(\mathrm{ac})}$ derived in [7] is also ultraviolet divergent. All other counterterms in eq. (1) are supposed to be specified in the framework of PWR approach.

In [9,10] the first order self-energy has been expressed as the sum of two contributions, a logarithmic and a sign terms. Numerical calculations reveal that the logarithmic term yields the most dominant contribution in the case of low-Z systems ($Z \leqslant 10$). However, the sign term turns out to dominate in the energy shift for high values of Z. A numerical evaluation of the one-loop self-energy shift demonstrates that the sign term yields indeed about 95% of the total result for $Z = 92$. Therefore, we keep all the sign terms only in order to estimate the two-photon self-energy in highly charged heavy ions. What we call *sign approximation* was tested for the irreducible part of SESE (a). Compared with the exact result for this contribution [3,4,6] the sign-approximation yields about 60% of the total result for $Z = 92$. One may assume

Table 1
Lamb shift contributions for the ground state of hydrogen-like $^{238}U^{91+}$ ions (in eV). The reduced mass correction has not been conventionally included.

Correction	Numerical value	Reference
Finite nuclear size[a]	198.82 ± 0.10	[2]
Self-energy	355.05	[15]
Vacuum polarization	-88.60	[16]
SESE irreducible (a)	-0.97	[3,4,6]
SESE reducible (a)[b]	0.01 ± 0.005	this work
SESE (b)	-0.05 ± 0.025	this work
SESE (c)	0.51 ± 0.25	this work
VPVP	-0.97	[16,17]
SEVP	1.27	[16,18,19]
Relativistic recoil	0.16	[20]
Nuclear polarization	-0.2 ± 0.1	[21]
Total theory	465.03 ± 0.48	
Experiment	470 ± 16	[1]

[a]For a Fermi distribution with $\langle r^2 \rangle^{1/2} = 5.860 \pm 0.002$ (fm).
[b]Evaluated together with the additional counter term.

that within the sign approximation a comparable level of accuracy will be achieved for the other SESE corrections as well.

For the numerical evaluation all terms in eq. (1) were expanded into double sums over partial waves. Accordingly, all individual partial-wave contributions are finite. Thus we avoid the appearance of the divergent expressions in our calculations. In sign approximation, the terms $\Delta E_n^{(\mathrm{in})}$ and $\Delta E_n^{(\mathrm{cr})}$ appear to be separately finite. Only $\Delta E_n^{(\mathrm{red})}$ and $\Delta E_n^{(\mathrm{ac})}$ are still divergent. To ensure correct cancellations both contributions have to be calculated at once. For the evaluation of the sums over intermediate electron states, the B-spline approach [13] with the minimal set of the parameters was employed.

In table 1 we compile the various contributions to the ground-state Lamb shift in hydrogen-like uranium. Our estimates for contributions of the $\Delta E_{1\mathrm{s}}^{(\mathrm{in})}$, $\Delta E_{1\mathrm{s}}^{(\mathrm{cr})}$, and $\Delta E_{1\mathrm{s}}^{(\mathrm{red})} + \Delta E_{1\mathrm{s}}^{(\mathrm{ac})}$ terms are given separately. The crossed-loop term seems to dominate strongly, a result which is consistent with estimates obtained earlier for low-Z systems [14]. According to the sign approximation we obtain $\Delta E_{1\mathrm{s}}^{(2)\mathrm{ren}} = 0.47 \pm 0.28$ (eV) for $Z = 92$. We also note, that in [5] the value which represents only one (probably not the dominant) part of $\Delta E_{1\mathrm{s}}^{(2)\mathrm{ren}} = -0.325$ (eV) has been reported. Because of the inherent uncertainty of the sign approximation of about 40% together with the numerical inaccuracy of the approach ($\simeq$10% (see [6]) we assign a total inaccuracy of about 50% to the presented results. This estimate reduces the existing theoretical uncertainty in the Lamb shift for hydrogen-like ions. However, the necessity to present a complete calculation of all SESE contributions remains.

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