Higher Order QED Contributions to the Atomic Structure at Strong Central Fields

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In honor to Professor Gerhard Soff

Abstract: An accurate determination of the precise structure of highly charged, very heavy ions is crucial for understanding QED at strong fields. The experimental advances in the spectroscopy of very heavy, highly charged ions – in particular H-, He- and Li-like species – are reviewed: Presently the ground state Lamb shift for H-like U ions is measured on a 1% level of accuracy; the screening terms in two-electron QED have just been touched by experiments for He-like U; and two-loop QED terms have been determined with ultimate accuracy for Li-like heavy species. The different approaches on QED measurements in strong fields will be discussed and the results compared to theory.

Introduction
The mean atomic field probed by a 1s electron increases in first approximation with the third power of the atomic number, \( \approx Z^3 \), due to the shrinking of the orbit and increase in nuclear charge. Whereas a 1s electron in a hydrogen atom sees on its orbit a mean field in the order of \( 10^{10} \) V/cm, this field increases for a H-like uranium ion (\( Z = 92 \)) by six orders of magnitude to a value of \( 1.8 \times 10^{16} \) V/cm [1]. This strong field almost touches the so-called Schwinger limit [2], i.e. a field where by moving the electron only over its Compton wavelength energy of the electron rest mass is involved. This extremely strong field is difficult to provide otherwise than through heavy atomic systems. For instance, the highest laser fields presently possible are at least three orders of magnitudes smaller, i.e. below \( 10^{13} \) V/cm. At the strong atomic fields for high \( Z \) perturbative approaches to QED are not valid any more, rigorous treatments are compulsory [1]. Here, the question arises whether the normal QED is still valid or whether field dependent higher terms have to be included. However, the author likes to emphasize that no deviation from the standard QED formalism was found for the strong field case until now.

In a perturbative approximation the QED contribution to the binding energy of ns electrons, the ns-Lamb shift \( L_{ns} \) in a one-electron ion is given by [3]

\[
L_{ns} \sim \alpha/\pi \cdot (Z\alpha)^7/n^3 \cdot F(Z\alpha) \cdot m_0c^2 \tag{1}
\]

Here \( \alpha \) is the fine-structure constant, \( n \) the main quantum number for the electronic shell considered, \( F(Z\alpha) \) a general function given as power series expansion in \( Z\alpha \), and \( m_0c^2 \) the electron rest mass. Moreover, it is found that the QED contribution is mainly determined by the strongest field part near the nuclear surface.

As the electron binding energy in a shell depends roughly on \( (Z/n)^2 \) the relative QED part on binding energy increases considerably with atomic number. For \( U^{91+} \) the ground state binding energy is about 130 keV, and the ground state Lamb shift is in the order of 1/3% (= 460 eV). For higher shells the QED contributions decrease with \( 1/n^3 \) – as the relativistic contributions do. Nevertheless, with increasing atomic number \( Z \) the QED contribution to intra shell transitions (\( \Delta n = 0 \)) can be appreciable, e.g. up to 20% for intra L-shell transitions (2p\(_{1/2}\)\( \rightarrow \)2s\(_{1/2}\)) in Li-like \( U^{89+} \). However, the question arises whether the higher shell electrons probe similar strong fields as the 1s electrons do. In order to answer this question we display
in Fig.1 the radial electron density distribution for K- and L-shell electrons in Bi [4]. Obviously, the radial dependence of the electron distribution near the nucleus is similar for 1s and 2s electrons; only the absolute value is reduced by the $1/n^3$ law for the density probability at the nucleus. This dependence is exactly reproduced in the formula (1) for $L_{ns}$. That means that the QED contribution is primarily determined by the strongest field probed by the electron near the nucleus, however its magnitude depends directly on the probing probability of this field, here by $1/n^3$. In this sense the strong field QED can similarly be probed by ns electrons in higher shells as well as by 1s electrons.

![Fig.1: Radial density distribution for the innermost electrons in a highly charged Bi ion.](image)

In the present communication emphasis is given to the heaviest few-electron systems, i.e. to H-like, He-like and Li-like systems. For clarity in Fig.2 level diagrams with the relevant transitions are given for the different systems. For the case of uranium the K→L transition energies are in the region of 100 keV, whereas the $2p_{1/2}→2s_{1/2}$ intra-L-shell transition for Li-like ions is in the region of 280.5 eV. Hence, for inter-shell or ground state transitions one is in the hard x-ray region whereas for intra-shell transitions, the $\Delta n = 0$ transitions, we are in the soft x-ray or extreme ultra-violet (EUV) region. Correspondingly, different experimental approaches are indispensable [5]. For the hard x-ray region energy dispersive solid state detectors (Ge(i)) are generally used; whereas different methods are applied for the EUV region, ranging from wavelength dispersive grating spectroscopy [6 – 8] via Doppler tuned spectroscopy [9] to dielectronic resonance spectroscopy [10].
In order to provide the heaviest few-electron ions for experiments two different approaches are competing, the fast ion beam technique and the ion trap technique [11]. With the unique storage and cooler rings built for heavy ions, the fast beam technique provided a lot of exiting results in the domain of strong field QED in the recent years. The draw back of this fast ion method is the Doppler effect limiting the final spectroscopic accuracy. On the other hand the ion source and trap developments – EBIT – all over the globe make highly charged ions available at rest. The draw back there of low ion intensities for the heaviest few-electron ions will hopefully be overcome in near future by the new developments as e.g. at the EBIT facilities in Heidelberg, Tokyo and Shanghai. In the present paper emphasis is given to fast ion techniques and to results from the heavy ion storage / cooler ring ESR at GSI in Darmstadt.

**Ground state Lamb shift – H-like heavy systems.**

Fast beams of bare U^{92+} ions were produced by foil stripping at a few hundred MeV/u after the heavy ion synchrotron SIS at GSI in Darmstadt; then these ions were injected into the ESR storage ring, decelerated to lower energies down to typically 40 – 70 MeV/u and cooled by elastic scattering of electrons in the cooler target at the proper energy [11]. A small fraction of ions recombines radiatively with an electron (RR: radiative recombination). In the next down-stream magnet of the ring these down-charged H-like U^{91+} ions are separated from the coasting bare ions and are then monitored in an inserted particle detector, cf. Fig.3. The recombination populates also excited levels, which stabilize radiatively to the ground state. The electron target region can be viewed by solid state detectors close to 0\(^0\) and 180\(^0\), respectively. By x-ray coincidences with the down-charged ions the photon detection is restricted to transitions associated with H-like U^{91+} ions; moreover by time of flight window restrictions the active x-ray emission region is constrained to the target area itself [12]. In Fig.4 such a clean coincidence x-ray spectrum is displayed for H-like U^{91+} at 43.6 MeV/u and 0\(^0\) observation; lab photon energies are given in the figure. Beyond the Lyman lines, Ly-\(\alpha_1\) and Ly-\(\alpha_2\), direct RR transitions to the K shell (K-RR) are also present.

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**Fig.2:** Level diagrams for H-, He- and Li-like very heavy ions and the involved transitions.
Fig. 3: Experimental arrangement for photon – particle coincidence measurements at the electron cooler of the heavy ion storage ring ESR.

Fig. 4: A coincident x-ray spectra from down-charged U$^{91+}$ ions. Initially bare U$^{92+}$ at 43.6 MeV/u recombine with electrons from the electron cooler.

The Ly-$\alpha_1$ line gives the single and well-separated $2p_{3/2} \rightarrow 1s_{1/2}$ transition, most adequate for determining the ground state Lamb shift. After correction for Doppler shift and subtracting the corresponding Dirac transition energy for a point-like U nucleus an experimental ground state Lamb shift of 459.8 ± 4.8 eV is found [12]. This value comprises for historical reasons beyond the relevant QED contributions also terms caused by the finite size of the nucleus (about 198.82 eV). The main QED contributions (cf. Fig. 7a below) are the one loop self energy (SE, the emission and re-absorption of a virtual photon) – also described as renormalization of electron mass (about 355.05 eV), and the one loop vacuum polarization (VP, the coupling to a virtual electron-positron pair) – also described as renormalization of...
charge (about 88.60 eV) [13]. Two-loop QED terms (SE-SE, VP-VP, SE-VP, S(VP)E) are in the order of 1 eV and can just not be approached within the present experimental accuracy. The present experiment determines the ground state Lamb shift in H-like U\(^{91+}\) – and hence the corresponding QED terms – with an accuracy of one percent. It is emphasized that with this result the experimental accuracy improved by almost a factor of 30 within the last decade [14 – 17]. Further improvements utilizing crystal diffraction techniques are anticipated [18]. For lower Z heavy atoms like Pb or Au the present accuracies have not been reached [19, 17].

Two-electron QED contributions – He-like heavy systems
Using – as discussed above – the same coincidence technique at the electron cooler target of the ESR, transitions in He-like systems can be monitored too utilizing radiative recombination into initially H-like U\(^{91+}\) ions. Unfortunately, all the lines observed in heavy He-like systems cannot be assigned to single transitions by solid state detectors; the lines separate only according to the different total angular momentum \(j\) of the active L-shell electron; cf. Fig.2. However the direct K-RR line, i.e. the transition from the continuum boundary to the ground state, measures uniquely the ground state binding energy without any blending. Comparing two cases, RR into initially bare and H-like ions at exactly the same velocity, gives the binding energy difference of the electron in the ground state in H-like and He-like ions, in U\(^{91+}\) and U\(^{90+}\), respectively. The electron cooler guaranties that for both the beams ion momentum and geometry are identical making such a comparison to a high-precision experiment.

![Graph](image)

**Fig.5:** A comparison of H-like and He-like spectra of U under the same experimental conditions as in Fig.4.

In Fig.5 the corresponding spectra for uranium are compared. From this a ground state binding energy difference for the K electrons of 2248 ± 9 eV results [20]. This is within the experimental uncertainties in best agreement with theory predicting a value of 2245.92(9) eV
[21]. It is emphasized that in this comparison all single-electron terms cancel; only the two-electron terms remain. (For various graphs of the different contributions see Fig.7b below.) Most of the measured difference is caused by normal screening, the standard electron-electron interaction; higher order screening terms with two-photon exchange (also called non-radiative QED terms – not shown in Fig.7b) is in the order of 12 eV; whereas the true 2-electron self energy and 2-electron vacuum polarization contributes –9.78 eV and +4.25 eV, respectively. Hence, the measurement is just at the threshold of getting sensitive to two-electron QED. Certainly, the present accuracy can be improved in future using the present experimental method as well as further by an anticipated diffraction spectroscopy. There are additional measurements on the two-electron QED contributions for He-like heavy systems ranging from Kr, via Xe up to Pb [22, 23]. The accuracy with respect to the true 2-e QED terms of these measurements performed at the super-EBIT in Livermore is in the same order as the fast beam experiment for the heavier U ions.

Two-loop QED terms – Li-like heavy systems

As was pointed out already the QED contributions to intra L Shell transition are relatively large; for the 2p_{1/2} → 2s_{1/2} transition we have for U^{89+} a total transition energy of about 280.5 eV with a QED contribution of about 55 eV, i.e. 20% of the total energy. Measuring this transition energy to high precision gives here an ultimate accuracy for the QED in particular for more-loop terms and that indeed for the strong field case as elucidated above. There are different experimental methods to approach this accuracy goal. A quite new technique is the dielectronic resonance spectroscopy applied in the storage cooler ring at the ESR [10]. The energy of the electrons of the cooler target is intermittently (with a cycle of 20 ms) detuned from the cooling energy to the measuring position and the recombination rate of the cooled ions is monitored behind the next down-stream magnet as function of the de-tuning energy, cf. Fig.3. The recombination rate is determined by both the radiative recombination (RR) and the so-called dielectronic recombination (DR). RR is the time-reversed photo-ionization process, and likewise DR is the time-reversed Auger process, where a resonant capture of a free electron under simultaneous excitation of a bound electron yields to a doubly excited state which finally may stabilize radiatively. For instance, a free electron is captured by electron-electron interaction to a high Rydberg level nl under the resonant excitation of the 2s_{1/2} electron to the 2p_{1/2} level; here the energy of the free electron has to match the energy condition for the 2s_{1/2} → 2p_{1/2} excitation. Tuning the electron energy correspondingly many Rydberg levels may be probed by this technique.

In Fig.6 an example for initially Li-like Au^{76+} ions coasting in the ESR is depicted. On a smooth background caused by RR, Rydberg resonances for 27 ≤ n ≤ 41 show up for the DR process:

c + Au^{76+} (1s^2 2s_{1/2}) → Au^{75+} (1s^2 2p_{1/2} nl) → + stabilizing photon

(2)

The energy scale given in the figure is already transformed to the center of mass system of the ion. Extrapolating the Rydberg levels to the series limit one just yields the pure 2s_{1/2} → 2p_{1/2} transition energy for Li-like Au^{76+} ions. An experimental energy of 216.134(96) eV results with an accuracy of 4·10^{-4} [10]. In this case, the one-loop QED contributions (SE, VP) are in the 10% region of the transition energy, the two-loop QED terms are in the 0.5% region [24]. The accuracies of the calculations are on the 10^{-4} level, i.e. on the same accuracy level as the experiment. Moreover, experiment and theory concur on this level of accuracy. This is also true for the neighboring Li-like systems Bi^{85+} and U^{96+} [10]. Here the strong field QED is confirmed on the two-loop level with high precision.
e⁻ + Au⁷⁶⁺(1s² 2s₁/₂) → Au⁷⁵⁺(1s² 2p₁/₂ nlᵣ)

ΔE = E_{kin} - E_{n_i}

**Fig.6:** Dielectronic recombination spectrum for Li-like Au⁷⁶⁺ measured at the electron cooler target at the ESR. The recombination rate is given as function of the relative kinetic energy between electron and ions.

For lighter heavy elements the 2p₁/₂→2s₁/₂ transition energy was determined using EUV grating spectroscopy in beam foil excitation experiments at the heavy ion accelerator UNILAC for Li-like ions of Ni, Zn, Ag, Sn and Xe [6 – 8]. Here, even a higher accuracy level of 7·10⁻⁵ was achieved, giving perfect agreement with the theoretical predictions over the total Z region investigated.

For the heaviest system Li-like U⁸⁹⁺ there is also an other, outstanding earlier measurement on the 2p₁/₂→2s₁/₂ transition energy using a Doppler tuned technique in a beam foil experiment [9]. Similar accuracy as for the above mentioned DR resonance spectroscopy was achieved yielding to QED results in accordance with each other. Just recently, the EUV grating spectroscopy was applied in a complementary ion trap experiment at the Livermore EBIT [25]. There the experimental accuracy is stated to be comparable to the EUV experiments at lower Z, i.e. appreciably better than the values documented for the heaviest ions in the literature until now. Once more, the experimental uncertainties are here appreciably smaller than the possible systematic errors claimed by theory.
Summary and achievements
In Fig. 7 we show various graphs for the main possible QED contributions:

Fig. 7: Possible QED contributions for (a) H-like, (b) He-like, and (c) Li-like atomic systems accessed by experiments at strong fields.

Part a) gives the leading one-loop terms which were mainly discussed for H-like ions: Self energy (SE) and vacuum polarization (VP). For the heaviest system, U^{91+}, these contributions are experimentally determined on the percent level. There is the hope to achieve in future an accuracy of around 1 eV, i.e. a factor of five better than the present accuracy.
Part b) displays two-electron QED contributions in He-like systems. Beyond the screening terms (non radiative QED part) – the two-loop screening terms are not shown in the figure – screened SE and VP are the essential QED contributions. For $U^{90+}$ the experimental accuracy is presently just on the order of the QED contributions of screened SE and VP. Also here agreement with theory was found. In this case an improvement of experimental precision by a factor of 10 seems feasible in near future determining the main two-electron terms possibly on a 10% level of accuracy.

Part c) shows a bunch of possible QED contributions for Li-like systems. On the one hand screening for the QED terms has to be considered, however also pure two-loop QED terms like SE-SE, VP-VP, SE-VP, and S(VP)E have to be taken into account. Up to about four dozens of graphs had to be included into the calculations [24]. Here also a perfect agreement can be stated between theory and experiment. The experimental accuracy is so advanced that even the two-loop terms are confirmed with an accuracy of roughly 1%; here experiment is ahead of theory concerning accuracy.

In summary we can state that for all the considered cases the present day understanding of QED is completely confirmed also at the strongest possible atomic fields around $10^{16}$ V/cm. Most of the experimental results have been achieved at the heavy ion storage / cooler ring ESR at GSI in Darmstadt. However, the advances in EBIT technology will deliver in future higher intensities of heavy and highly charged ions and these ions are at rest. Hence, there outstanding advances can be expected from measurements at the EBIT facilities in future. An impressive example was given just now by the new result from the Livermore EBIT for Li-like U [25], yielding the most accurate QED measurement ever performed in the strong field case. Hence, EBIT facilities will have a bright future also in this field of research.

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