REVIEW / SYNTHÈSE

Precision energy-level measurements and QED of highly charged ions [1]

Peter Beiersdorfer

Abstract: A review is given of measurements involving the K-shell ($np \rightarrow 1s$) transitions of hydrogenlike ions. In many experiments carried out, for example, on electron-beam ion traps and tokamaks, the calculated energies of the Lyman-series lines are utilized as calibration standards for measuring the energies of lines from more complex ions. Examples given include measurements of the transition energies of L-shell lines in neonlike ions. The Lyman lines of low-Z ions are also used as a bootstrap for measuring the contributions of quantum electrodynamics (QED) in very high-Z ions, such as U^{81+} and U^{89+}. The lowest energy member of the Lyman series, Lyman-α, is commonly the target of absolute-energy measurements so as to test the reliability of the calculations of atomic structure in general and of the $1s$ QED terms in particular. A review of 42 measurements of $1s$ QED measurements indicates an apparent bias toward wanting to agree with calculations.

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Résumé : Nous passons en revue des mesures impliquant les transitions dans la couche K ($np \rightarrow 1s$) dans les ions de type hydrogène. Dans plusieurs expériences, utilisant par exemple des pièges ioniques à faisceau d'électrons ou des tokamaks, les énergies calculées pour les lignes de la série Lyman sont utilisées comme standard de calibration pour mesurer les énergies de lignes dans des ions plus complexes. Des exemples incluent la mesure de lignes dans la couche L d'ions de type néon. Les lignes Lyman d'ions de faible Z sont aussi utilisées comme point de départ pour mesurer les effets de l'électrodynamique quantique (QED) dans les ions de Z élevé, comme U^{81+} et U^{89+}. L'élément de plus basse énergie de la série Lyman, Lyman-α, est souvent le sujet de mesures absolues en énergie, de façon à pouvoir tester la validité de calculs en structure atomique en général et en particulier du terme $1s$ en QED. Une révision de 42 mesures du $1s$ en QED indique un biais résultant d'un désir d'être en accord avec les valeurs calculées.

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1. Introduction

The K-shell X-ray emission from one-electron, hydrogenlike ions is well known both experimentally and theoretically [1]. The strongest transition proceeds from the $2p_{3/2}$ upper configuration to the $1s_{1/2}$ ground configuration and is commonly labeled Lyman-α_1. The second strongest line is Lyman-α_2, which proceeds from the $2p_{1/2}$ upper configuration to the ground configuration and has about half the intensity of Lyman-α_1. Weaker lines in the Lyman series proceed from np configurations with $n \geq 3$ to ground and are designated alphabetically with a Greek letter in accordance with increasing principal quantum number n.

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P. Beiersdorfer. High Temperature and Astrophysics Division, Lawrence Livermore National Laboratory, Livermore, CA 94550-9234, USA (e-mail: beiersdorfer@llnl.gov).

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Hydrogenlike ions are the simplest atomic system with one bound electron. Thus, difficult-to-calculate electron–electron correlations are nonexistent, and their energy levels are expected to be most reliable. For example, calculations of ions with atomic number $Z \leq 20$ were performed by Garcia and Mack [2]; subsequent calculations were performed by Erickson [3] and Mohr [4]. The results differed from each other only slightly and most of the difference could be traced to changes in the value of the atomic constants. Calculations that extended to essentially all elements available in the laboratory, i.e., those with atomic number $Z \leq 110$, were given by Johnson and Soff [5]. The results in this paper include both the Dirac energies as well as the one-loop quantum electrodynamics (QED) and finite nuclear-size contributions, which for the $1s$ level of uranium U^{91+} are as large as 460 eV. These calculations thus include essentially all the physics needed to produce very accurate results. Missing physics is limited to higher order QED effects, i.e., two-loop QED, which mixes self-energy and vacuum polarization, and yet higher order loops [6]. These contributions are miniscule for all but the highest-Z elements.

The accuracy of the calculations of hydrogenlike transitions make the Lyman lines ideal references for measuring the energies of lines from more complex ions, as we discuss in the next section. This method, which I shall dub the "bootstrap" method,

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has been widely used by the author and his co-workers in various studies on tokamaks and electron-beam ion traps. Tests of the accuracy of the theoretical predictions of the Lyman-α lines and thus of the predictions for the $1s$ QED contributions have also been carried out, as we discuss in Sect. 3. Comparisons with the results of Johnson and Soff [5] show excellent agreement. In fact, the 42 measurements performed in the first 20 years since the publication of the paper by Johnson and Soff have found agreement that is better than expected from statistical consideration. This implies that experimentalists may have avoided publishing measurements that differed from the calculations.

2. Transition-energy measurements using the bootstrap method

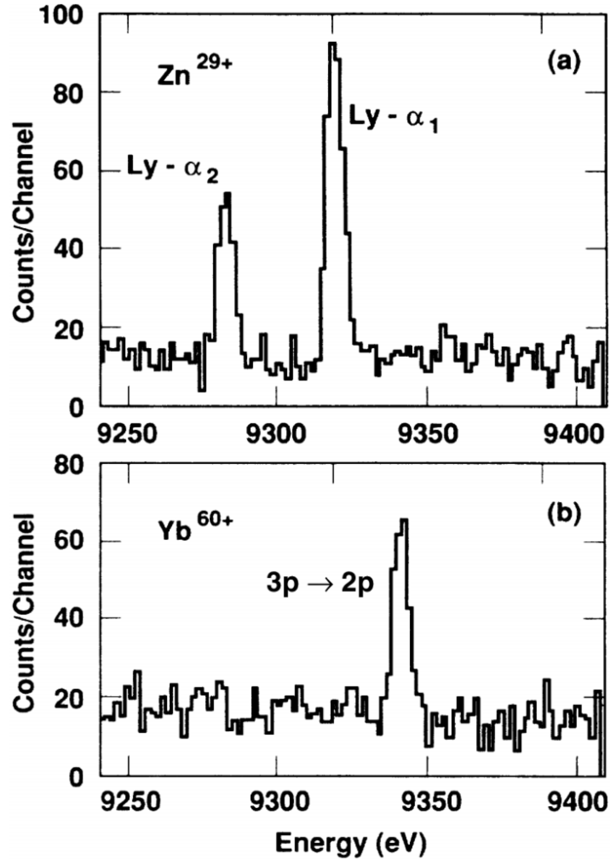
Making transition-energy measurements that are absolutely calibrated is a difficult and arduous task. One main reason is the absence of readily available calibration techniques, and those available are very difficult to implement. In fact, there is a noticeable absence of highly reliable reference standards in the X-ray regime, as, so far, a highly accurate transfer of the length standard from laser light in the visible to the X-ray range has not been accomplished. The use of X-ray lines from hydrogenic ions as reference standards whose transition energy is well known from theoretical calculations is thus a natural alternative.

An illustration of the use of the Lyman-α lines for measuring the energy of lines in a more complex ion is given in Fig. 1. Here, we show the Lyman-α_1 and Lyman-α_2 lines of hydrogenlike zinc, Zn^{29+}, recorded on the Livermore EBIT-I electron-beam ion trap, as reported earlier [7]. In the example shown in Fig. 1 the energies of the hydrogenic lines calculated by Johnson and Soff [5] were used as reference standards to determine the energy of the $1s^22s_{1/2}2p^63p_{3/2} \rightarrow 1s^22s^22p^6$ transition in neonlike ytterbium Yb^{60+}. This allowed an 18.4 ± 0.8 eV determination of the self-energy contribution to the $2s$ level [7]. Similarly, a systematic effort to measure the energies of the L-shell lines of neonlike ions between Ag^{37+} and Eu^{53+} had been performed earlier at the Princeton Large Torus (PLT) tokamak [8, 9]. The L-shell lines measured here were situated in the range from 2 to 4 Å, and Lyman lines from hydrogenlike Ar^{17+}, K^{18+}, Sc^{20+}, Ti^{21+}, V^{22+}, and Cr^{23+} were employed as reference standards. Some of the L-shell lines measured on PLT, notably the $3 \rightarrow 2$ lines of neonlike xenon, Xe^{44+}, were later used in turn in measurements on the Tokyo electron beam ion trap as reference standards for determining the energy of L-shell lines of close-by neonlike ions such as I^{43+} and Cs^{45+} [10].

EBIT-I, as well as EBIT-II and SuperEBIT subsequently built at Livermore [11], have been used extensively for transition-energy measurements in essentially all wavelength bands. Measurements have been carried out for X-ray astrophysics [12, 13], X-ray laser research [14], magnetic fusion [15], inertial fusion and laser-produced plasma research [16], as well as for tests of QED and the determination of atomic–nuclear interactions [17–19]. The use of hydrogenlike reference standards based on the calculations of Johnson and Soff [5] has been common in these measurements.

Figure 2 shows measurements carried out on EBIT-I to make an accurate inventory of lines in the extreme ultraviolet range for the analysis of observations made with the Chandra X-ray Observatory [20]. The K-shell emission from low-Z contaminants is readily observed. In particular, the Lyman-α line of carbon C^{5+} is seen in second, third, fourth, and fifth order and may serve as a reference standard in this spectral region for measuring the transition energies of lines from complex ions, such as those of highly charged neon also shown in Fig. 2.

Fig. 1. Spectrum of (*a*) the Lyman-α lines of Zn^{29+} and (*b*) the $1s^22s_{1/2}2p^63p_{3/2} \rightarrow 1s^22s^22p^6$ transition in Yb^{60+}. The spectra were measured with a crystal spectrometer on the EBIT-I device at Livermore.



The K-shell emission from heliumlike ions may also serve as wavelength references, because the wavelength of these lines are also rather well known from first principles. Calculations by Drake [21] and Johnson et al. [22, 23] have provided excellent reference standards, especially for the K-shell lines of low-Z heliumlike ions, such as those from carbon C^{4+}, N^{5+}, and O^{6+}. In fact, the K-shell transitions from heliumlike C^{4+} and O^{6+} together with the Lyman-α lines of hydrogenlike O^{7+} have been used in either first- or second-order reflection to determine the energy of the $1s^22p_{1/2} \rightarrow 1s^22s_{1/2}$ transition in lithiumlike U^{89+}. The result was 280.645 ± 0.015 eV [24], which to date represents the most accurate determination of QED in a highly charged system, as illustrated in Fig. 3. In fact, this measurement tests the roughly 42 eV prediction for the QED contribution to within 3.6×10^{-4}. Most importantly, the ± 0.015 eV measurement of the $1s^22p_{1/2} \rightarrow 1s^22s_{1/2}$ transition provided a very accurate test of the 0.22 ± 0.07 eV contribution from two-loop QED to the $2s$ level [24]. The accuracy of this test is comparable to what is achieved in atomic hydrogen using sophisticated laser probing [25]. A test of the two-loop QED

Fig. 2. Grazing-incidence grating spectrometer measurement of (*a*) background emission of K-shell lines from carbon and nitrogen in the Livermore electron beam ion traps and (*b*) of the L-shell emission of Ne^{4+} – Ne^{7+} ions. Lines are identified by charge state and order (in parenthesis) of diffraction.

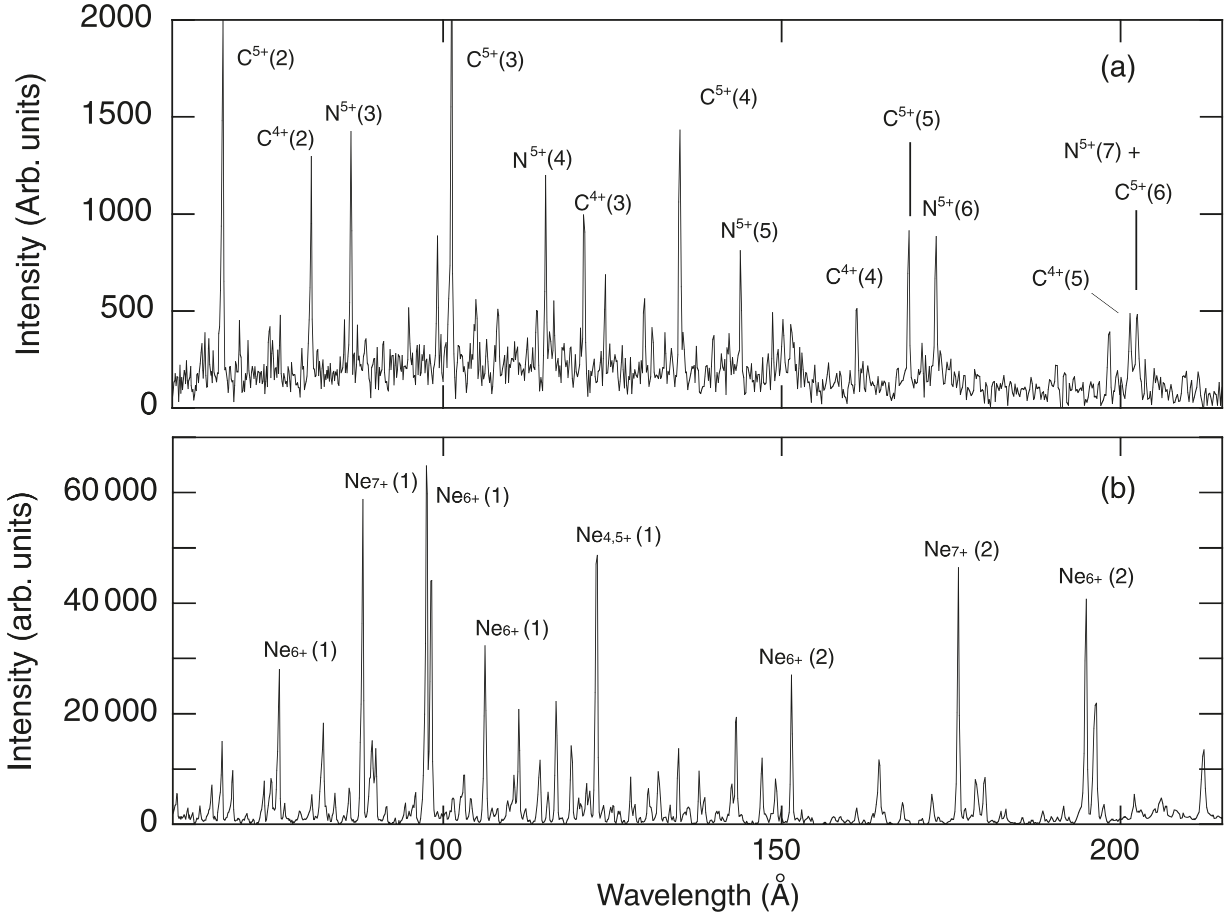
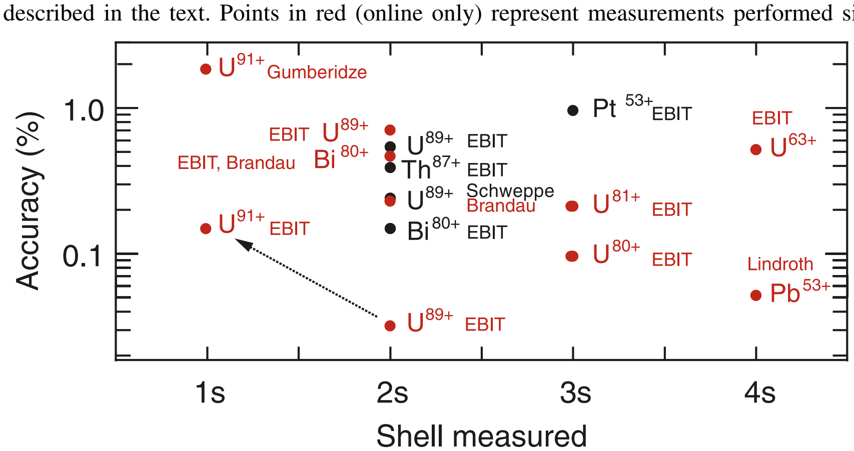


Fig. 3. Overview of the precision achieved in measurements of the QED terms in high-*Z* ions by studying transitions in different shells. The *y*-axis shows the experimental accuracy of a given measurement divided by the size of the total QED contributions. The points measured at the Livermore electron-beam ion trap facility are labeled "EBIT" and are from refs. 24, 31–35. Others are labeled by the first author's name [36–39]. The U^{91+} datum labeled "EBIT" represents an estimate of the 1*s* two-loop QED derived from the 2*s* QED measurement of U^{89+}, as described in the text. Points in red (online only) represent measurements performed since 2000.



contribution in atomic hydrogen is limited by the fact that the proton radius is not known to very high accuracy. In fact, the uncertainty in a single proton radius measurement, for example, $r_p = 0.862 \pm 0.012$ fm [26], introduces an uncertainty of 32 kHz in the theoretical predictions [27]. However, several measurements of the proton radius have been made [26, 28, 29], and these do not agree within their respective error bars. The spread in the different proton measurements introduces an uncertainty of 152 kHz. This uncertainty is about a quarter of the predicted size of the two-loop QED contribution in atomic hydrogen. For comparison, the ±0.07 eV uncertainties in the theoretical estimates of the three-photon exchange in U^{89+} limit a test of the two-loop QED contribution in this system to about 30% [24].

The two-loop QED derived from our bootstrap measurements of the U^{89+} transition can be used to estimate the two-loop QED contribution to the 1*s* electron in hydrogenlike U^{91+}. To do so, we scale the two-loop QED of the 2*s* level the same way theory predicts the scaling for the one-loop QED term [40]. This means we have to multiply the results for the $1s^22p_{1/2} \rightarrow 1s^22s_{1/2}$ transition by −6.39 and obtain −1.27±0.45 eV. The error limits associated with this result reflect the scaled uncertainty of the theoretical values needed to extract the $2s_{1/2}$-$2p_{1/2}$ two-loop Lamb shift in U^{89+} from our measurement of the $2s_{1/2}$-$2p_{1/2}$ transition energy; it does not reflect the experimental error bar. As illustrated in Fig. 3, the uncertainty associated with this procedure is nevertheless an order of magnitude better than the best direct measurements of 1*s* QED in U^{91+}, none of which is yet sensitive to two-loop effects.

The results derived for the two-loop QED term in U^{91+} clearly illustrate the power of using hydrogenlike lines for reference standards. The accuracy of theoretical calculations — in this case that of low-*Z* hydrogenlike oxygen O^{7+} — is sufficient to even derive the QED contributions for very high-*Z* hydrogenlike systems with high accuracy.

3. Test of the 1*s* Lamb-shift calculations

With the advent of suitable ways of producing highly charged ions, absolute transition-energy measurements were undertaken to test the theoretical values for the energy levels in hydrogenlike ions. About 42 absolute measurements have been made in the first 20 years since the publication of the paper by Johnson and Soff. These measurements were performed on heavy-ion accelerators [39, 41–57], tokamaks [58, 59], and electron-beam ion traps [60–63].

At Livermore, two measurements were performed to test the calculations of Johnson and Soff on low-*Z* hydrogenlike ions, i.e., Mg^{11+} and Si^{13+} [60, 62]. An absolute determination of the Lyman-α_1 and Lyman-α_2 transition energy was accomplished by using a monolithic crystal [64] with two reflecting surfaces, which were separated by a well known distance, and an accurately measured lattice spacing. The results from these measurements and others involving close-by ions for the Lyman-α_1 transition are shown in Fig. 4. Good agreement is found with the calculations. In fact, not a single measurement appears to disagree with the calculations by Johnson and Soff outside its error bar.

One may ask how well the combined 42 measurements have tested the theoretical results of Johnson and Soff. Most measurements claim an uncertainty limit of one standard deviation. Thus, we define a quantity Δ, which expresses the difference between the measured value E_{expt} and the calculated value E_{theor} in terms of the stated uncertainty limits of the measurement E_{error}:

$$\Delta = \left| \frac{E_{\text{expt}} - E_{\text{theor}}}{E_{\text{error}}} \right| \qquad [1]$$

The quantity Δ thus expresses the agreement or disagreement between experiment and theory in terms of the error bar, i.e., in units of one σ.

Fig. 4. Comparison of the measured QED contributions to the Lyman-α_1 transition energies in various low-*Z* ions (solid circles) with the calculations of Johnson and Soff (continuous curve).

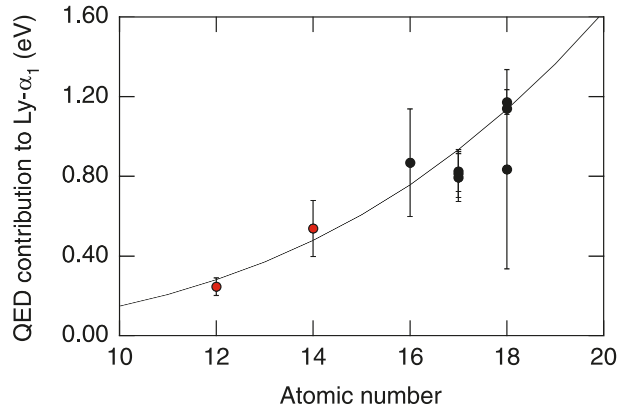
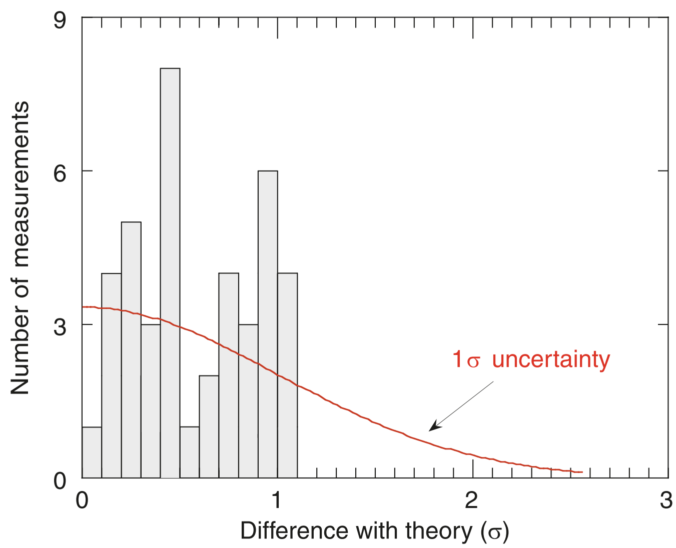


Fig. 5. Expected (continuous line) and actual (histogram) frequency of 1*s* QED measurements reporting a particular difference between experiment and calculation in units of one standard deviation. Data are binned in terms of 0.1σ.



In Fig. 5, we plot the expected frequency of Δ by binning the values of Δ in 0.1σ intervals. For comparison, we plot the number of times a given measurement was reported with a particular value of Δ. From Fig. 5, it is clear that essentially no measurement deviated from the calculations by Johnson and Soff by more than the stated error bar. The few measurements that did differ did so by less than a tenth more than the 1-σ error bar. In other words, no one reported a measurement that disagreed with the calculated numbers.

We can only speculate why no measurements have been reported that differ from the calculations of Johnson and Soff by more than the width of the error bar. Whatever the reason, it is clear that the community has great trust in these calculations. In my opinion, this is a great tribute to the quality of the work of Walter Johnson.

4. Conclusion

The calculations by Walter Johnson, both of hydrogenlike and heliumlike ions, have served in many ways as an anchor for making very accurate measurements of the energies of lines in complex highly charged ions. The calculations of the Lyman-α transitions of hydrogenlike ions themselves have been subjected to a multitude of tests, and no disagreement was found outside the experimental error limits. These calculations will thus continue to serve the atomic physics community for years to come as reference standards in the X-ray regime.

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