Recent developments in X-ray tests of quantum electrodynamics[1]

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Abstract: Experimental tests of quantum electrodynamics (QED) have developed dramatically for simple systems of hydrogen and helium, but there has also been significant progress for medium-Z hydrogenic and helium-like atoms over the last few years. In this area, tests are often based on X-ray spectroscopic measurements, and here we review some key developments. Of particular interest is the status of few-electron QED in the medium-Z regime, the fine-structure Lamb shift from X-ray measurements, tests of two-electron QED, and of np subshell and excited state QED. We discuss some recent secondary tests of the data to confirm the quality and different approaches to experimental development to address the dominant systematics in this area.

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Résumé : Les tests expérimentaux de QED dans des systèmes simples comme l'hydrogène et l'hélium ont augmenté rapidement, mais il y a eu aussi des progrès notables pour des atomes de Z intermédiaire de type hydrogène ou hélium. Ces tests sont souvent basés sur des mesures spectroscopiques X et nous en passons ici en revue les développements clés. Particulièrement intéressants sont les effets QED dans les système à quelques électrons avec une valeur intermédiaire de Z, le déplacement de structure fine de Lamb par mesure X, les tests QED pour deux électrons, ainsi que pour les états de la sous-couche np et excités. Nous analysons quelques tests secondaires sur les données afin d'en confirmer la qualité et différentes approches pour développer les expériences qui visent les aspects les plus importants du domaine.

[Traduit par la Rédaction]

1. Introduction

Experimental tests of quantum electrodynamics (QED) are experiencing a major renaissance, because theoretical uncertainties are now known to be comparable to experimental accuracy [1, 2]. Recent calculations of high-order terms have concluded that the two expansions in $\alpha(\frac{\alpha}{\pi})$ and $Z\alpha$, based on the evaluation of successive Feynman diagrams, may both be only asymptotically convergent [3]. Therefore, higher order terms may yield corrections as large or larger than lower order terms. Recent theoretical development has been based "in view of the probable divergence of quantum field theory in higher order" [4]. Alternative theoretical approaches to QED yield different results [5], testable with current experimental precision both in low-Z and medium-Z systems.

Normal spectroscopic tests of QED in hydrogen have been limited by uncertainty in nuclear form factor and nuclear polarizability. This area has been reviewed recently [6]. Lowest-order QED terms scale as $(Z/137)^4 n^{-3}$, with higher-order terms scaling to the sixth and higher powers. Such higher terms may only be a few percent of the lowest-order terms, and yet these are the critical areas of current theoretical development and also are the region where the convergence of all higher-order terms remains ill-defined, which may be probed by medium-Z experiments.

Medium-Z measurements also probe higher-order (photon exchange) QED theory, in particular the $\alpha^2(Z\alpha)^6$ and $\alpha^2(Z\alpha)^7$ terms causing recent dilemmas. These expansions are not analytic at low or high Z [7]. The medium-Z regime is not limited by nuclear form factor uncertainties, which limit low-Z and high-Z measurements [8]. Hence, a relative accuracy of 1 ppm [10^{-6}] in a medium-Z atomic system with Z = 30 will be as sensitive to some of these terms as an experiment in hydrogen with a relative accuracy of 10^{-12} or 10^{-15}.

Helium-like systems measure both correlation effects and two-electron QED that are inaccessible to hydrogenic studies. The status for helium itself has been reviewed [9]. In general, few-electron systems test correlation effects and several different computational formalisms. Results from different experimental groups in the medium-Z region are inconsistent, and the problem of correlation in three-body systems is complex and unresolved.

Recent motivation has involved reassessments of the fundamental constants of nature via the CODATA efforts [10], including discussions of alternative interpretations [11, 12]. Numerical calculation of $G_{SE}(Z\alpha)$, for Z = 1–5, differed by 13 kHz for hydrogen 1S, showing that high orders in perturbation are really large [13, 14]. Two-loop $\alpha^2(Z\alpha)^6 m$ terms are dominated by the single logarithm term (B_{61}). Estimates of uncalculated terms is an art, rather than a science [14], implying that direct experimental tests of convergence are always important. The numerical error of B_{60} is 15% [15]

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and is in major disagreement with the numerical calculation without expansion in $Z\alpha$ [16]. For radiative-recoil contributions, a key single loop term $\alpha(Z\alpha)^6\ m/M$ is known, but other terms of similar order are not. Proton radius remains a key issue for hydrogen itself, and non-S state higherorder terms remain of significant importance and are bound up in direct experimental confirmations for higher-Z.

Recently, it has been observed that EBITs have led to a new opportunity in the possibility of testing two-electron QED effects [17]. A significant realisation of recent years is that complementary endeavours are investigating different fundamental issues and making major contributions to different fields. Modest increases in experimental precision over current work — by a factor of three in an appropriate system — may demonstrate the limitations of current theoretical approaches and may suggest a more sound theoretical approach to QED.

Accuracy of helium-like QED contributions by some four main different calculation approaches has been a source of difficulty in that terms may not be adequately renormalized, leading to difficulties in convergence [18–21]. The problem of isolating contributions from different correlation diagrams in these few-electron systems has compounded this difficulty in some cases. Partial wave expansion may hold thepromise of being able to address some of these concerns for many-electron or molecular systems [22].

In the medium-Z range of current discussion, spectroscopic tests may investigate hyperfine structure and shifts, laser resonance studies, or X-ray spectroscopy of core transitions.

There has been excellent work developing laser resonance experiments at accelerators and recently at EBITs [23–26]. Part of this area has been reviewed recently [27]. Significant unexplained anomalies between theory and experiment remain in this field and it is an area of active interest.

Other tests in this regime have pursued lifetime or quench studies, which may be based on laser-optical or X-ray transitions [28], or on radiative recombination and radiative electron capture [29], and related processes involving X-ray or visible emission from continuum states. This review will concentrate on X-ray spectroscopic transitions between discrete levels, where narrow natural widths permit high-resolution measurements.

2. Recent approaches to X-ray tests

The main X-ray tests of QED have been spectroscopic measurements of the Lyman α transition in medium- and high-Z atomic systems and corresponding measurements of the w, x, y, and z transitions in Helium-like medium-Z atomic systems. Recently, these have been augmented with investigations of Li-like systems, with associated development of theoretical techniques to enable useful QED investigations.

2.1. Hydrogenic medium Z measurements using X-ray spectroscopy

Figures 1 and 2 give comparisons of key 1s-2p Lamb shift measurements of hydrogenic systems in the medium-Z region using X-ray spectroscopy.

The simplest method used is absolute spectroscopy of a beam-foil source. In these experiments, the Lyman α measurement is calibrated against an external source (KCl K and Cl, and Ar Kα X-rays for Z = 18, 16, and 17, Co Kα for Z = 26, Cu Kα for Z = 28, and for example Cr Kα for Z = 36). This requires identical source locations in the spectrometer for reference and beam radiation, precise angular linearity for scanning spectrometry, and corrections for diffraction effects. Bragg diffraction has been used in all these experiments; diffraction crystals used were Si 111 curved crystals (Johann mounting) [30, 32], Ge 220 curved crystals [33], Si 111 flat crystals [35], Si 220 flat crystals [37], curved Ge 220 crystals [41, 43], and flat Si 220 crystals in second order [44]. The curvatures involved were $2Rz$ = 800–1896 mm. Flat-crystal scanning measurements involve an additional requirement for the stability of the beam. Reference Kα components are usually unresolved and must be fitted carefully, and anode conditions must be precisely controlled. The main problem with this technique is the Doppler shift between reference and beam transitions, dependent on the beam energy, foil stopping power, and spectrometer alignment. This is augmented by the presence of satellite contamination from poor excitation conditions or intrinsic to the excitation method used.

The figures give comparisons with the theory of Johnson and Soff [45]. The theory of Mohr [46] could have been used equally well. It is important to realise exactly what most of these experiments are, as they can be misquoted in the literature. They are measurements of a discrete X-ray inner-shell transition, 1s-2p. The Dirac energies are subtracted, being well-defined and known quantities, primarily leaving reduced mass corrections and QED contributions. For many experiments, this 1s-2p QED result (or "1s-2p Lamb Shift") is quoted as a 1s Lamb shift measurement. In all systems, the contribution of the upper state is nonzero and observable, so there is an explicit assumption that the excited stated QED is known exactly. In the case of hydrogenic ions, this distinction is clear and well-formed; however, the same interpretation is often made in helium-like and lithium-like QED tests, where the separation of these two ideas is both dubious and fraught.

These difficulties in beam-foil spectroscopy are similar for Tokamak measurements. Tokamak measurements used von Hamos diffraction geometry; all these absolute spectroscopy measurements used position-sensitive proportional counters or backgammon detectors. A space-charge build-up between Lyman components can occur at high count rates in the Tokamak measurements, requiring correction [31, 34], with thermal broadening decreasing the resolution to 1000. The measurement of hydrogenic Cl observed a 11% contamination of Lyman peaks with satellites [31], which for Ar gave an estimated 4% contamination [34]. An additional problem with the absolute spectroscopy method in these two measurements was the rotation of the spectrometer for calibration. The possibility of net motions in the plasma is discussed in these papers and could give an uncorrected Doppler shift.

Satellite contamination was approximately 20% and 50% of the Lyman peaks in other early measurements [30, 33], the latter being a recoil measurement, where 5.9 MeV/amu U^{66+} bombards Ar to produce highly-stripped argon ions with negligible recoil velocities. This solves the Doppler

Fig. 1. Comparison of theory and experiment for the 1s-2p Lamb shift. Points are marked according to the detection methods used. In general, Von Hamos geometries have higher flux and statistics but more complex problems regarding calibration; flat crystal measurements can have very high resolution, relatively low flux, but are extremely sensitive to small systematics regarding calibration and alignment. Results are paired with Lyman α_1 ($1s\text{-}2p_{3/2}$) followed by Lyman α_2 ($1s\text{-}2p_{1/2}$), where reported. In order of Z, references are: $Z = 17$ [30]; [31]; [32]; $Z = 18$ [33], [34], [35]; $Z = 22$ [36]; $Z = 26$ [37], [38], [39], [40] ; $Z = 28$ [41]; $Z = 32$ [42].

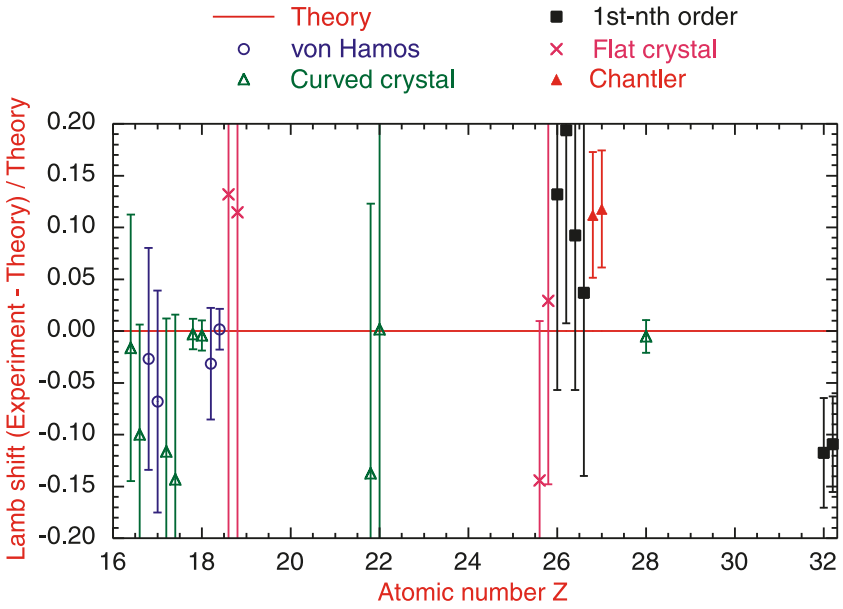
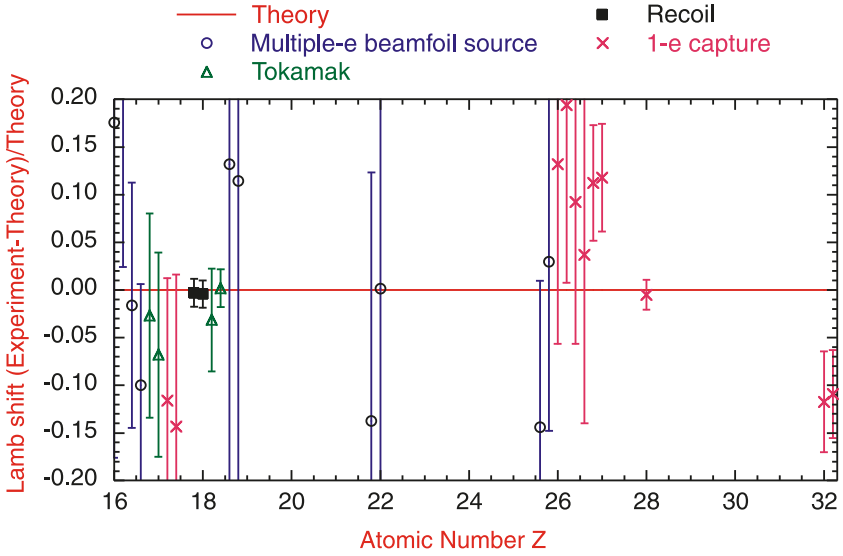


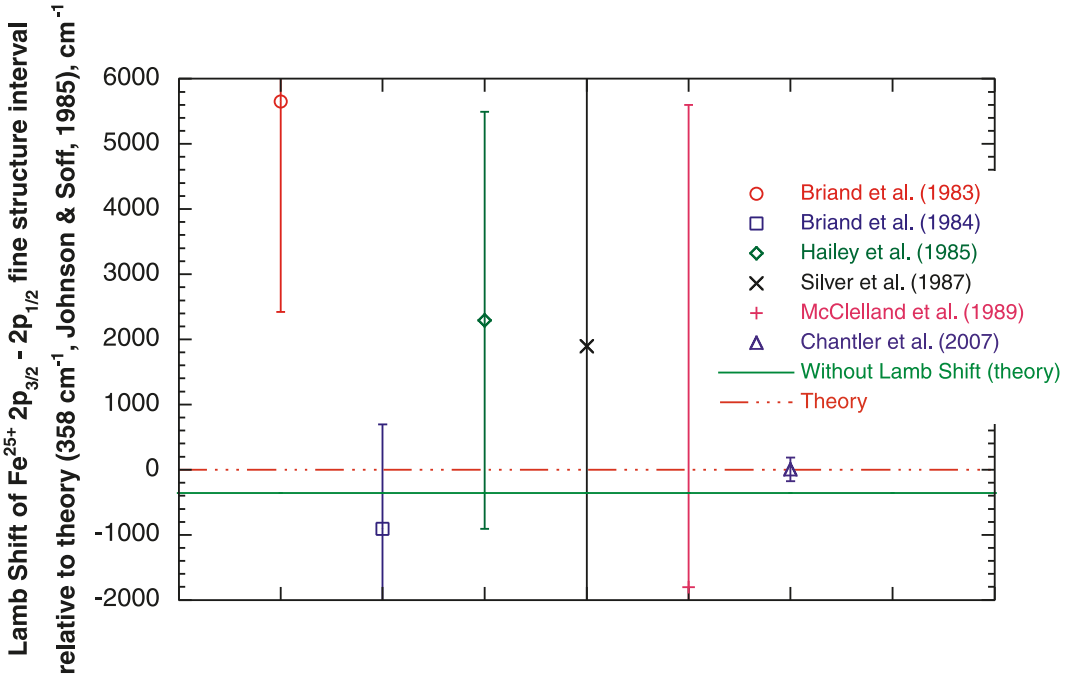
Fig. 2. Comparison of theory and experiment for the 1s-2p Lamb shift, as for the previous plot. Here, points are marked according to the type of source used. Results are paired with Lyman α_1 ($1s\text{-}2p_{3/2}$), followed by Lyman α_2 ($1s\text{-}2p_{1/2}$). References are given in the text and in Fig. 1.



problem, but observed satellite contamination was fitted empirically with seven peaks of arbitrary widths and intensities and gave the dominant error. The quoted 1.5% error on this measurement of the Lamb shift is the smallest in Fig. 1, but the use of different profile widths or forms (e.g., Lorentzians convolved with slits) would give larger errors. The most precise measurement of Lyman α transitions in medium Z ions remains that of [33]. The recoil-ion technique resulted in a measurement of the Lyman α transitions in hydrogenic argon [33], with an experimental precision of 5 ppm, or a 1.5% test of the $1s_{1/2}$ Lamb shift. Note however, that this experiment was limited by contamination, there was no modelling of the processes involved in the analysis, and significant additional possible systematic error cannot be ruled out.

A measurement for $Z = 36$ [44] does not provide a spectrum or discuss satellites, but the technique used produced 28% of the helium-like state prior to excitation with a second foil, with 50% hydrogenic and only 22% of the (optimum) bare charge state. It is therefore expected to show significant contamination. This measurement requires an additional first-to-second order diffraction correction. A measurement at $Z = 22$ is unpublished [36] and was also one of the early absolute spectroscopy measurements. A measure-

Fig. 3. Direct and indirect measurements of the $2p_{1/2}$-$2p_{3/2}$ fine structure interval in hydrogenic iron, compared with theoretical work of Johnson and Soff [45] and Mohr [46]. References are: Briand et al. (1983) [37]; Briand et al. (1984) [57]; Hailey et al. (1985) [58]; Silver et al. (1987) [38]; McClelland et al. (1989) [39]; Chantler et al. (2007) [40].



ment at $Z = 16$ has the largest quoted errors (and the largest discrepancy), because Lyman components were not resolved, and the conditions (and contamination) was designed for a helium-like measurement.

Briand et al. [35] measured Lyman α in argon with a mixture of 20% bare, 42% hydrogenic, and 29% helium-like ions incident on the target foil, at equilibrium for the energy used. Spectra do not show strong contamination by satellites, but helium-like lines are clearly stronger than hydrogenic spectra, the peak Lyman α_2 channel has only 120 counts, the two components overlap at the 25 count level, and satellite contamination give effects below this level. The earlier measurement of iron by Briand et al. [37] attempted to minimize helium-like contamination by using the maximum available energy. Good statistics were obtained. There appears structure in Lyman α_1, the authors noted the problem of satellite contamination, and they varied target thickness and composition "to control the number of outermost shell spectator electrons" and chose "conditions where the lines were free of satellites". There is certainly an improvement over other earlier work. A concern lies with the use of Co Kα peak channels to calibrate the measurement despite a strong 1 eV asymmetric structure, 3 eV resolution, and possible anode problems, yet yielding quoted 0.15 eV or half-channel precision. The authors observed a discrepancy for the 2p fine-structure splitting, which has not been supported by later work.

The remaining measurement in the lower Z region is that of Deslattes et al. [32] for $Z = 17$. Again, the method of absolute spectroscopy is used, but (as noted in Fig. 2), bare Cl^{17+} captured an electron from a differentially-pumped helium target. This avoids many solid-target effects, minimizes multiple capture, and hence provides very clean spectra. In addition, the accel–decel method was used to choose a range of energies $\beta = 0.038$–0.067 and derive improved estimates for β. The calibration lines were poorly resolved, but the spectrometer geometry allowed uncertainties in the angle to the beam to provide large uncertainties in the Doppler correction, leading to the final errors.

The effective sequel to this experiment [41, 43] involved bare Ni^{28+} at four (accel–decel) energies, capturing a single electron (mainly) from a differentially pumped argon target, followed by cascade transitions from a higher n state through Lyman α. β is measured more accurately than before, and the alignment is extremely good. The two-dimensional detector has high resolution, yielding the very precise result quoted in the Fig. (1.5%). Effects of crystal curvature and multiple capture, especially at the low energies used to extrapolate to $\beta = 0$, are not discussed. Further, the crystal suffered from major mechanical deformation, which may be unmodellable with a dynamical diffraction approach and could yield large systematic errors. The experiment was unable to observe both Lyman components, which is of concern relating to the determination of the dispersion relation.

At higher energies it is more common to use Ge(Li) detectors [47] and a 20% measurement of the 1s-2p hydrogenic xenon Lamb shift measurement has been reported. This experiment had significant helium-like contamination, and the spectrometer resolution was inadequate to separate helium-like and hydrogenic transitions. The in-beam comparison technique was used (versus the absolute spectroscopy method), following Hänsch and Silver [38, 48]. The absence of a high-resolution two-dimensional detector is a serious difficulty, and the poor excitation conditions lead to unknown satellite contamination.

Some problems appear intrinsic, such as the Tokamak and Ar-recoil satellite contamination, while other methods may be able to provide large improvements in precision soon.

Table 1. Selected w ($1s2p\ ^1P_1$-$1s^2$) helium-like transition energies (eV) for vanadium and surrounding medium Z ions.

Z	Drake w (eV)	Author, year, reference
15	2 152.43	Safranova 1980 [65]
16	2 460.64	Schleinkofer et al. 1982 [66]
16		Aglitsky et al. 1988 [60]
18	3 139.58	Briand et al. 1983 [59]
18		Deslattes 1984 [59]
19	3 510.45	Beiersdorfer 1989 [61]
20	3 902.37	Aglitsky et al. 1988 [60]
21	4 315.41	Beiersdorfer 1989 [61]
22	4 749.63	Beiersdorfer 1989 [61]
23	5 205.15	Beiersdorfer 1989 [61]
23		Aglitsky et al. 1988 [60]
24	5 682.05	Beiersdorfer 1989 [61]
24		Aglitsky et al. 1988 [60]
26	6 700.40	Briand 1984 [57]
26		Chantler 1990 [52]
26		Beiersdorfer 1989 [61]
26		Aglitsky et al. 1988 [60]
27	7 242.08	Aglitsky et al. 1988 [60]
28	7 805.57	Bombarda 1988 [68]
28		Aglitsky et al. 1988 [60]
29	8 391.00	Aglitsky et al. 1988 [60]
30	8 998.48	Aglitsky et al. 1988 [60]
31	9 628.16	Aglitsky et al. 1988 [60]
32		MacLaren 1992 [62]
32	10 280.14	Chantler 1990 [52]
36	13 114.34	Briand 1984 [67]
36		Indelicato 1986 [69]
36		Widmann 1995 [70]
38	14 669.43	Aglitsky et al. 1988 [60]
39	15 481.98	Aglitsky et al. 1988 [60]

Other sources, such as EBIS and EBIT devices, may avoid contamination and Doppler problems in the near future but may reveal other difficulties.

No precision measurements of vanadium Lyman α have been published, and the best beam-foil measurement for the closest element, titanium, is a 30% measurement of the Lamb shift [36].

The most recent reported measurement in the lower range is an EBIT measurement [49] of hydrogenic titanium, using a curved Ge (220) crystal, where the statistical precision was very high and towards the ppm level, with a single vanadium K α calibration spectra. Satellite contamination appeared to be very minor, and Doppler shifts are negligible in this source. Limitations arise relating to the calibration of the vanadium spectrum [50] of 20 ppm plus the limited calibration of the dispersion axis.

The remaining measurements did not use absolute spectroscopy (except as a rough calibration) and did not use proportional-counter detection. They used the one-electron pick-up method, and were made by research groups including the first author. In comparison with the hydrogen and 2s-2p measurements, this general field is relatively new, and there are numerous improvements that can be made to most experiments [51]. A trend can be seen in the plot for the development of the accuracy and consistency of these measurements, especially for $Z = 26$ (iron).

In the most recent analysis [40], a long and complex experiment collected a large data set on high-resolution X-ray emulsions using curved-crystal diffraction. Neither crystal defects nor photographic linearization were significant limitations to the accuracy, compared with earlier work. Statistics were excellent (a few ppm). The development of linearization modelling and the collection of data beyond the Lyman α – Balmer β intercomparison method were crucial for the accuracy obtained. A key development over previous medium-Z QED X-ray investigations was the characterization of dynamical diffraction effects, shifts and profiles [52–54], especially for use of calibration lines in different orders of diffraction, compared with the highly charged lines and for any curved crystal geometries [55]. The Lyman α – Balmer β intercomparison technique developed by Silver automatically cancels several systematic effects including Doppler shifts, though secondary cancellations involving paired circles and two-dimensional detectors were also necessary to achieve the final accuracy. Several systematics around the part per million level were assessed for the first time, including dielectronic satellites, Lyman γ contributions, 2s-1s, and 4f-2p transitions.

The simultaneous measurement of wide ranges of the Balmer and Lyman series is new and serves to constrain and define the dispersion function of the spectrometer to a much higher level than before. A major investigation related to the population mechanisms in beam-foil excitation; this modelling resolved some long-standing ambiguity [56] and constrained the uncertainty in particular due to down-stream deexcitation arising from (quite significant) Yrast decay. This was the dominant source of uncertainty; followed by fitting uncertainty, diffraction corrections, and statistics.

This led to good accuracy for direct measurements (a 5.7% measurement of the hydrogenic 1s-2p Lamb shift in iron) but also allows highly accurate intercomparisons, because most of the systematics relate to common deexcitation locations or satellites. Hence this yielded measurements of the $2p_{1/2}$-$2p_{3/2}$ fine structure and Lamb shift (Fig. 3). The fine structure yields a measurement of the QED component of the fine structure at the 51% level and a new type of test.

2.2. Helium-like medium Z measurements

A survey of key experimental measurements across medium-Z helium-like resonance lines of $1s^2$-$1s2p\ ^1P_1$ is shown in Tables 1 and 2 and Fig. 4 and compared with QED theory.

The most precise absolute measurement of medium Z helium-like ions is attributed to Deslattes and co-workers [59], with a 12 ppm measurement of the w transition in argon ($Z = 18$). The x and y transitions were measured in this work to similar accuracy, but the z transition was not observed, presumably because of limitations in bandpass. The experiment made use of an external X-ray calibration standard lying close to the wavelength of interest to minimize calibration uncertainty by extrapolation. The recoil-ion experimental method used therein also eliminates the need for Doppler corrections and uncertainties in that work, as opposed to numerous other experiments. The experimental arrangement produced Ar^{16+} by collisions of MeV U^{66+} ions with an argon gas target [33]. A Johann curved crystal spectrometer was employed with a position-sensitive proportional counter

Table 2. Selected w ($1s2p\ ^1P_1$-$1s^2$) helium-like transition energies (eV) for vanadium and surrounding medium Z ions.

			Theoretical transition energies						
Z	Experiment	Ref.	Unified [18]	AO [20]	CI [19]	MCDF [21]	ΔTh (ppm)	QED (eV)	2e QED (ev)
18	3 139.553(38)	[59]	4 749.63	4 749.64	4 749.71		23	1.055	0.09
22	4 749.74(17)	[61]	5 205.15	5 205.16			17		
23	5 205.10(14)	[17]	5 682.05	5 682.06	5 682.15			2.474	0.16
24	5 682.32(40)	[61]	6 700.40	6 700.43	6 700.54	6 700.60	18		
26	6 700.08(24)	[52]	10 280.14	10 280.19	10 280.39		30		
32	10 280.70(22)	[62]					24	7.674	0.40

Note: In this work: ΔTh: Maximum discrepancy between theories. QED: QED contribution to ground state ($1s^2\ ^1S_0$) [18]. 2e QED: Two electron QED contribution extrapolated (see text) [71].

of the backgammon type. This spectroscopic method has systematic errors associated with the geometry and detector type and position, unless these corrections are quantified [17].

Three-electron satellite contamination in these observations was considerably reduced by adjusting the gas target pressure. The contribution of the residual satellite contamination to the overall precision of wavelength determination was estimated to be 3 ppm. However, as with all spectra with strong satellites, the limiting uncertainty is difficult to quantify. Argon is at the lower end of the medium Z elements, where QED effects are smaller relative to the transition energies.

An extensive survey of helium-like transitions was reported by the Russian groups, under difficult circumstances using a low-inductance vacuum spark plasma (LIVS) [60]. A double Johann spectrograph was used to record spectra. Unusually, characteristic lines were used for calibration but based upon the reference wavelengths of Cauclois. In general, these measurements lie higher than theory; but for example the accuracy of the w line in vanadium was reported as 105 ppm, including strong satellite features and reporting only the w lines.

A second survey of helium-like spectra was made by Beiersdorfer and colleagues [61] at the Princeton Large Torus. Helium-like transitions were observed concurrently with hydrogenic lines, which were used as the wavelength reference for calibration. From these observations, values were obtained for the w ($1s2\ ^1P_1$-$1s^2\ ^1S_0$) transition, but the other $n = 2$ to $n = 1$ transitions (x, y, and z) were not reported. The uncertainty reported for vanadium, for example, was 40 ppm. From the plot, this survey generally reports measurements higher than the theory of Drake and suggests that this may be a systematic discrepancy of theory.

An earlier Tokamak measurement reported all components [63] but was defined relative to the w component, had no long-range calibration of dispersion, large satellite structure, and anomalous intensities. One question relates to all Tokamak measurements, namely, how is the contamination by higher charge states treated? Contamination in hot plasmas is often the major limiting uncertainty on the precision of energy measurements [28]. Bulk motions can be very fast and vary between charge states [31].

A fourth helium-like Vanadium observation comprises a study of the K X-ray spectra of helium-like vanadium performed at the Lawrence Livermore EBIT in 1991 by Beiersdorfer et al. [64]. Significant associated dielectronic satellite emissions from lithium-like, beryllium-like, and boron-like ions were observed. Wavelengths were measured for the w, x, and z transitions and for the y–$^3P_0$ blend, which could not be resolved in these observations. When determining the theoretical value for the y–$^3P_0$ blend, an estimated relative intensity of 4:1, respectively, was used, based on private communications [64]. The theoretical separation of y and $^3P_0$ is about 290 ppm of their transition energy, so any uncertainty level in the intensity ratio at the 3% level will shift the theoretical value of the y–$^3P_0$ value by 10 ppm.

Calibrations were performed using the Lyman α doublet of hydrogenic vanadium and the w line of helium-like vanadium. As such, they constitute a relative measurement that also assumes QED theory for one-electron systems are understood. As noted above, no experimental verification of vanadium Lyman α energies has been published. The value used for the w calibration line is semi-empirical and based upon the previous work by this group [61]. Perhaps more importantly, any measurement of helium-like transitions calibrated to the corresponding elemental hydrogenic transition represents an extrapolation of the dispersion function by 10–30 times the interpolated calibration region (the fine structure separation of the Lyman components), depending upon Z (e.g., 17–19 times for vanadium, 12–14 times for iron). The possibility of major extrapolation error or uncertainty is significant.

The experimental uncertainty claimed in this work is between 40 ppm and 60 ppm, although the uncertainty in wavelength determination is optimistically reported to be 40–80 ppm. Care should be taken when comparing these relative measurements to absolute measurements, where calibration has been performed to well-determined reference lines.

Several of the additional measurements reported [65–69] were made under similar conditions as discussed above, with satellite contamination, LIVS complexity, and issues relating to calibration and bandpass. All were developments and important results. Some of the most critical recent measurements are reported in more detail in Table 2.

It should be clear by now that bandpass and calibration are crucial to accurate measurements, and that helium-like studies in the medium-Z region have often been strongly affected either by satellite contamination, bandpass limitations, or possible diffraction or calibration offsets.

Compared with this, [52] and [17] show two examples of extensive calibration of the dispersion relation, including diffraction corrections with minimal satellite contamination and (very) large bandpass. The first used one-electron pickup on the bare iron nucleus in a beam-foil source, so

Fig. 4. Measurements of the w ($1s^2p\ ^1P_1$-$1s^2$) transition in medium Z ions: comparison with theoretical work of Drake [18]. Paterson et al. 1989 [17] (◆); Beiersdorfer et al. 1989 [61], Z = 32, MacLaren et al. 1992 [62] (○); other sources (●) (see refs. cited in Table 1).

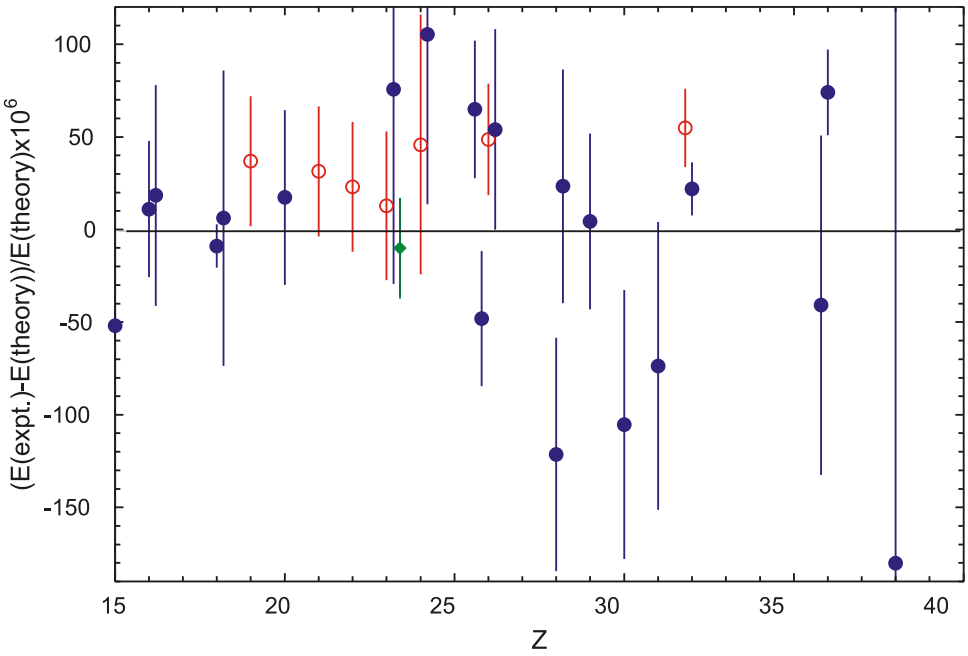
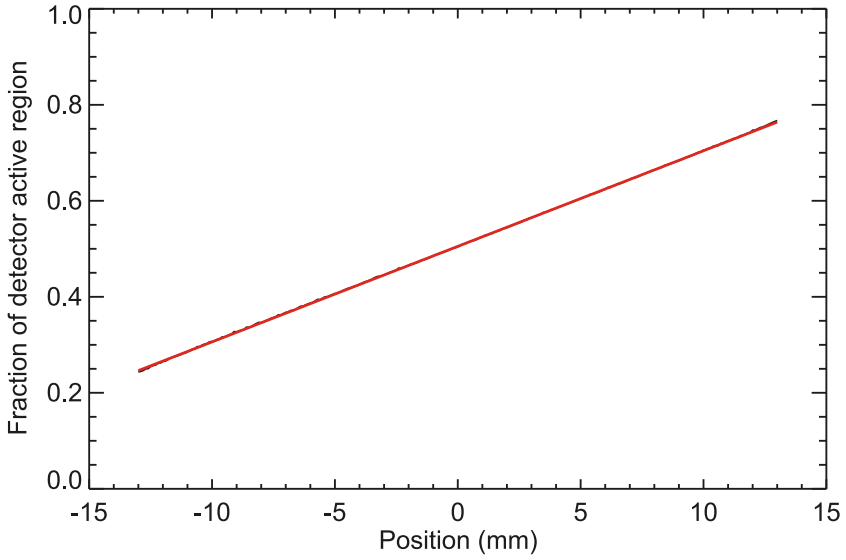


Fig. 5. A plot of the recorded spectral peak centroid location as a function of exposed position across the face of the backgammon-type MWPC. The linearity is better than 0.001% or 2.8 μm.



that the helium-like spectra were relatively weak but very clean; the uncertainty is dominated by statistics (see Table 9 of ref. 40).

The second experiment at an electron beam ion trap (EBIT) has no Doppler shift nor any significant separation of source location from different components. Spectra (w, x, y, and z) are clean with reasonable statistics and represent a 27–40 ppm determination of the helium-like resonance lines with absolute calibration to characteristic lines and the metre. Additionally, this is sensitive to two-electron QED and is sensitive to the excited state 2s level, in part because of the stability of the dispersion calibration. However, the determination of the x component ($^3P_2$) was limited by statistics, the dominant limitation of the strong w and z components was the dispersion function determination (in part limited by statistics of the calibration lines and their bandpass), and a third major limitation (at the 12 ppm level) was the ability to determine the reference lines and their co-location.

Table 2 summarizes the fact that recent experiments are becoming sensitive to both QED components, discrepancies between different computational formalisms, correlation effects, and two-electron QED components.

The uncertainty of theoretical calculations including the estimation of missing or uncalculated terms has been receiving increasing scrutiny as techniques have advanced. One of

the most recent two-electron Lamb shift calculations by Persson et al. [71] estimates missing correlation effects in QED contributions at 0.1 eV for all elements or 20 ppm of transition energies in medium-Z ions. In earlier work, Drake [18] claimed uncertainty for $Z = 23$ was <0.005 eV or 1 ppm of helium-like resonance lines due to uncalculated higher-order terms. Some of the latest theoretical calculations for the w transition in medium Z ions are summarized in Table 2. The discrepancy between theories is indicated, and the maximum discrepancy ranges from 23 to 30 ppm for $Z = 18$–26, and differences are consistent. Our measurements are at this level of uncertainty.

As a simple estimate, we have estimated the two-electron Lamb shift for helium-like ions of Z less than 32 by extrapolating the results of Persson et al. for $Z = 32$–92, using a power law fit (2e QED = aZ^b). The Z power dependence is interestingly found to be $b \approx 2.5$. Derived results for $Z = 18$ and 23 are tabulated with Persson's result for $Z = 32$ in Table 2. Theory might expect a power law dependence of $b \approx 4$, but the sum of all computed contributions gives this result. For vanadium, the two-electron Lamb shift is 0.16 eV or 31 ppm, slightly larger than the experimental uncertainty of 0.14 eV of our measurements. The agreement between this result, obtained from extrapolation of the results of Persson et al. and the value obtained by direct calculation from Johnson and Soff and Drake, is excellent (0.01 eV difference). For $Z = 32$, where the comparison can be made directly without extrapolation, the difference is 0.09 eV, remarkably consistent with the uncertainty estimate (0.1 eV) of Persson et al. for contributions from missing correlation effects in QED. In terms of basic physical effects included, the calculations of Drake and of Persson et al. are equivalent up to all terms of order α^3 (assuming that the many body perturbation theory expansion has converged sufficiently well) and also terms of order α^4Z^6, and α^4Z^5. Any difference between the two calculations should therefore scale as α^4Z^4, at least through the intermediate range of Z.

The calculation of Drake accurately treats the $1/Z$ expansion of the nonrelativistic two-electron QED shift but not the αZ expansion of relativistic and correlation corrections. The calculation of Persson et al. is improved for the αZ expansion, but not the $1/Z$ expansion of the nonrelativistic correlation terms. For larger Z, the calculations of Persson et al. may be preferred, and for smaller Z the calculations of Drake may be preferable.

Because of these issues and motivations, we have spent a significant part of the last few years characterizing systematics and how to address them. In particular, we have been developing highly linear efficient detectors [72–75] and characterization of diffraction theory and (several hundred part per million depth penetration and other) systematics to new levels [55, 76], particularly for application to EBIT sources at NIST and Oxford [77]. EBIT sources can be tuned to have very low satellite contamination and no Doppler shifts but have potential limitations of modest flux and an extended line source shape. For our curved crystal Johann geometry, the systematics and statistical precision associated with these can readily be reduced to below 1–2 ppm.

The use of curved crystals (Johann geometry) dramatically increases the statistics, and also makes the experiment insensitive to positional misalignment of 5–500 μm (major limitations of other techniques). We have recently designed and constructed a prototype two-dimensional backgammon detector in Melbourne (based on NIST and Japanese precursors), promising the best performance (resolution and area) of this flexible type of X-ray detector. Detector development programmes have been designed and implemented to address a number of deficiencies that reduce the efficiency and resolution of the detector system. This has involved the optimization of the internal detector configuration and the re-design of the data acquisition system [74, 75].

Recently, important developments have addressed the linearity of response in backgammon detectors. Improvements have been achieved by carefully modelling the wiring configurations and optimizing the internal electric field. This has resulted in an improvement in the linearity (shown in Fig. 5) and a significant (2–3 fold) reduction in the broadening of the spectral lines [78]. Analysis of the residual structure in the linearity experimental data set (Fig. 5) has revealed additional understanding of these detector types. Modelling studies have confirmed the observed residual structure in the linearity profile and have identified several factors that can be employed to further enhance the linearity and therefore the ultimate spatial resolution. The removal of nonlinear effects has also minimized post-acquisition data analysis and has reduced the likelihood of unwanted systematics increasing the uncertainty in the spectral line position on the detector [77]. New CCD detectors have excellent two-dimensional resolution and are complementary to our backgammon prototypes and will be investigated by the Oxford links.

However, it is crucial to use an array of calibration lines spanning the dispersion of the spectrometer [50]. We recommend a set of four elements including K α and K β lines. One difficulty that then remains is that the Bearden and Deslattes tabulations do not provide profiles and may have accuracies of only 5–20 ppm, which may well limit the measurement accuracy. Hence these must in some cases be remeasured or recalibrated. Maintaining statistics with adequate bandpass to give highly accurate calibration of the dispersion relation is certainly nontrivial, and reducing this below 5–10 ppm by any method is difficult. One of the immediate goals, as mentioned, is to address different helium-like computational formalisms that differ by some 20 ppm in the medium-Z regime, another is to be more critically sensitive to two-electron QED, and a third longer-term objective is to investigate higher-order QED in the medium-Z regime. All of these objectives are showing promise in the medium-term future.

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