# Testing Three-body Quantum Electrodynamics with Trapped $Ti^{20+}$ Ions: Evidence for a Z-Dependent Divergence between Experiment and Calculation

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We report a new test of quantum electrodynamics (QED) for the $w$ ($1s2p\ ^1P_1 \rightarrow 1s^2\ ^1S_0$) X-ray resonance line transition energy in helium-like titanium. This measurement is one of few sensitive to two-electron QED contributions. Systematic errors such as Doppler shifts are minimised in our experiment by trapping and stripping Ti atoms in an Electron Beam Ion Trap (EBIT) and by applying absolute wavelength standards to calibrate the dispersion function of a curved-crystal spectrometer. We also report a more general systematic discrepancy between QED theory and experiment for the $w$ transition energy in helium-like ions for $Z > 20$. When all of the data available in the literature for$Z = 16 - 92$ is taken into account, the divergence is seen to grow as approximately $Z^3$ with a statistical significance on the coefficient that rises to the level of five standard deviations. Our result for titanium alone, 4749.85(7) eV for the $w$-line, deviates from the most recent *ab initio* prediction by three times our experimental uncertainty and by more than ten times the currently estimated uncertainty in the theoretical prediction.

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Quantum electrodynamics (QED) is a cornerstone of modern theoretical physics. New activity on this topic has been stimulated by the announcement of a five-sigma inconsistency between a 15 ppm (parts per million) measurement of an atomic transition frequency in muonic hydrogen [1] and independent measurements of the proton size, linked together by QED calculations. The high sensitivity of such a measurement to QED is derived in part from the large mass of the bound lepton which shrinks the orbital radius. Another way to reduce the orbital radius and study magnified QED effects is to measure transitions in highly charged ions of increasing $Z$. QED processes scale as various powers of $Z\alpha$ and significantly affect the quantum observable, namely transition energies. Moreover, in the high-$Z$ range, some of the perturbative expansions fail, so that theoretical methods very different from those used for hydrogen are required. Since QED treatment of low-$Z$ and high-$Z$ systems are undertaken with significantly different starting points and mathematical techniques, precise measurements for ions in the mid-$Z$ range will guide the long-pursued development of a unified computational methodology with very accurate predictions for the entire domain $Z < 100$ [2, 3].

Advances in QED theory have been sufficient that one can go beyond one-lepton systems (either free or bound) and explore the three-body quantum problem to high precision, including the investigation of helium-like atomic systems with two electrons bound to a nucleus. Here the two-electron QED contributions that are entirely absent in one-electron systems can be probed and compared to various theoretical formulations. In this work, we report a measurement of the strongest resonant transition $1s2p\ ^1P_1 \rightarrow 1s^2\ ^1S_0$ in He-like Ti ($Ti^{20+}$), and present a divergence that is becoming evident between precision measurements and the most complete theoretical formulations of transition energies for He-like ions in the mid-$Z$ range between S and Kr.

The context of this report is the systematic investigation of medium-$Z$ two-electron systems that is underway by several research groups [4–8]. New results are infrequent, owing to the need to account for all known systematic effects to ever-exacting levels of precision and the scarcity of run time available at the few facilities capable of producing such highly charged ions. Improvements in measurement precision not only help distinguish between theoretical methods which treat few-electron atomic systems, but also check the consistency of various experimental approaches which have very different methodologies (using empirical, semi-empirical, relative or absolute calibration schemes). A very useful outcome would be if measurements that are traceable to the definition of the meter, as the present one, would be found to agree with measurements done relative to transitions in H-like systems (convenient and precise fiducials in many highly charged ion experiments) that themselves have been calculated using two-body QED [4, 8, 9]. Such a closing of this measurement loop could help establish hydrogen-like lines of highly charged ions as a new class of transfer

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standards in x-ray spectroscopy [10, 11].

The present work was undertaken at the Electron Beam Ion Trap (EBIT) facility at the National Institute of Standards and Technology (NIST) [12] using wavelength dispersive spectroscopy from the University of Melbourne to obtain precision diffraction profiles of the $w(1s^2(^1S_0)\rightarrow 1s2p(^1P_1))$, $x(1s^2(^1S_0)\rightarrow 1s2p(^3P_2))$, $y(1s^2(^1S_0)\rightarrow 1s2p(^3P_1))$ and $z(1s^2(^1S_0)\rightarrow 1s2s(^3S_1))$ transitions in He-like Ti (labels are standard notation). Earlier work [8, 13–15] demonstrated that a thorough understanding of diffraction conditions, dispersion relations and source systematics can allow the determination of transition energies in highly charged ions to a precision limited by statistics [5, 16].

For energy-scale calibration, an electron fluorescence x-ray source was used to provide high-intensity, neutral x-ray lines that are tabulated and traceable to the definition of the meter [17, 18], thus providing an absolute measurement, rather than one relative to other spectral lines whose positions are calculated. Scandium, titanium, vanadium, chromium and manganese target foils provided characteristic K transition energies (ten K$\alpha$:$2p \rightarrow 1s$). The crystal spectrometer employed a Ge(220) crystal bent to 218 cm radius of curvature in reflection geometry. The calibration lines produced diffraction angles that spanned the spectrometer angular rotation range, with manganese K$\alpha$ near the high-energy limit or the smallest angle of diffraction (31.7°), and scandium K$\alpha$ at the low-energy limit with the largest angle of diffraction (49.4°); the $Ti^{20+}$ spectrum was centred around 41.1°. Several clinometers mounted on the spectrometer provided detector and source arm positions relative to the Earth's local gravitational field yielding diffracting angles accurate to arc-seconds. Because inner shell neutral atomic lines are asymmetric due to underlying atomic processes [19, 20], an extensive investigation of K$\alpha$ peak shapes was undertaken to provide a robust fitting procedure [21] to accurately determine peak profile turning points as well as modelling the doublet as the sum of six Voigt functions. Finally, diffraction angles and detector positions were calculated using a curved crystal dynamical diffraction modelling code [13, 14] to determine photon energy as a function of photon diffraction angle and detector position.

Figure 1 shows the fitted helium-like Ti spectrum accumulated over several days of experimentation and weeks of calibration. The six observed peaks correspond (from left to right) to the titanium helium-like $z$, lithium-like $r$, lithium-like $q$, helium-like $y$, helium-like $x$ and helium-like $w$ transitions. Given that the key components defining the analysis system are the detector and spectrometer, the main two elements of uncertainty relate to an experimentally determined detector response function treated in [22] and references therein, and an experimentally determined dispersion function of clinometer reading versus angle.

The fitted function is the sum of six Voigt profiles and a quadratic background, with the instrumental Gaussian

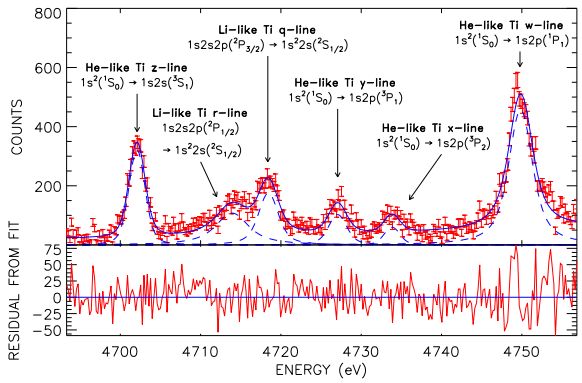


FIG. 1: Fitted summation of helium-like titanium data. Dashed peaks represent individual peak profiles. Solid line gives the fit including the background. Residuals from the fit are indicated below. The $\chi^2_r$ was 2.9.

| SOURCES | | UNCERTAINTY eV | ppm |
|---|---|---|---|
| (i) | Ti angle statistics | 0.046 | 9.7 |
| (ii) | Calibration angle statistics | 0.035 | 7.3 |
| (iii) | Ti X-ray spectra statistics | 0.0285 | 6 |
| (iv) | Detector systematics | 0.024 | 5.1 |
| (v) | Ti fit systematics | 0.012 | 2.6 |
| (vi) | Calibration line spectra statistics | 0.0016 | 0.3 |
| (vii) | Dynamical diffraction corrections | 0.00033 | 0.07 |
| | TOTAL | 0.07 | 15 |

TABLE I: Sources contributing to the final uncertainty in the energy of the $w$-transition in helium-like titanium.

contribution to the total width common to all lines. To suppress correlation error, the width of the weak $r$-line is fixed to a physical value, and the quadratic background is centred around the minimum background region of the $z$-transition.

Table I lists the dominant contributions of uncertainty in our measurement of the $w$-line. The two largest contributions (i and ii) are due to the statistical uncertainty in the clinometer readings which enter into the determination of the diffraction angles for both the x-ray calibration lines and the He-like Ti lines. The third largest contribution (iii) is due to the statistical uncertainty in the fit shown in figure 1. Detector systematics (iv) include non-linearities and channels/mm translational scale [23]. Systematic errors in the Ti spectral fit (v) were estimated by an extensive investigation of the effect of changing the assumed form of the fit function, weights, and $r$-line width in the fit. Statistics relating to the centroid determinations of the calibration lines (vi) and to the dynamical diffraction theory [13, 14] and functional form of the dispersion relation (vii) are minor.

The $w$-line was thereby determined to be 4749.85 eV ± 0.07 eV. Under our experimental conditions for a nom-

inal electron beam energy of 10 keV, satellite contamination does not significantly interfere with this spectral line position [5] as confirmed by calculations with the present EBIT conditions using the FAC [24] and NOMAD codes [25].

Our measurement of the $w$ transition energy in $Ti^{20+}$ has an uncertainty smaller than the magnitude of the two-electron QED contributions to the transition energy [26] and therefore offers insight into the current status of agreement between three-body QED theory and experiment. Fig. 2(a) compares the present result with earlier measurements of this line in helium-like Ti. Fig. 2(b) puts this result in the broader context of all available measurements for this line in ions with $Z > 15$ in comparison with theoretical predictions.

Drake's [2] pioneering comprehensive calculation of the lowest few energy levels of all helium-like ions from $Z = 2$ to $Z = 100$ using the Unified approach has sufficient accuracy that it has stood as a standard reference for decades. More recently, several groups have built upon previous work with a variety of methods for including additional QED corrections to ever-higher orders. The work of Artemyev et al. [26] for example includes two-electron QED corrections and is one of the most complete treatments to date, so is presented as the reference theory in Fig. 2(b). The theory results of Cheng et al. [27] and Plante et al. [28] are detailed relativistic configuration interaction and relativistic many-body perturbation theoretical treatments of He-like systems that cover the range of mid-$Z$ and are therefore included for comparison. These 3 recent works are potential improvements upon Drake's calculation for $Z > 15$.

Fig 2(b) captures the overall state of affairs between experiment and theory for two-electron atomic systems, using the brightest resonance line in He-like highly charged ions as a function of $Z$. All reported experimental data are presented as averages for each $Z$, weighted by the published uncertainty estimates. Our new measurement dominates the average shown at $Z = 22$. For the measurement of Bruhns et al. [9], we use their claimed absolute uncertainty for direct comparison with our present results and with other claimed absolute measurements. The data are plotted as points relative to the theory of Artemyev et al. [26]; theoretical predictions of [28] and [27] are also shown as dotted lines beneath and dashed lines above the zero line, respectively. While the theoretical predictions diverge between themselves by less than 10 ppm at $Z = 36$, a much larger and statistically significant deviation exists between the theoretical predictions and the experimental results. This deviation appears to grow systematically with $Z$. The statistical significance of the deviation does not necessarily grow with $Z$ due to the difficulty of maintaining a similar experimental uncertainty as the total transition energy also grows roughly as $Z^2$. The $w$ line has also been reported at even higher $Z$ in helium-like Xe [42, 43] and U [44], with the former falling below and the latter falling above the $Z^3$ fit of Fig. 2(b). The reported uncertainties on

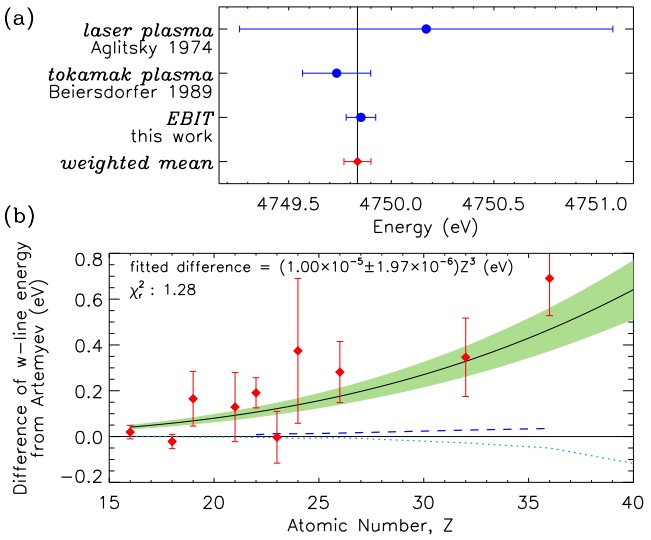


FIG. 2: (a) Measurements of the $w$-line transition energy in helium-like Ti, in temporal order and indicating the nature of the source [29, 30]. (b) Experimental results and theoretical predictions for the $w$-line transition energy in helium-like systems, plotted as a function of $Z$ after subtracting the theoretical values of [26]. The weighted mean of multiple measurements for each $Z$ is shown for clarity. The least-squares fit through the data has a $Z^3$ dependence relative to [26]. Included in the plot are EBIT data for $Z = 16$ [4], $Z = 18$ [9], $Z = 22$ [the present work], $Z = 23$ [5], $Z = 32$ [31], $Z = 36$ [6, 32]and non-EBIT results for $Z = 16$ [30, 33–35], $Z = 18$ [36–39] $Z = 19$ [29, 30], $Z = 21$ [29], $Z = 22$ [29, 30], $Z = 23$ [29, 30, 34], $Z = 24$ [29, 34], $Z = 26$ [8, 29, 34, 40], $Z = 32$ [10] $Z = 36$ [7, 34, 41]. Also shown are the theories of [27](positive dashed values) and [28](negative dotted values). $\chi^2_r = 1.28$, or 1.06 considering only EBIT data.

these high-$Z$ measurements, however, are large enough that they do not distinguish between the fitted curve and the theory. Both are included in the fit of Fig. 2(b).

Fits of the global data set shown to various powers of $Z$ produced $\chi^2_r$ (goodness of fit) that exhibited a optimum at $Z^3$ with a positive coefficient (given in Fig. 2(b)) and demonstrating a deviation from the calculation of [26] at the five standard error level. Our result considered alone deviates from [26] at the three standard error level. Shown is the $Z^3$ fit along with a shaded region indicating the 68 % confidence intervals of the fit. If the fit shown in Fig. 2(b) is restricted to only the eight EBIT measurements, the fit coefficient is virtually unchanged but the $\chi^2_r$ improves from 1.28 to 1.06.

The $1/Z$ expansion [2] to the nominal $Z^4$ scaling of the Lamb shift gives a $Z^3$ dependence to first order. While the $Z^3$ dependence is consistent with the expected scaling of uncalculated screening corrections to the two-loop Lamb shift [e.g. Lindgren et al., unpublished], the magnitude is unexpectedly large. $Z^3$ is the best phenomenological description of the divergence given the present accumulated data. The origin of any divergence between experiment and theory could be more complex, involving

a variety of QED effects, orders, and $Z$ dependencies. Isotope and nuclear size uncertainties are negligible at $Z = 22$, so we have used ordinary Ti which can be assumed to be approximately 74% $^{48}$Ti.

Our measurement of the strongest resonance line on the helium-like isoelectronic sequence results in one of the most statistically significant discrepancies from theory for the 1s2p $^1P_1 \rightarrow 1s^2\ ^1S_0$ transition energy. Both the precision of this measurement and its strategic location on the $Z$-axis have enabled a fresh assessment of the overall agreement between experiment and theory along this sequence. By averaging all available experimental data at each value of $Z > 15$, a general trend of divergence from prediction presents itself at the level of five standard errors. The evidence for systematically-low predicted transition energies suggests that missing terms in three-body QED calculations are much larger than presently anticipated or there is an error in the calculated terms.

In closing we note directions for future work. Although unaccounted-for systematic errors may tend to cancel when results from different research groups are averaged, a critical evaluation of individual results would provide a necessary complementarity. Work on argon ($Z = 18$), for example, discussed evidence of dominating satellite line contamination under certain experimental conditions [36–39]. While it is believed that the associated uncertainty has been reduced dramatically in recent work on argon [9], detailed independent modeling is important to confirm relative positions and magnitudes of possible satellites which could affect the positions of the $w$-line [45, 46]. In addition, new measurements in the unexplored range $Z = 27$ to $Z = 31$ would enable verification and systematic parameterization of apparent discrepancies with theory, pointing towards better ways of extending QED calculations beyond the two-body problem and into the extreme, high-field regime of highly charged ions. Such work will complement activity in other fields in which high power lasers are also being used to probe the quantum vacuum, as discussed in [47, 48].

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