Two-loop QED contributions tests with mid-Z He-like ions

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Abstract. We report about high-precision wavelength determination of H-like and He-like ions at the Heidelberg Electron Beam Ion Trap (HD-EBIT). The experiment was carried out with a novel flat crystal (Si-111) spectrometer applying a reference technique without collimation. The result for the transition energy of the 1s2p1P1 → 1s2 1S0 resonance line in He-like Si14+ agrees with theoretical predictions with an experimental accuracy five times higher than earlier experiments. The same line in Ar16+ was measured with a relative uncertainty of δλ/λ = 2 × 10⁻⁶, a factor of 2.5 more accurate than any X-ray wavelength in highly charged ions ever reported, and for He-like ions probes QED two-electron and two-photon radiative corrections. Beside relative wavelength measurements absolute ones were carried out using the Bond method. The results point at the possibility of establishing absolute Lyman-α transition X-ray wavelength standards in the future.

1. Introduction

Any experiment intended to test QED and the small effects it predicts have to be very precise. In 2005 T.W. Hänisch was awarded the Nobel Prize for his determination of the frequency of the 1s − 2s transition in hydrogen with a relative accuracy of 2 parts in 10¹⁴ [1, 2]. Current theory can predict nearly all decimal figures of the experimental result correctly, but is affected by limitations in the knowledge of the internal structure of the proton, which presently introduces the largest uncertainty in the calculations.

Highly charged ions (HCIs) offer important advantages for studying QED effects scaling with the nuclear charge Z to fourth power, thus increasing with higher charge state of an ion and becoming easier to measure. Moreover, in such systems the electric field strength experienced by the 1s electron can go up to 10¹⁶ V/cm (U⁹¹⁺). This strength of the interactions between electrons and the nucleus cannot be described anymore in the perturbative approach which has been very successful in the case of the hydrogen atom. In addition, due to the high binding energy of their electrons for an accurate description of those ions relativistic effects become essential.

Further theoretical challenges arise in systems involving more than one bound electron. Paramount examples for relativistic systems strongly affected by QED are highly charged ions belonging to the He isoelectronic sequence. In order to predict the energies of electronic states there, one has to solve a many-body problem, which can be treated only approximately. There
are various theoretical approaches to that end. For He-like ions, accurate correlated two-electron
non-relativistic wave functions perturbatively corrected for QED and relativistic effects are
applied by the unified method (UM) of Drake [3]. The all-order (AO) method of Plante [4] has a
different ansatz, namely employing a fully relativistic two-body calculation accounting for QED
and electronic interaction by introducing the Breit approximation. While AO calculations use
the QED corrections derived from the UM, a recent calculation by Artemyev et al. [5] generates
a new, \textit{ab initio} QED prediction within an all-order approach here referred to as bound-state
QED (BSQED). Notice that the UM should describe systems at low $Z$ more accurately since in
this regime correlation effects are more relevant than relativistic ones, while the AO and BSQED
methods are to be expected better at high $Z$, where relativistic effects become dominant. For
medium $Z$ ions, $Z \approx 26$, both relativistic and correlation effects are of comparable size and
therefore accurate description of all relativistic, correlation and QED effects is necessary.

From an experimental point of view, the strongest transitions in HCI appear in the X-ray
region. The most accurate transition wavelengths in that region ($K_{\alpha}$ lines) are known with
an accuracy of $\sim 1$ ppm [6] only, ten orders of magnitude lower than in the visible range. For
He-like systems several measurements of the $1s^22p^1P_1 \rightarrow 1s^21S_0$ ("w" [7]) resonance transition
ranging from $S$ ($Z = 16$) [8] to Kr ($Z = 36$) [9] have been carried out. Deslattes et al. [10]
reached an accuracy of $(\Delta \lambda/\lambda = 12$ ppm) for Ar$^{16+}$ ($Z = 18$), the hitherto highest for such
a measurement. To distinguish among the various theoretical approaches, the uncertainty has
to be reduced by a factor of 5 compared to this experiment. The current experiment at the
Heidelberg Electron Beam Ion Trap (HD-EBIT) contributes to alleviate this situation.

2. The experiment
The classical crystal spectrometer is still widely used to study X-ray transitions at high
resolution, since there are currently no appropriate laser sources available in the X-ray region.
Since X-ray spectrometers using curved crystals have a complicated focussing geometry and are
difficult to describe, a flat crystal spectrometer type with rotatable crystal (Si-111) was chosen
for in our experiment.

Transition energy determination implies measuring the Bragg angles which becomes a quite
challenging task if an accuracy at the low ppm is aimed, since an offset of the angular scale
cannot be avoided. In contrast, angular differences can be determined very precisely. Thus, for
high precision measurements X-ray reference lines are usually required, normally $K_{\alpha}$ transitions
of copper, molybdenum and tungsten [11], limiting the accuracy which can be reached to the
precision to which their energies are known, $\sim 1$ ppm. These transitions as reference lines,
however, have serious limitations at higher levels of accuracy. Since to generate such lines
neutral atoms embedded in the bulk have to be excited, multi-electron effects caused by all bound
electrons, i.e. so called satellite transitions, lead to asymmetric lineshapes. These asymmetries
cannot be predicted by theory at the required level of accuracy. Therefore it has been proposed
[12, 13] to use other lines not affected by these problems as reference lines. Suitable transitions
are the Ly$\alpha$ transitions (used in our experiment), since they can be determined reliably by
theory.

In our experiment we use the HD-EBIT for the production of HCI. The advantage of our
method in comparison to others such as the measurements applying the recoil ion technique
[29, 10], deceleration and electron capture method [14] or using tokamak plasmas [15] is the
spectral purity, i.e. satellite-free lines (Fig. 1) and the absence of Doppler shift. Thus using an
EBIT for the production of the ions studied later on it should be possible to establish Lyman-$\alpha$
wavelengths as high-precision, calculable atomic X-ray standards. This standard is requested
compulsory with regard to future laser resonance fluorescence studies at synchrotron facilities
and free-electron lasers [16] as well as for the development of X-ray microcalorimeters [17].

Normally, performing high precision measurements on transition wavelengths in the X-ray
Figure 1. X-ray spectrum of the Lyman-α$_1$ (7) and Lyman-α$_2$ (5) lines in Ar$^{17+}$ (HD-EBIT) fitted with a Voigt profile shown together with predicted [18] satellites (1-4, 6, 8) on a logarithmic scale. One can see that satellite “6” could have an influence on the peak position of the Lyman-α$_1$ line which can be calculated by fitting a Gaussian to satellite “2” since the excited state is the same for both satellites. The transition probability of satellite “2” (E1 transition) is $\sim 80$ times larger than the one of satellite “6” (M1 transition). With the branching ratio mentioned above, the intensity of satellite “6” is $< 0.03\%$ of the intensity of the Lyman-α$_1$ transition, i.e. insignificant. Notice also that the resolution is better than FWHM $< 1.8 \text{ eV}$ at 3323 eV.

region the incoming direction of the X-rays is fixed by collimation with slits which leads to a decreasing X-ray flux, not desirable in the view of the low intensity (generated by $\sim 1$ million of trapped ions) emitted by an EBIT. To avoid these problems, in our experiment a reference method avoiding collimation, the “a/b-method” [19, 20], developed in our group by J. Braun and H. Bruhns was applied.

2.1. The a/b-method using light fiducials

The central idea of this new measuring is to monitor the incoming direction of the X-rays without significant loss of X-ray flux using two laser beams originating from a virtual source overlapping with the trapped ions as angle and direction references (“fiducials”). These laser beams are reflected by the same crystal onto a CCD detector according to the usual optical reflection law. The ratio of the distances from the X-ray position on the detector to the light fiducial positions is a function of the incoming direction of the X-rays and depends on the Bragg angle. A central advantage of the a/b-method is that this ratio, as a result of similar triangles’ theorem, does not depend on the exact locations of the crystal or the camera, as long as the points from which the X-rays and the light fiducials originate coincide, thus generating triangles with a common vertex. To align the virtual source of the laser fiducials, two retractable lenses collect visible light emitted by trapped B-like Ar$^{13+}$ ions which is imaged onto the CCD detector. The virtual source is then adjusted to overlap with the imaged light. A detailed description of the a/b-method can be found in [19].

2.2. Combination of the a/b-method with the Bond method

To perform absolute wavelength measurements we combined the a/b-method with the Bond method [21]. The rotatable flat crystal reflects X-rays towards either one of two symmetrically arranged, windowless, cryogenically cooled CCD detectors. This angle is determined by the a/b-method, and still contains an offset. In a second step, a rotation by $180^\circ - 2\Theta_B$ where $\Theta_B$ is the Bragg angle of the line of interest leads to a reflection of the X-rays towards the other CCD detector. This second angle containing the same offset is also determined. In this way the exact Bragg angle $\Theta_B$ can be derived from the measured angular difference in the crystal angle.
2.3. Experimental parameters

For the production and trapping (trapping region: cylindrical volume of 100 µm diameter and 4 cm length) of Ar$^{16+}$, Cl$^{16+}$, S$^{14+}$ needed for the measurements in our experiments the electron beam current was set to about \( \sim 400 \) mA at an electron beam energy of \( E_e = 9.5 \) keV. In order to keep the temperature-stabilized laboratory undisturbed for several days during our measurements, the EBIT and the spectrometer were computer controlled and worked without operator intervention during the runs.

3. Results and conclusions

For alignment of the crystal, the angle \( \phi \) between the Si (111) plane and the crystal surface was determined in a separated setup to be \( \phi = 0.0585^\circ \pm 0.002^\circ \) [28]. The crystal is mounted on a holder which allows to rotate it around the surface normal axis. This way the orientation of \( \phi \) can be adjusted perpendicular to the scattering plane thus not having any influence on the measured difference angle. The orientation of the Si (111) plane with respect to the crystal shape needed for this purpose was known with a precision of \( \pm 2^\circ \). After performing this alignment procedure the remaining error contribution caused by this process was calculated to be 0.5 ppm [20]. Smaller errors arise from the change of the lattice spacing due to temperature fluctuations, adjustment of the visible light assembly (see 2.1), alignment of the spectrometer with respect to the trap center and stability of the light fiducials.

Besides counting statistics, the remaining leading error contribution to our absolute measurements is caused by the fact that the EBIT trapping volume is a line source emitting X-rays which generate a series of circular segments on the CCD cameras after Bragg reflection. Therefore a projection of the X-ray spectra on the energy dispersive axis results in intrinsically asymmetric line profiles leading to a calculable shift of the line centroid to about 40 ppm higher energies [20]. A direct observation of the line bending is not possible since symmetric line broadening effects, e.g. thermal broadening effects, lead to a modification of the line shape. If the X-ray emission center lies outside the scattering plane this shift is partially compensated, in our case by \( \sim 15 \) ppm [28], since both the effective crystal lattice spacing and the line curvature shift are modified, and a final uncertainty of the absolute wavelength measurements of \( \sim 20 \) ppm cannot be eliminated. Performing relative wavelength measurements the final uncertainty can be significantly reduced by putting these systematic contributions leading to a shift of the line centroid in a correction angle \( \Delta \Theta_{\text{corr}} \) and adding it to the absolutely measured Bragg angle \( \Theta_a \) of the line of interest. \( \Delta \Theta_{\text{corr}} \) is obtained as the difference between the predicted Ar$^{17+}$ Lyman-\( \alpha_1 \) Bragg angle \( \Theta_t \) derived from the theoretical wavelength \( \lambda_t \) [22] and the measured absolute Lyman-\( \alpha_1 \) Bragg angle. A detailed description of this procedure can be found in [28]. A scaling from \( \Theta_t \) to \( \Theta_a \) was necessary since the correction angle \( \Delta \Theta_{\text{corr}} \) depends on the Bragg angle. The scaling factor was derived from a ray-tracing simulation [20] of the X-ray trajectories.

Our results listed with 1σ error bars are shown in Table 1. The results were converted to energy using the conversion factor \( hc = 1.239841875(31) \times 10^{-6} \) eV m [11]. Figure 2 shows

| Transition | \( E_{\text{theo}} \) (eV) | \( E_{\text{exp}} \) (eV) | Error (ppm) |
|------------|-----------------|-----------------|-------------|
| Cl$^{16+}$ Ly-\( \alpha_1 \) | 2962.352 [22] | 2962.344(30) [28] | 10.0 |
| S$^{14+}$ w | 2460.629 [5] | 2460.641(32) | 13.0 |
| Ar$^{16+}$ w | 3139.582 [5] | 3139.583(6) [28] | 1.9 |
the relative deviation of the experimentally measured $\Delta E_{1s}^{exp}$ and theoretically predicted $\Delta E_{1s}^{theo}$ Lamb shift [22] in hydrogenlike ions as a function of the nuclear charge $Z$. Within the error bars all experimental results agree with the theoretical calculations, especially good for hydrogen and uranium while unfortunately for the mid-$Z$ region experimental precision is much lower (as well as the accuracy reached for our results of the chlorine Lyman-$\alpha$ transition energy [28]), not allowing to establish transitions in hydrogenlike ions as X-ray standard lines. For this purpose theoretical predictions still have to be tested on a higher level of accuracy. Consequently, currently huge efforts are made to align the spectrometer in such a way that the line source center lies inside the scattering plane in order to minimize the above mentioned uncertainty of our absolute wavelength measurements. Nevertheless, as we compare our 2007 result for the chlorine Lyman-$\alpha$ transition energy with former results [23, 24, 25], all results reported earlier had an uncertainty bigger than 100 meV. Our result has an error bar of only 30 meV [28], enabling to test the vacuum polarization contribution to the $1S_0$ state of 68 meV [23]. Our recent result for the $S^{14+}$ w transition, $\lambda_w = 5038.695(74)$ mÅ, or $E_w = 2460.641(32)$ eV, has an error of only 12.8 ppm, a factor of $\sim 3$ better than the former most precise measurement of this transition energy [8]. This result is in excellent agreement with all theoretical predictions [3, 4, 5] within its $\sim 13$ ppm uncertainty. However, the error bar has to be reduced in ongoing experiments to be able to distinguish between the different theoretical calculations on a level of (finally) 1 ppm. We would like to point out our 2007 result [28] for the $Ar^{16+}$ w transition, $\lambda_w = 3949.066(8)$ mÅ, or $E_w = 3139.583(6)$ eV, which has an uncertainty of only 2 ppm [28]. This is 6 times more accurate than the most precise measurement in any He-like ion, namely in $Ar^{16+}$ recoil ions [10] and until now a factor 2.5 better than any X-ray wavelength in HCIs ever reported [29]. To calibrate our spectra we used the theoretical $Ar^{17+}$ Lyman-$\alpha_1$ wavelength instead of the experimental one obtained [29] because the uncertainty of that experimental value, 5 ppm, exceeds the theoretical one by far. While the measurement of Deslattes et al. [10] gave an indication that the w transition energy could be smaller than the predicted theoretical values, our result is in excellent agreement with state-of-the-art BSQED calculations by Artemyev et al. [5] and the results of the AO method [4] within its 1σ error estimate. The UM prediction [3] lies just inside our 2 ppm error bar. This could be due to an incomplete description of relativistic effects at $Z = 18$ in UM [28]. Table 2 lists theoretical one- and two-electron QED contributions to the $1s2p^1P_1$ and $1s^21S_0$ states in the $Ar^{16+}$ ion (from [5]). As seen there, our result probes, at a level of 6% of their total, all two-electron QED contributions to the $1S_0$ ground state energy, i.e., screened self-energy, screened vacuum polarization and two-photon exchange diagrams. For example, the change of the ground state energy due to vacuum polarization effects (7.2 meV) is
Table 2. Theoretical one- and two-electron QED contributions (in eV) to the $1s^2 2p^1 P_1$ and $1s^2 1S_0$ states in $\text{Ar}^{16+}$ (BSQED taken from [5]). Total 1-el.: sum of one-electron contributions; Scr. SE: screened self-energy; Scr. VP: screened vacuum polarization; 2-ph. exch.: exchange of two virtual photons; total 2-el.: sum of two-electron contributions.

| State  | Total 1-el. | Scr. SE | Scr. VP | 2-ph. exch. | Total 2-el. |
|--------|-------------|---------|---------|-------------|-------------|
| $1S_0$ | -1.1310     | 0.1116  | -0.0072 | -0.0091     | 0.0953      |
| $1P_1$ | -0.0062     | 0.0031  | -0.0001 | 0.0001      | 0.0031      |

1.2 times larger than our present experimental accuracy. Our experimental value is also sensitive to the total one-electron QED correction of the $1P_0$ excited state, but the uncertainty is still too low to probe the total 2-electron contribution (3 meV). Thus, although our results now agree excellently with the predictions of BSQED [5] on the present level of accuracy, and are in good agreement with [3] and [4] at $Z = 18$, further tests require extending measurements over a broader range of elements.

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