Direct double ionization of the He-like B^{3+} ion by a single photon

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Within a joint experimental and theoretical research project, double photoionization of the He-like B^{3+} ion by a single photon was studied in the energy range from approximately 350 to 1160 eV. With the parent-ion beam in the experiment containing both $1s^2\ ^1S$ ground-state (90.9%) and $1s2s\ ^3S$ metastable B^{3+} ions (9.1%), two contributions to the apparent single- and double-ionization cross sections, $\sigma_{34}^{\mathrm{app}}$ and $\sigma_{35}^{\mathrm{app}}$, respectively, are involved in the measurements. Ratios $Y(5+)/Y(4+)$ of double- over single-ionization yields were experimentally determined. By multiplying the measured ratios by the known cross section $\sigma_{34}^{\mathrm{app}}$, the apparent cross section $\sigma_{35}^{\mathrm{app}}$ for double ionization was inferred. Using the information thus obtained, the measured yield of B^{5+} ions produced from hydrogenlike B^{4+} could also be normalized. The results show good agreement with theoretical benchmark cross sections σ_{45} for single photoionization of B^{4+}. Convergent close-coupling calculations were performed to determine double-photoionization cross sections σ_{35} for $B^{3+}(1s^2)$ and $B^{3+}(1s2s)$ ions. The result for the ground state agrees very well with theoretical data obtained previously with an intermediate-energy *R*-matrix approach. Within the systematic uncertainty of the normalized experimental cross sections, calculated and measured data are in agreement with one another.

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I. INTRODUCTION

Direct, or nonsequential, double ionization of an atom, molecule, or ion by a single photon is one of the most fundamental many-body processes. This phenomenon, known as photo double ionization (PDI), has been extensively studied both experimentally and theoretically, particularly in neutral helium—the simplest atom accessible for such investigations ([1–5] and the numerous references therein). Theory has gone beyond the neutral He atom and also treated two-electron ions [6–13] to explore the importance of electron correlation relative to the electron-nucleus interaction in the PDI process. These theoretical attempts have remained untested so far by experiment. A single relative measurement of photo double detachment yields of H^- [14] only covering an energy range of a few hundred meV around the threshold could not challenge the vigorously pursued theoretical treatments of two-electron removal from H^- [6,10,15–21]. Not a single experiment has been reported to date on PDI of a heliumlike positive ion.

Even PDI of ions with more than two electrons, which can be produced more easily, has been studied only for very few examples. Like in H^-, measurements of photo double detachment (PDD) from He^- [22] and K^- [23] were restricted to very narrow energy ranges of a few hundred meV just above the respective PDD thresholds. The theoretical interpretation of a measurement of double-photodetachment cross sections of F^- [24] suggested a dominant contribution of PDD at energies around 50 eV. However, the experiment did not yield a clear distinction between individual contributions of PDD versus 2*s* inner-valence-shell ionization with subsequent Auger decay. Similarly, evidence for contributions of PDD could be found in multiple photoionization experiments on Fe^- [25] but, again, quantifying and separating PDD from other possible double-detachment channels could not be achieved.

Clear-cut evidence of PDD of negative ions over an extended energy range could be provided together with the measurement of absolute cross sections for F^- [26] and C^- [27]. The first measurement of an absolute PDI cross section of a positive ion was achieved in an experiment addressing the removal of two *M*-shell electrons from the Ar^+ ion [28]. Extensive measurements on multiple (*m*-fold) ionization of Ar^+ ions (with $m = 1, 2, \ldots, 6$) [29] could be disentangled by employing a theoretical approach to PDI [30]

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including direct two-electron removal processes of electrons residing in any of the $2s$, $2p$, $3s$, and $3p$ subshells.

Reasons for the lack of experimental data for PDI of ions have been the relatively small cross sections for PDI, the low densities generally achievable with ionic targets, and the limitations in photon flux available at synchrotron radiation facilities. Free-electron lasers [31] can provide photon beams with extremely high photon densities exceeding the capabilities of synchrotron light sources by many orders of magnitude. However, such levels of photon density facilitate multiphoton absorption by a single atom or ion which is in conflict with the condition of single-photon interaction for (double-ionization) cross-section measurements.

An unexpected result had been obtained for PDI of the K shell of C^- evidenced by the observation of C^{4+} product ions with an obvious contribution from the simultaneous removal of both K-shell electrons and subsequent Auger decays [27]. The inferred PDI cross section for $1s + 1s$ electron removal from C^- reaches a maximum of approximately 3 kb. This is roughly a factor of 30 above the theoretical prediction of PDI of He-like C^{4+} [12]. Half of the difference may be rationalized by the reduced threshold energy for K-shell double ionization of $\approx$670 eV for C^- as compared to $\approx$880 eV for C^{4+}; however, the remaining discrepancy by more than an order of magnitude needs to be explained. As a first step towards resolving such a disturbing discrepancy, an experimental verification of the theoretical approaches to PDI of a He-like ion is desirable. However, measurements on PDI of He-like ions are particularly difficult because the associated PDI cross sections are minimal. Moreover, with the exception of singly charged Li^+ [32,33] and H^-, their technically achievable production yield is low compared to that of ions with more electrons.

The peak cross sections for PDI of heliumlike ions are predicted to drop approximately proportional to Z^{-4} [6] which, with respect to signal rates, would have favored a lower-Z element. However, Li^+ with its PDI threshold energy of about 198.1 eV would have been outside the available photon-energy range of our experimental setup, as would have been H^-. The next more highly charged ion, Be^{2+}, was not a viable choice due to safety concerns. Thus the He-like B^{3+} ion with its relatively small atomic number $Z = 5$ was chosen for the present experiment.

Since the parent-ion beam in our experiment contained both ground-state and metastable B^{3+} ions, the measured yields of bare B^{5+} ions resulted from the following two PDI processes:

$$h\nu + B^{3+}(1s^2\ ^1S) \rightarrow B^{5+} + 2e^-, \tag{1}$$

$$h\nu + B^{3+}(1s2s\ ^3S) \rightarrow B^{5+} + 2e^-. \tag{2}$$

Within the frame of the present project, the cross sections for both of these processes were calculated by employing the convergent close-coupling (CCC) method. Three mechanisms for direct two-electron removal from a heliumlike system have been discussed: the so-called two-step one (TS1), the shake-off (SO), and the quasifree mechanism (QFM) (see Ref. [3] and references therein). In TS1 a photoelectron is ejected which, on its way out, knocks out a second electron. This mechanism dominates PDI at lower photon energies and the cross section is reminiscent of electron-impact ionization. At higher energies SO takes over and QFM is generally a very small contribution [3]. The present experiment particularly provides a test of the calculations for PDI of ground-state B^{3+} at energies where TS1 dominates. Theory and experiment are in satisfying agreement.

The present paper is organized as follows. Next to this introduction, in Sec. II, the experimental procedures are outlined. In Sec. III, the theoretical approach to PDI is briefly described. Section IV presents and discusses the theoretical and experimental results. The paper ends with a summary and conclusions (Sec. V).

II. EXPERIMENT

The experiment was conducted at the soft-x-ray beamline P04 [34] of the synchrotron lightsource PETRA III [35] operated by DESY in Hamburg, Germany. The permanent endstation PIPE (Photon-Ion Spectrometer at PETRA III) [36] of beamline P04 provided the complete experimental setup needed for the present measurements. The photon-ion merged-beams technique [37] was employed. The experimental procedures for the measurement of cross sections at PIPE have been previously described in great detail [38,39]. The present measurements were part of an experimental campaign aiming at photoionization of boron ions. First results and the techniques employed in that campaign have already been published [40]. Therefore, the present description of the experimental procedures is kept at a minimum.

The double-ionization threshold for ground-state B^{3+} is 599.600 43 eV [41,42]. The maximum PDI cross section for $B^{3+}(1s^2\ ^1S)$ was previously predicted to be only about 200 b [12] at a photon energy of about 750 eV. The beamline is equipped for such experimental conditions with its very high photon flux ϕ_{ph} of up to 10^{14} photons per second at $E_{ph} =$ 750 eV. The photon-ion merged-beams interaction length of 1.7 m available at PIPE supports the measurement of small cross sections. An additional experimental asset helped facilitate the measurement of extremely small signal rates. The single-particle detection of B^{5+} product ions was accompanied by extremely low background. Neither the ion beam nor the photon beam alone produced a measurable count rate on the B^{5+} product-ion detector. This was made possible by the careful design of the charged-particle optics of PIPE preventing stray particles and photons to reach the detector and by the low pressure near 10^{-8} Pa in the experiment suppressing two-electron stripping in residual-gas collisions. Hence it was essentially only the detector dark-count rate that produced background. The design, the construction, and the operation of the detector unit [43,44] were aimed at the suppression of spurious counts from microdischarges in the vicinity of the robust channel electron multiplier used to generate measurable electronic pulses. Dark counts were measured for 40 000 s accumulating 682 counts which results in a dark-count rate of 0.01705(65) Hz, where the numbers in parentheses stand for the uncertainty of the last two digits.

Beams of isotopically purified 18-keV $^{11}B^{3+}$ ions, filtered by a magnetic-dipole analyzer, were collimated to a diameter of about 1 mm and merged with the counterpropagating photon beam provided by beamline P04. Photoionized B^{5+}

product ions were separated from the parent $^{11}B^{3+}$ ions by a second dipole magnet and then detected with almost 100% efficiency. All parent ions were collected in a large Faraday cup and their electrical current was measured by a sensitive electrometer. The flux ϕ_{ph} of the transmitted photon beam was recorded by a calibrated photodiode. Typical $^{11}B^{3+}$ ion-beam currents I_{ion} in the interaction region were between 2.5 and 3 nA. The product-ion detector recorded approximately 0.05 true signal counts per second under these conditions.

The parent $^{11}B^{3+}$ ion beam extracted from an electron cyclotron resonance ion source (ECRIS) consisted of two components: $^{11}B^{3+}(1s^2\ ^1S_0)$ ground-level and long-lived $^{11}B^{3+}(1s2s\ ^3S_1)$ excited-level ions [40]. Hence double-ionization signals from both beam components had to be expected [see Eqs. (1) and (2)]. The fraction of metastable ions in the parent-ion beam was previously determined to be $f = 0.091 \pm 0.016$ [40], which is in good accord with the findings of a preceding experiment on electron-impact ionization of B^{3+} ions [45] employing an identical ECRIS.

A blazed 400 lines per millimeter grating with Pt coating was used to achieve the highest possible photon flux. With a monochromator exit-slit width of 1000 μm the photon beam had an energy spread of about 1 eV at $E_{ph} = 750$ eV. The photon energies were calibrated by employing very accurately known resonances in the single photoionization of B^{3+} ions [40]. The energy axis for the present yield and cross-section data is accurate within an error margin of ± 0.1 eV. The Doppler shift of photon energies by approximately a factor of $1 + v_{ion}/c = 1.00188$ due to the counterpropagating photon and ion beams was corrected for, considering the ion velocity $v_{ion} = 5.62\times10^5$ m/s and the vacuum speed of light c.

Absolute photoionization cross sections $\sigma_{qq'}$ for changing the ion charge from q to q' by removal of $(q' - q)$ electrons can be determined from measurable quantities linked with one another by the following equation:

$$\sigma = R_{q'} \frac{q\, e\, v_{ion}}{\eta\, I_{ion}\, \phi_{ph}\, \mathcal{F}}, \tag{3}$$

where $R_{q'}$ is the detector count rate of product q'-charged ions, e the elementary charge, η the detector efficiency, and $\mathcal{F}$ the beam-overlap factor (form factor) [37]. In the present experiment, product-ion yields

$$Y_{q'} = \frac{R_{q'}}{I_{ion}\, \phi_{ph}} \tag{4}$$

were determined without measuring $\mathcal{F}$.

Rates R_4 of B^{4+} and R_5 of B^{5+} ions produced as a result of single-photon absorption by B^{3+} parent ions were recorded in separate energy-scan measurements covering a photon-energy range from approximately 350 to 1160 eV. The photon flux and the ion current were monitored at the same time for normalization of the signal. From the resulting yields, ratios $r = Y_5/Y_4$ were determined. Assuming that the form factor $\mathcal{F}$ did not change with time, the measured ratios r can also be interpreted to be the ratios of apparent cross sections $\sigma_{35}^{app}/\sigma_{34}^{app}$. These cross sections are "apparent" because they depend on the experiment-specific fractions f of metastable and $1 - f$ of ground-level B^{3+} parent ions. Consequently, the apparent cross sections addressed in the experiment can be represented as

$$\sigma_{3q'}^{app} = f\sigma_{3q'}^{ms} + (1 - f)\sigma_{3q'}^{gs}, \quad q' = 4, 5, \tag{5}$$

where the superscripts ms and gs identify the connection of the cross sections with either the metastable or the ground-state ions, respectively.

As demonstrated in the preceding publication [40], the apparent cross section σ_{34}^{app} is well understood and can be employed to determine the apparent PDI cross section σ_{35}^{app} for He-like B^{3+}. The later discussion in this paper will provide evidence that the present σ_{35}^{app} is almost equal to σ_{35}^{gs} at energies above the PDI threshold and therefore provides a good test of calculations of the PDI cross section for ground-state B^{3+} ions. In order to obtain σ_{35}^{app}, the cross-section ratio has to be multiplied with the known σ_{34}^{app}.

Since the overlap factor $\mathcal{F}$ could not be separately determined and monitored (and is inherently associated with an uncertainty of about 15% anyway [38]), one cannot exclude that it changed with time. In order to overcome this problem, the ratio r was measured by switching directly between $q' = 5$ and $q' = 4$ at a photon energy of 761.5 eV. For the measurement, the photon beam was chopped and the "on" and "off" phases were separately evaluated. Within the associated total time span of approximately 1 h for the measurement of the yield ratio, $\mathcal{F}$ could be safely assumed to remain constant. Therefore, the ratio $\sigma_{35}^{app}/\sigma_{34}^{app}$ was directly obtained from $Y_5/Y_4 = (4.38 \pm 0.49)\times10^{-3}$ at 761.5 eV. From the energy-scan yield measurements that were recorded up to two days apart from one another, a ratio $Y_5/Y_4 = (5.25 \pm 0.79)\times10^{-3}$ at 761.5 eV was inferred. Therefore, we applied a correction factor of 0.834 to the cross-section ratios obtained from energy-scan measurements to match them with the separately determined cross-section ratio.

The directly determined ratio $\sigma_{35}^{app}/\sigma_{34}^{app}$ and the corrected ratios from the energy-scan measurements were multiplied with the known apparent cross section σ_{34}^{app} to obtain the desired σ_{35}^{app} PDI results. The apparent single-ionization cross section is almost exclusively determined by the contribution of ground-state ions. It is shown in Fig. 11 of our preceding publication on single photoionization of heliumlike B^{3+} [40]. For the present purposes, it was reconstructed from the present CCC calculations following Eq. (5) and considering the fraction $f = 0.091$ of metastable parent ions in the experimental B^{3+} ion beam.

On the basis of the procedure described above, a normalization function for measured product-ion yields can be easily constructed and used to determine cross sections on an absolute scale. The condition is that the collimation of the ion beam and the geometry of the photon beam are not changed thus constraining possible variations of the form factor. This concept was also applied in the preceding publication on single photoionization of B^{3+}. The correction function A_{corr} is simply based on the high accuracy of calculated cross sections σ_{34} for direct single ionization of heliumlike $B^{3+}(1s^2\ ^1S)$ and (with less emphasis) of $B^{3+}(1s2s\ ^3S)$ and can be represented as $A_{corr} = \sigma_{34}^{app}/Y_4$.

This concept was also applied to single photoionization of hydrogenlike B^{4+}

$$h\nu + B^{4+}(1s\ ^2S_{1/2}) \rightarrow B^{5+} + e^- \tag{6}$$

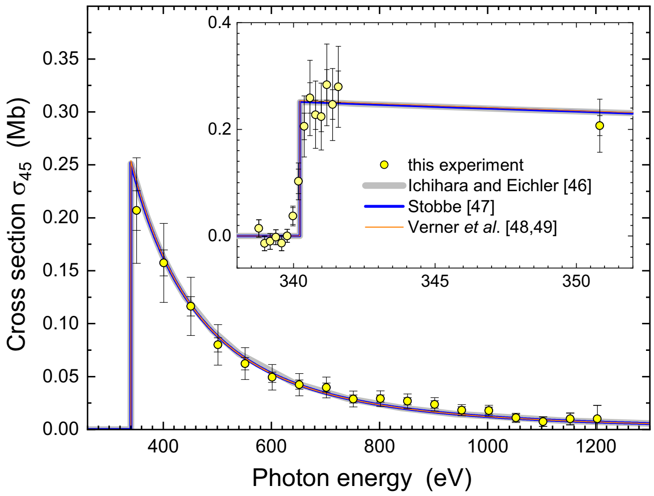

FIG. 1. Cross sections σ_{45} for the photoionization of hydrogenlike ground-level $B^{4+}(1s\,^2S_{1/2})$ ions. The open circles with yellow shading represent the present experiment for which the statistical and total error bars are shown. The solid curves result from the theoretical calculations by Ichihara and Eichler [46] (the thick gray curve), by Stobbe [47] (the solid blue line), and by Verner *et al.* [48,49] (the thin red line). The inset highlights the threshold region.

for which B^{5+} product-ion yields were determined as a function of the photon energy without changing the geometry of the B^{3+} experiments. Since the cross sections for photoionization of hydrogenlike ions are known by theory without doubts, the derivation of such data from experiments can serve as a validity test of the data-taking and data-analysis procedures. Of course, uncertainties of the proposed technique have to be considered. On the basis of our previous work on single photoionization of B^{3+} [40] we infer a relative uncertainty of $\pm 10\%$ for the calculated $\sigma_{34}^{\mathrm{app}}$ in the energy region of interest in the present investigation. Systematic uncertainties also arise from possible variations of $\mathcal{F}$ in time. These uncertainties are estimated to be $\pm 20\%$.

We conclude this experimental section with presenting the result of the test measurement of the cross section σ_{45} for single photoionization of H-like $B^{4+}(1s\,^2S_{1/2})$ in which the described procedure for data normalization was applied. Naturally, the injected beam contained only ground-state ions. The measurements were performed by just switching the magnetic analyzer from transmitting $^{11}B^{3+}$ to transmitting $^{11}B^{4+}$ ions into the interaction region without changing the collimator settings. The product-ion analyzing magnet was set to direct the B^{5+} ions to the detector. In the data analysis, the change of the ion velocity υ_{ion} was considered. The resulting cross section is compared in Fig. 1 with the results of theoretical calculations.

Two photon-energy scans were performed. One of these covered the energy range from about 350 to 1200 eV in steps of 50 eV; the second scrutinized the threshold region between 338.5 and 341.5 eV in steps of 0.2 eV. The resulting absolute cross sections for single photoionization of B^{4+} are shown as open circles with yellow shading in Fig. 1 together with their statistical and total uncertainties. The threshold energy of 340.226 022 5(6) eV [41] is clearly mapped out by the experiment (see the inset of Fig. 1).

Calculations of cross sections for the photoionization of hydrogen and hydrogenlike ions date back as far as the era of the development of quantum mechanics. Stobbe [47] was first to apply quantum theory to that fundamental problem. More elaborate calculations were performed much later by Verner *et al.* [48,49]. Then Ichihara and Eichler [46] presented results of an exact relativistic description. All these calculations are in perfect agreement with one another, underpinning the present understanding that photoionization of hydrogenlike atoms and ions as well as its time-reversed process, radiative recombination, are theoretically well understood.

Within the experimental uncertainties, the present experimental cross sections for the photoionization of hydrogenlike B^{4+} ions in their ground level agree with the theoretical benchmark cross sections. The comparison shown in Fig. 1 can be taken as a confirmation of the validity of the experimental procedures employed in the present study.

III. THEORY

The convergent close-coupling (CCC) approach to calculating single and double photoionization of helium and heliumlike ions was developed by Kheifets and Bray [6,50]. A broader review is available [51], as are some recent developments focusing on the near-threshold behavior [52]. The CCC approach was employed in the present investigation. Briefly, upon photoabsorption, the final photoelectron-ion interaction is calculated by expanding the ionic wave functions in an orthogonal Laguerre basis. For each orbital angular momentum $\ell \leqslant \ell_{\max}$, this basis has the following two parameters: (1) basis size N_ℓ and (2) exponential fall-off parameter λ_ℓ. We rely on the completeness of the basis to ensure that convergence, to a desired precision, is obtained by simply increasing the basis size. In order to reduce the number of free parameters, we typically set $N_\ell = N_0 - \ell$ and $\lambda_\ell = \lambda$, thereby reducing convergence testing to just the three parameters $\ell_{\max}$, λ, and N_0. The photoelectron-ion wave function is then obtained via the CCC method, which solves the resulting close-coupling equations in momentum space. The photoionization amplitude is then formed by evaluating the dipole operator between the target ground state and the CCC-calculated wave function. This is evaluated in the three gauges of length, velocity, and acceleration. When both the initial target state wave function and the CCC-calculated final wave function are sufficiently accurate, then the three forms yield indistinguishable, converged results.

In the present case of $\gamma - B^{3+}$ interaction, the hydrogenlike B^{4+} wave functions are obtained by setting $\ell_{\max} = 4$, $\lambda = 3$, and $N_0 = 35$. Only open states are retained as the contribution of closed states was found to be insignificant. This means the size of the calculations rapidly increases with photon energy. Nevertheless, with modern computational resources the calculations take no more than just a few minutes per photon energy.

The initial-state description for the $B^{3+}(1s^2\,^1S)$ ground state was provided by a 20-parameter Hylleraas-type wave function [53]. Such a description ensures the complete gauge convergence of the CCC results with the length, velocity, and acceleration gauges being practically indistinguishable. For metastable $B^{3+}(1s2s\ ^1S)$ and $B^{3+}(1s2s\ ^3S)$ states, Hylleraas-type wave functions can only be used in the asymptotic region of infinitely large photon energies [54]. As a substitute, we employ a multiconfiguration Hartree-Fock (MCHF) expansion [55] generated using the GRASP software package [56]. The $1s2s\ ^1S$ wave function is spanned by 14 two-electron configurations, while the $1s2s\ ^3S$ state comprises 10 configurations. The smaller number of configurations for the triplet state results from Pauli exclusion of the diagonal terms. The convergence of the MCHF expansion is controlled by the condition that the total energy of the target ion reaches an accuracy better than 0.01%.

The use of the MCHF representation of the initial state limits the gauge convergence of the CCC results. The PDI results in the length gauge suffer the most because this gauge is particularly sensitive to large distances. The wave function at large distances is not represented sufficiently accurately by the MCHF expansion. Out of the remaining two gauges, it is the velocity gauge that retains its accuracy from the threshold to the asymptotic limit of large photon energies. This is confirmed by comparing the asymptotic CCC double-to-single cross-section ratios with the Hylleraas results of Forrey *et al.* [54].

With the use of the MCHF representation of the initial state, the CCC results become noisy with the individual data points being scattered more than with the Hylleraas ground-state description. This deficiency can be countered by describing the whole set of PDI cross sections, calculated at multiple photon energies, with a single shape function as introduced by Pattard [57]. This shape function fits the CCC data with an accuracy better than 5% for the metastable singlet state and better than 10% for the triplet state. In addition, there is a systematic difference between the velocity and acceleration gauges for the triplet state which requires an upscaling of the acceleration gauge by 20% to match the velocity gauge results. We estimate the uncertainty of the cross section $\sigma_{35}^{\mathrm{ms}}$ of the metastable $B^{3+}(1s2s\ ^3S)$ ion in the velocity gauge to be definitely smaller than 20%.

IV. RESULTS AND DISCUSSION

Figure 2 shows theoretical PDI cross sections (in the velocity gauge) for B^{3+} in the initial levels $1s^2\ ^1S$, $1s2s\ ^1S$, and $1s2s\ ^3S$. The present CCC calculations addressed all of these levels, while a previous intermediate-energy R-matrix calculation [12] was restricted to the $B^{3+}(1s^2\ ^1S)$ ground level.

The two theoretical approaches for the ground state are in good accord with one another. The threshold energies for the two metastable excited levels are considerably lower than the onset of double ionization of ground-state B^{3+}. Previous theoretical work [41,42] provided the thresholds 396.795 30 eV and 401.032 20 eV for the $1s2s\ ^1S$ and $1s2s\ ^3S$ levels, respectively. This is in fairly good agreement with the CCC calculations as evidenced by Fig. 2. Obviously, the lower thresholds favor higher PDI cross sections and the $1s2s\ ^1S$ level supports a cross-section maximum of more than 1.1 kb, approximately a factor of 5.5 above the cross-section maximum for the $1s^2\ ^1S$ ground level.

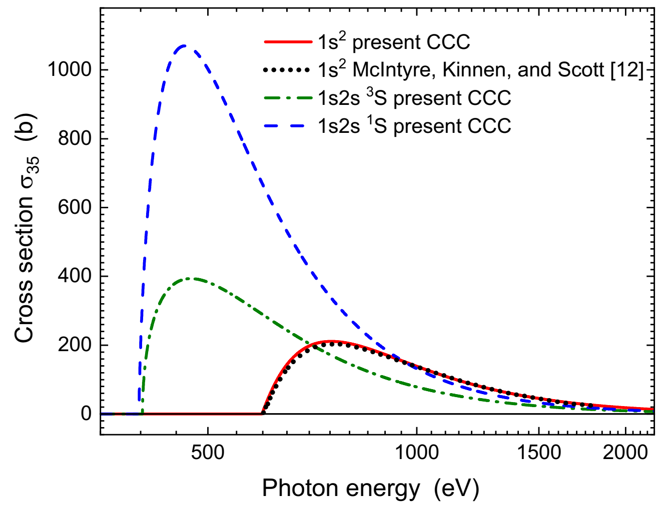

FIG. 2. Theoretical cross sections σ_{35} for PDI of B^{3+} in different initial states. The blue dashed line represents the present CCC calculation for the $1s2s\ ^1S$ initial level, the green dashed-dotted line is the result of the present CCC calculation for the $1s2s\ ^3S$ initial level, and the red solid line shows the CCC result for $1s^2\ ^1S$ ground-state ions. The dotted black line resulted from an intermediate-energy R-matrix method [12] applied to the ground state.

The apparent experimental and the associated theoretical model cross sections $\sigma_{35}^{\mathrm{app}}$ for PDI [see Eq. (5) with $q' = 5$] of a mixture of B^{3+} ions in the $1s^2\ ^1S_0$ ground level and in the $1s2s\ ^3S_1$ metastable excited level are displayed in Fig. 3. The experimental data derived from photon-energy scans are represented by the circles with light-blue shading. The large blue circle was obtained by the separate measurement of the cross-section ratio $r = \sigma_{35}^{\mathrm{app}}/\sigma_{34}^{\mathrm{app}}$ and subsequent multiplication with the apparent cross section $\sigma_{34}^{\mathrm{app}}$ for single ionization of B^{3+} known from theory. Each experimental cross section is shown with both the statistical and the total error bars as described in Sec. II. Due to their limited statistical quality, the experimental data points show much scatter and large relative uncertainties, particularly at energies below ≈600 eV and above ≈900 eV. At the lower energies, the apparent cross sections and, hence, the numbers of signal counts are very small and at the higher energies the photon flux in the experiment rapidly dropped from its maximum (reached at about 550 eV) so that the signal count rates were also dropping.

The theoretical model cross section $\sigma_{35}^{\mathrm{app}}$ is represented by the red solid line in Fig. 3. According to Eq. (5) and considering the known fraction f of metastable ions in the experimental ion beam, the model cross section is $0.091\sigma_{35}^{\mathrm{ms}} + 0.909\sigma_{35}^{\mathrm{gs}}$. For $\sigma_{35}^{\mathrm{ms}}$ the CCC results behind the green dash-dotted line in Fig. 2 are employed and for $\sigma_{35}^{\mathrm{gs}}$ the CCC cross section for ground-state PDI represented by the red solid line in Fig. 2 is used. The green dotted line in Fig. 3 shows the contribution of the metastable $B^{3+}(1s2s\ ^3S)$ ion component to the model cross section. It is relatively small in the energy range above 600 eV because $\sigma_{35}^{\mathrm{ms}}$ is rapidly dropping off beyond the maximum and the weight of 0.091 reduces its relative importance in the apparent cross section.

As discussed in Sec. III, the calculated cross section $\sigma_{35}^{\mathrm{ms}}$ has an estimated relative uncertainty of considerably less

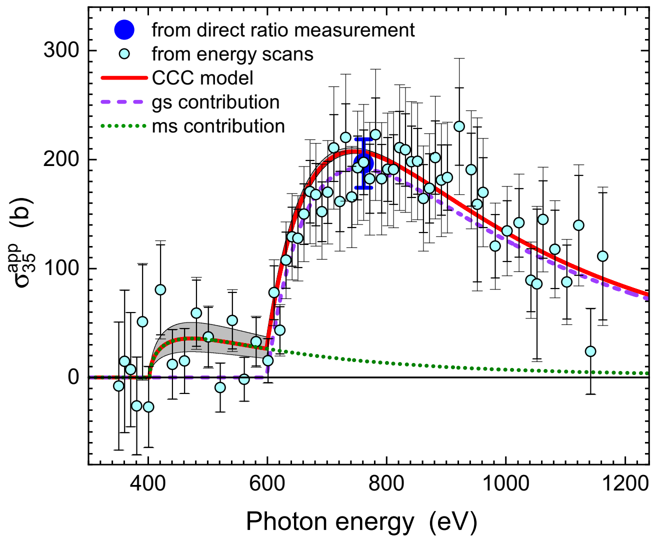

FIG. 3. Experimental and theoretical cross sections σ_{35}^{app} for PDI of a mixture of ground-level $B^{3+}(1s^2\ ^1S)$ and metastable $B^{3+}(1s2s\ ^3S)$ ions. Due to the statistical uncertainties of the observed numbers of detector counts, negative values of cross sections may result when the background is subtracted. The light-blue shaded circles were derived from energy-scan measurements. The solid blue circle was inferred from a direct measurement of the ratio $\sigma_{35}^{app}/\sigma_{34}^{app}$. The red solid line is the apparent cross section σ_{35}^{app} modeled according to Eq. (5) on the basis of the present CCC results. The light-gray shaded area around the red curve shows the maximum effect of an assumed 20% uncertainty of σ_{35}^{ms} and the 18% uncertainty of the fraction f of metastable ions in the parent-ion beam. The violet dashed line represents the contribution of ground-state PDI to the calculated apparent cross section. The green dotted line represents the contribution of metastable-state PDI to the calculated apparent cross section.

than ±20%. In addition, the fraction f of metastable ions in the experimental parent-ion beam is not exactly known: $f = 0.091 \pm 0.016$ [40]. It is elucidating to investigate the effect of the existing uncertainties on the model cross section σ_{35}^{app}. For this purpose the minimum and maximum contributions of σ_{35}^{ms} to the apparent cross section σ_{35}^{app} were considered assuming a maximum deviation of ±20% for σ_{35}^{ms}. Clearly, when $f = 0.091 - 0.016 = 0.075$ is assumed to be at its possible minimum, the fraction $1 - f = 1 - 0.091 + 0.016 = 0.925$ reaches its maximum so that the effects on σ_{35}^{app} partly cancel each other. The shaded area around the model cross section characterizes the maximum uncertainty caused by the possible 20% error of the calculated PDI cross section for the $B^{3+}(1s2s\ ^3S)$ ion component combined with the uncertainty that is due to the error margin of f.

In the investigated energy range below the threshold of ground-state PDI, i.e., below 599.6 eV, the uncertainty of the model cross section is quite large. The comparison with the experimental data is not conclusive since the uncertainty of the measured contribution of σ_{35}^{ms} to σ_{35}^{app} is excessively large in that energy region.

The situation drastically changes as one goes up in photon energy. The contribution of σ_{35}^{ms} to σ_{35}^{app} rapidly shrinks to insignificance. Thus it is almost correct to say that the experimental apparent cross section σ_{35}^{app} essentially tests the theoretical PDI cross section σ_{35}^{gs} for ground-level B^{3+} ions. Above the PDI threshold of ground-level B^{3+} the contribution of PDI of $B^{3+}(1s2s\ ^3S)$ does not play a significant role anymore, i.e., its influence on the measured cross section σ_{35}^{app} can be considered to be negligible.

Given the uncertainties of the experimental data, there is remarkably good agreement of the measured and the theoretical cross sections. There is no hint towards a discrepancy that might explain the unexpected, large cross section found previously for double-*K*-shell ionization in the C^- anion [27].

V. SUMMARY AND CONCLUSIONS

We present theoretical and experimentally derived cross sections for single-photon double ionization of heliumlike B^{3+} ions. There is no ambiguity in the interpretation that the measured cross sections describe the direct process of photo double ionization (PDI)—simply because there is no other pathway by which both electrons could be removed by a single photon. The fact that a mixture of $B^{3+}(1s^2\ ^1S)$ and $B^{3+}(1s2s\ ^3S)$ was present in the experimental parent-ion beam is insignificant for the test of the PDI cross section for ground-level B^{3+} ions. The comparison shows agreement between theory and experiment. Moreover, the present convergent close-coupling calculations on PDI of heliumlike boron agree with previous calculations employing an intermediate-energy *R*-matrix approach [10,12]. At least at the level of the relatively large uncertainties of the present experiment, PDI of heliumlike positive ions appears to be well understood theoretically.

The PDI experiment we performed was difficult due to the small cross sections involved, all below approximately 200 b. Accordingly, uncertainties of the order of ±30% remained for the experimental cross sections. This is not a principle limit of accuracy. We anticipate to have available much higher ion currents from a more state-of-the-art electron cyclotron resonance ion source that is presently being prepared for experiments with multiply charged ions. Much higher ion currents are expected compared to the present work. This will greatly facilitate the experiment by improving the quality of beam diagnostics and counting statistics. Moreover, an extension towards higher ion charge states will be feasible.

It is also possible to improve the determination of cross-section ratios by investing more time into switching back and forth between the detection of single- and double-ionization products from which not only the requirement of measurements with a constant form factor but also the statistical quality of the results will profit.

While the present investigation shows that PDI of heliumlike ions within the constraints of the present experiment is well understood by theory, our present results do not provide any hint towards an explanation of the previously observed, overly large cross section for double-*K*-shell ionization in the C^- anion [27]. A logical next step in the pursuit of this unresolved issue is to move on towards systems that have more than two electrons. The natural choice for further investigations is the photoionization of the lithiumlike B^{2+} ion. Different from heliumlike B^{3+}, three-electron B^{2+} can be produced with practically 100% of all ions in the parent-ion beam residing in the $1s^2 2s\,^2S_{1/2}$ ground level.

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