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2012 J. Phys.: Conf. Ser. 388 012036

(http://iopscience.iop.org/1742-6596/388/1/012036)

XXVII International Conference on Photonic, Electronic and Atomic Collisions (ICPEAC 2011) IOP Publishing
Journal of Physics: Conference Series **388** (2012) 012036 doi:10.1088/1742-6596/388/1/012036

Multiple ionization of atoms including post-collisional contributions

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Abstract. We present a theoretical study on multiple ionization on Ne and Kr by charged ions in the energy range (0.1-10) Mev/amu. We employed the continuum distorted-wave eikonal initial state and a Hartree-Fock description of the dressed-ion, together with photoionization branching ratios to include Auger-type post-collisional contributions. Results are good, especially for Kr targets. Some questions, such as limitations of the independent particle model or influence of the ion charge-state versus the ion nuclear-charge, are analyzed based on the different results for Ne and Kr targets. We found that single ionization is related to the ion charge-state while multiple-ionization shows that the nuclear-charge is weekly screened by the ion outer-electrons.

1. Introduction

Multiple electron processes in ion-atom collisions is one of the most interesting and challenging subjects to study. It demands elaborated theoretical methods, highly advanced experimental techniques to get absolute measurements of all possible channels and final states, and a detailed knowledge of the post-collisional processes which determine the ultimate charge measured by the experiments. Several reviews and books have been devoted to this subject, which compile the experimental and theoretical state of the art (for example [1]-[3] and references therein).

Coincident measurements of multiple-ionization cross sections separating direct ionization from capture channels play a mayor role in the study of these processes. Pioneering on this research is the experimental work on multiple ionization of rare-gases by DuBois, Mason and co-workers in the '80s [4]-[9]. But it was in the last decade that the combination of advanced experimental techniques and the inclusion of experimental rates of post-collisional electron emission within the theoretical models managed to describe the experimental cross sections of multiple ionization in the high energy regime [10]-[12], giving new impulse to the experimental and theoretical research on this subject [13]-[23].

There are different mechanisms of post-collisional ionization (PCI), i.e. Auger and Coster-Krönig processes, electron shake-off, excitation followed by double Auger, which were extensively studied in photoionization by Carlson, Krause and co-workers [24]-[29]. The advent of new experimental techniques in photoionization experimental research in the last two decades has contributed to a detailed knowledge of the Auger-type processes, the intermediate steps and cascades [30]-[44]. These experimental works provide accurate branching ratios of final charge states of the target atoms after single photoionization.

The Auger-type processes are time-delayed electron emissions, which depend on the target initial vacancy and not on the projectile. This means that the branching ratios of charge state distribution after single photoionization experiments may be introduced in ion-atom multiple-ionization to include PCI [11, 12]. An important condition is that the experiment guarantees the creation of only a single initial vacancy [18].

Multiple electron transitions are basically many-body processes which involve correlation among the electrons and time dependent potentials. In the case of helium, this turned out to be a key point [45]-[51] and some models have been developed to describe it. However, the extension to other targets is out of the present possibilities. For targets heavier than He, the independent particle model (IPM) is the one most employed. It approaches the multiple electron processes from single electron ones in a statistical way. How far the IPM applies to multiple processes, how important the correlation among electrons may be, if the IPM can be equally applied to Ne target with 10 electrons or Kr with 36 or, what is more important: the ion charge-state or the ion nuclear-charge, are some of the questions that move the present work.

In this work we present here new results for single to quintuple ionization cross sections of Ne and Kr bombarded by different ions with charge states +1 and +2, in the intermediate to high energy range. The present contribution combines the calculation of the ionization probabilities using the continuum distorted-wave eikonal initial state (CDW-EIS), with the Hartree-Fock description of the dressed-ion potential, and with recent photoionization branching ratios.

2. Theoretical model

The CDW-EIS, initially proposed by Crothers and McCann [52] and extended by Fainstein *et al* [53], is one of the most reliable approximations within the IPM to deal with calculations of ionization probabilities in the intermediate to high energy regime [54].

In this work we follow previous contributions where impact parameter probabilities for single ionization were calculated. Our previous calculations [18],[54]-[56] were improved in two senses. First, the amplitude of transition as a function of the impact parameter was calculated using the well known eikonal approximation; in this case the maximum number of magnetic quantum numbers m was extended considerably to avoid aliasing. Second, when dealing with dressed projectiles, the ion potential was calculated using the Hartree-Fock wave functions for positive ions given by Clementi and Roetti [57]. The matrix element of the residual potential was taken into account (see Eq.(15) of Ref [56] in the CDW-EIS approximation.

Within the IPM, direct multiple ionization can be related to the single ionization probability as a function of the impact parameter, via the multinomial distribution [18]. We introduce the branching ratios for postcollisional ionization (PCI) in a simple way by considering that

$$1 = \sum_{k=0}^{k_{max}} F_{nl,k}, \tag{1}$$

where $F_{nl,k}$ is the branching ratio of single-ionization of a certain nl-subshell followed by PCI of k electrons of the outer-shells (Auger cascades), ending with an ion charge state $k+1$ [18]. This is included as a factor multiplying the ionization probability within the multinomial equation. The addition of probabilities is rearranged in order to put together those terms that contribute to the same number of final emitted electrons [18]. The branching ratios employed in the present calculations are those of Table 1 in Ref. [18].

3. Results and discussions

We present new results for multiple ionization cross sections of Ne and Kr targets and different impinging ions with charge +1 (H^+, He^+) and 2+ (He^{2+}, B^{2+}). In general we have calculated up to quintuple ionization, both with CDW-EIS and with first Born approximation, for direct multiple-ionization and for multiple-ionization including PCI.

3.1. Krypton

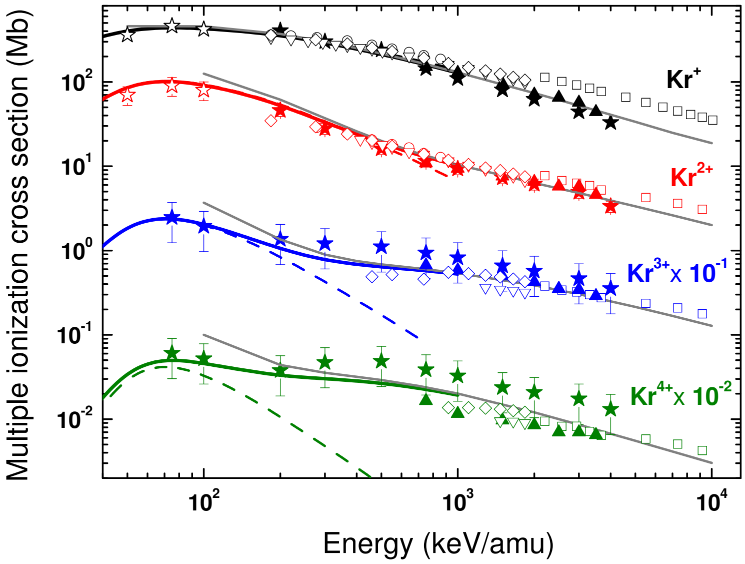

Figure 1. [color online] Single to quadruple ionization cross sections of Krypton by H^+ impact. Curves, Thick-lines, CDW-EIS results with (——) and without (- - - -) PCI; thin-grey-lines, Born results including PCI. Experimental data: proton-impact, full-triangles Cavalcanti *et al* [13], full-stars DuBois *et al* [5], hollow-stars DuBois [4]; electron-impact, ○ Syage [58], □ Schram *et al* [59], ▽ Rejoub *et al* [60], ◇ Krishnakumar *et al* [61].

Note that in Fig. 1 we display theoretical and experimental results for proton impact on Kr including data for electron impact at high energies.

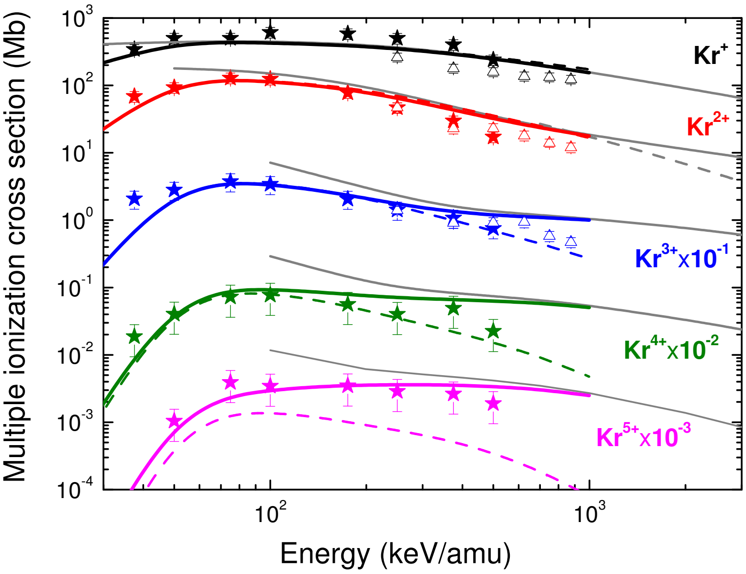

Figure 2. [color online] Single, double, triple, quadruple, and quintuple ionization cross sections of Krypton by He^+ impact. Curves, as in figure 1. Experimental data: △Santos *et al* [10], full-stars DuBois [7].

In Figs. 1, 2 and 3 we display the results for multiple ionization of Kr by H^+, He^+ and He^{2+}. In the three figures the comparison with the experimental data shows a good agreement, with the results of He^+ impinging on Kr being actually very good. A point to note is the clear separation between the results including PCI and those of only direct ionization. This separation begins at lower energy as the order of ionization increases from single to quintuple.

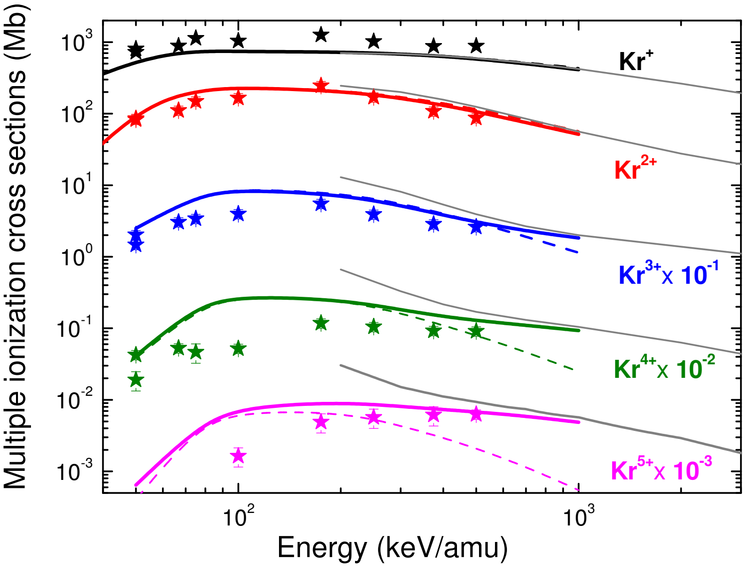

Figure 3. [color online] Single, double, triple, quadruple, and quintuple ionization cross sections of Krypton by He^{2+} impact. Curves, as in figure 1. Experimental data: full-stars, Dubois [6].

The comparison of these three systems also shows that the minimum energy for which PCI contribution begins to be important grows from H^+ to He^+ and to He^{2+}. PCI does not depend on the ion but the direct ionization does, so the relation between them changes. This fact was theoretically predicted by Tachino *et al* [22] for molecular targets, and it is now corroborated by the comparison of theoretical calculations and experimental data for different ions.

In Fig. 3 we can note that the agreement for He^{2+} impact is not so good as for H^+ and He^+. However it describes correctly the tendency of the experimental data by DuBois, even for quintuple ionization. It must be mentioned that this is the first theoretical calculation for multiple ionization of Kr by He^{2+}.

3.2. Neon

In Figs. 4, 5 and 6 we display the results for multiple ionization of Ne by H, He^+ and He^{2+}. For this target previous IPM results by Galassi *et al* [20] and by Kirchner *et al* [12, 62, 63] are included. The former use the CDW-EIS approximation with an effective potential for H^+ in Ne. The latter are performed for H^+, He^+, and He^{2+} in Ne, by solving numerically the time-dependent Schrodinger equation using de basis generator method. Kirchner *et al* [12, 62, 63] results include ionization and capture, which is important at low to intermediate energies (around or less than 100 keV/amu for proton impact, but up to 200 keV/amu for He^{2+} impact). Capture importance relative to pure ionization increases with the ionization degree (see the experimental data for capture by DuBois [4, 6]). In Fig. 6 we include the curves of Ref. [63] for He^{2+} in Ne only in the region where pure ionization dominates.

The CDW-EIS results are valid for high energies and tend to underestimate the cross sections in the intermediate energy region, which is the expected behavior of the model. In general, Figs. 4, 5 and 6 show a good description of the experimental data.

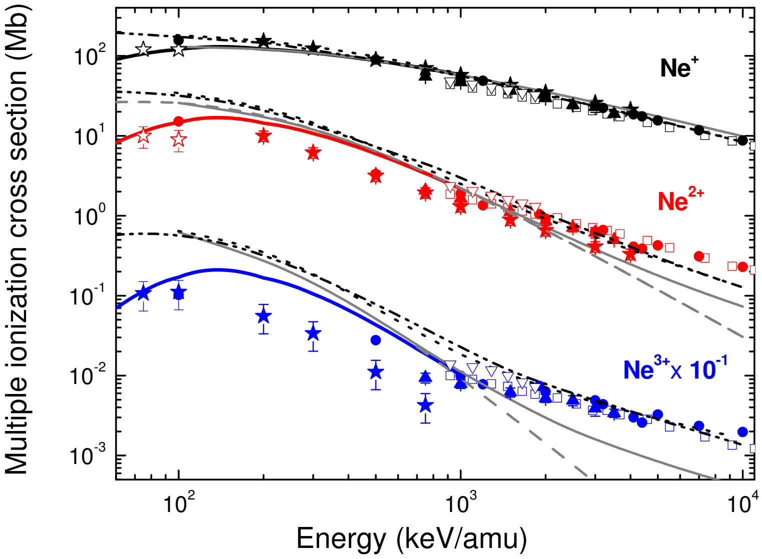

Figure 4. [color online] Single, double and triple ionization cross sections of Neon by H$^+$ impact. Curves: Thick-lines, CDW-EIS results with PCI; thin-grey-lines, Born results with (——) and without (- - - -) PCI; — · · —Spranger *et al* [12]; · · · · · ·Galassi *et al* [20]. Experimental data: for proton-impact, full-triangle Cavalcanti *et al* [11]; full-stars DuBois *et al* [5]; hollow-stars DuBois [4]; ● Andersen *et al* [64] normalized to theoretical total cross sections; for electron-impact, □ Schram *et al* [59], ▽ Rejoub *et al* [60].

The results in Fig. 4 for protons on Ne underestimate the data for double and triple in the high energy region, where PCI is important. In our calculation only PCI following initial K-shell vacancy is included. The curves by Spranger and Kirchner [12] and by Galassi *et al* [20] include Carlson *et al* [25] branching ratios for photoionization of the L-shell, which includes double-photoionization [18].

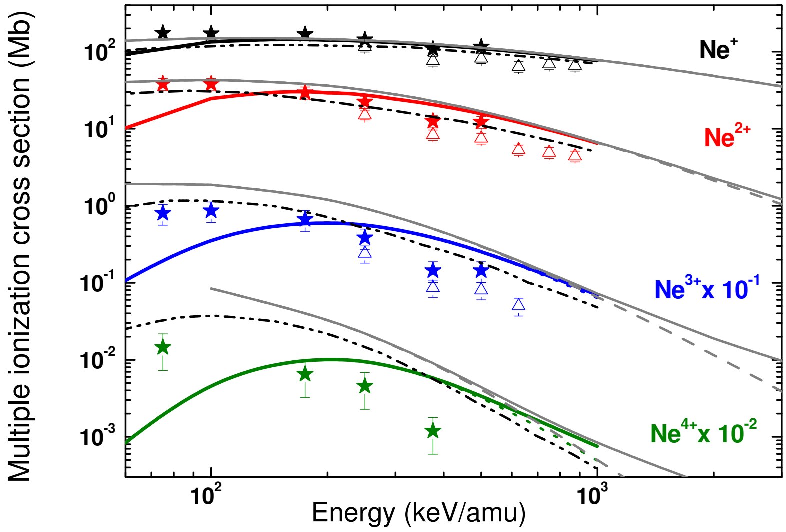

Figure 5. [color online] Single, double, triple and quadruple ionization cross sections of Neon by He$^+$ impact. Curves, Thick-lines, CDW-EIS results with PCI; thin-grey-lines, Born results with (——) and without (- - - -) PCI; — · · —Kirchner *et al* [62]. Experimental data: △, Santos *et al* [10]; full-star, DuBois [7].

We found a tendency of the CDW-EIS to overestimate the multiple ionization of Ne in a region around 300-500 keV/amu as observed in these figures. This energy region is dominated by the direct multiple ionization, where PCI contributions are negligible. As can be noted in the figures, this is a general behavior of the different IPMs. The good description obtained for Kr

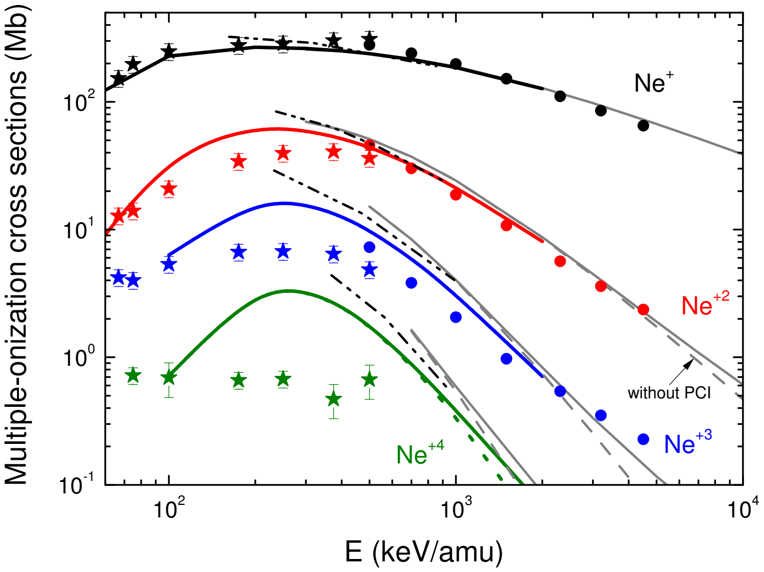

Figure 6. Single, double, triple, quadruple, and quintuple ionization cross sections of Ne by He^{2+} impact. Curves, Thick-lines, CDW-EIS results with PCI; thin-grey-lines, Born results with (——) and without (- - - -) PCI; — · · —Kirchner *et al* [63]. Experimental data: full-stars, Dubois [6]; ● Andersen *et al* [64] normalized to theoretical total cross sections.

contrasts with these theoretical results for Ne and open new questions about possible different statistics to deal with Ne and Kr atoms, about the relative importance of electron correlation in each target, or about the differences in the atomic potential when 4 electrons are emitted from a Ne target or from a Kr target. These are interesting questions that deserve future research.

The comparison of Figs. 1, 2 and 3 for Kr and Figs 4, 5 and 6 for Ne shows another interesting feature. For single ionization the charge state of the ion dominates. We note similar theoretical and experimental results for single ionization by H^+ or He^+ impact. On the other hand, for higher ionization degrees the ion-nuclear charge is important, i.e. the He^+ results are between the H^+ and He^{2+} results for double and triple ionization; and for quadruple ionization He^+ cross sections are close to He^{2+} values.

To study this point, in Fig. 7 we display the comparison of multiple ionization of Ne by bare He^{2+} ions and B^{2+} ($1s^2$,$2s^1$) ions.

Again we obtain similar results for single ionization by He^{2+} and B^{2+} ions and an increasing separation for higher orders of ionization, as observed in Fig. 7. In fact, we found that for triple ionization of Ne, B^{2+} theoretical values are very similar to those of Li^{3+} ions. These are interesting results to study experimentally.

This behavior is to be expected if we consider direct multiple ionization as the product of impact parameter probabilities. Very close collisions are important, and the ion outer-electrons weekly screened the nucleus. The ion-nuclear charge will be increasingly important for higher degrees of multiple ionization.

To show this we define the effective charge of the B^{2+} ion for the different Ne^{+q} final charge-states as

$$Z_{eff}(q) = 2\left(\frac{\sigma(B^{2+})}{\sigma(He^{2+})}\right)^{1/2q}, \tag{2}$$

and plotted it in Fig. 8. As observed, both theoretical an experimental results follow the tendency of increasing effective charge with increasing ionization of the Ne target.

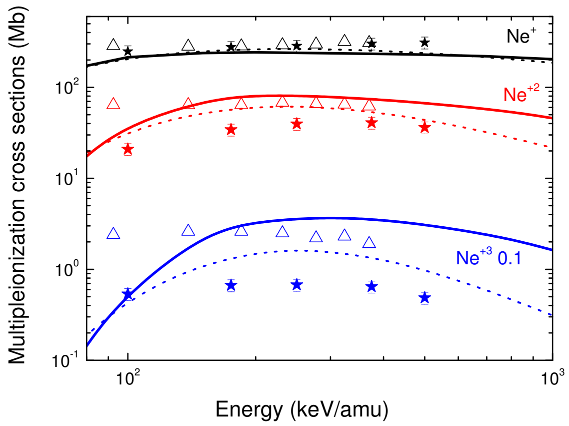

Figure 7. Single, double and triple and ionization cross sections of Neon by ——B^{2+} and ······He^{2+} ions, calculated with CDW-EIS including PCI. Experimental data: △Wolf *et al* [65] for B$^{(}$2+), full-stars, Dubois [6] for He^{2+}.

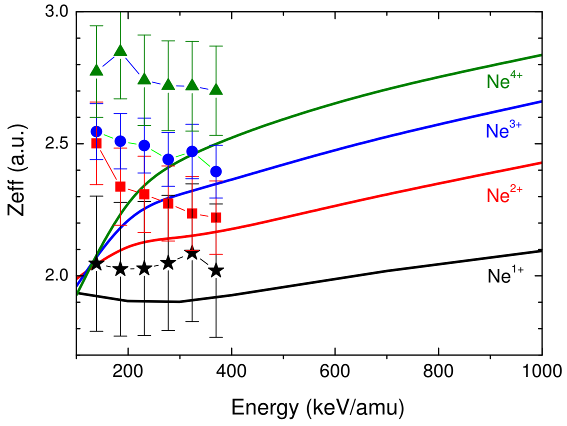

Figure 8. Effective ion charge for B^{2+} in Ne for different final charge-states of Ne^{+q}. ——present CDW-EIS results. Symbols, values obtained from the experimental data by Wolf *et al* [65] for B^{2+}, and by DuBois [6] for He^{2+}.

4. Conclusions

In this contribution we study multiple ionization by charged ions, considering the Ne and Kr cases. We combine the CDW-EIS results with branching ratios of final charge state in photoionization experiments. Results are good, especially for Kr targets. For Ne we found an overestimation in the region where direct ionization dominates. We showed that this behavior is common to different approaches within the IPM. In this sense Ne serves as a benchmark target for future multiple-ionization research to clear up questions such as the validity of multinomial statistics or the importance of correlation among electrons, questions that probed to have different answers for Kr and Ne. We also studied the influence of the ion charge-state and the ion nuclear-charge in multiple ionization probabilities, and noted that multiple-ionization is sensitive to the weekly screening of the ion by outer electrons.

Acknowledgments

This work was partially supported by the Argentinean CONICET, the Agencia Nacional de Promoción Científica y Tecnológica and the Universidad de Buenos Aires, and by the Brazilian Agencies CNPq and FAPERJ.

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