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Direct inner-shell ionization of atomic ions by electron impact

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Abstract

We study the higher-subshells effect on the direct ionization from inner 1s, 2s, 2p, 3s, 3p subshells of ions charged 5+ and more. The cross-sections analysed are those calculated in the relativistic distorted-wave (RDW) approach. For removal of an electron from a certain nl-subshell of ions, belonging to a sequence of ionization stages, we found approximate scaling of the cross-sections. The scaled cross-sections differ from each other by less than 50%. The difference depends on the number of electrons, N, bound above the nl-subshell undergoing the ionization. With an increase in N the scaled cross-sections decrease for projectiles of near-threshold energy and increase for high-energy (non-relativistic) projectiles. Dependence of the scaled cross-sections on a target ion (its chemical element, charge and level) is weak. For use in applications, we approximated the direct inner-shell ionization cross-sections by a simple formula with nl-dependent coefficients.

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1. Introduction

We study cross-sections of *direct* electron-impact ionization from *definite* nl-subshells of multiply charged atomic ions. This subshell may be 1s, 2s, 2p, 3s, or 3p. Let N be the number of electrons in higher (than nl) subshells of the target ions. In the present paper our main attention is on the dependence on N. For example, how do the cross-sections change along a sequence of ionization stages, in which N changes from zero up to a large number? To the best of our knowledge, the dependence on N has never been studied before.

The initial state of the target ion is assumed to be known. The electron configuration of the product ion is defined by that of the target ion and nl of the electron removed

$$A^{m+}(\alpha nl^k\gamma\ SLJ) + \mathrm{e} \rightarrow 2\mathrm{e} + A^{(m+1)+}(\alpha nl^{k-1}\gamma). \qquad (1)$$

Here $A^{m+}(\alpha nl^k\gamma SLJ)$ denotes the m-fold ionized atom of chemical element A on atomic level $\alpha nl^k\gamma^{2S+1}L_J$; k is the number of electrons in the nl-subshell undergoing the direct ionization, α denotes a group of subshells below nl, and γ denotes a group of subshells above nl. Electron configuration $\alpha nl^{k-1}\gamma$ may have a few levels $S'L'J'$. The cross-section for transition in a certain level is denoted below as $\sigma_{S'L'J'}(\varepsilon)$. Here, ε is the incident electron energy relative to the initial state. A quantity of interest for the present study is the sum over levels of the final configuration, i.e., the *total* (level-to-configuration) cross-section

$$\sigma(\varepsilon) = \sum_{S',L',J'} \sigma_{S'L'J'}(\varepsilon), \qquad (2)$$

which corresponds to scheme (1). This cross-section describes direct creation of a vacancy in the nl-subshell of $A^{m+}(\alpha nl^k\gamma SLJ)$ ions in the case where any level of the $A^{(m+1)+}$ ion is acceptable.

In the present paper, subshells belonging to α are assumed to be *closed* ones, while each subshell belonging to γ may be closed, partially filled, or empty. The $\gamma = 0$ case corresponds to ionization from the outermost subshell. In the case of inner-shell ionization, the removal of an electron from nl^k may occur simultaneously with changes in the angular momenta of γ. To illustrate this possibility and the dependence on $S'L'J'$, we show in figure 1 all nonzero $\sigma_{S'L'J'}(\varepsilon)$ that correspond to removal of a 2s electron from $1s^22s^22p^4\ {}^3P_1$ level of an Ar^{10+} ion,

$$\mathrm{Ar}^{10+}(1s^22s^22p^4\ {}^3P_1) + \mathrm{e} \rightarrow 2\mathrm{e} + \mathrm{Ar}^{11+}(1s^22s2p^4\ S'L'J'). \qquad (3)$$

Six level-to-level cross-sections correspond to six levels of $1s^22s2p^4$ configuration of the product ion. These levels are ${}^4P_{3/2}$, ${}^4P_{1/2}$, ${}^2D_{3/2}$, ${}^2S_{1/2}$, ${}^2P_{3/2}$, and ${}^2P_{1/2}$. Two more levels possible for $1s^22s2p^4$ configuration, namely ${}^4P_{5/2}$ and

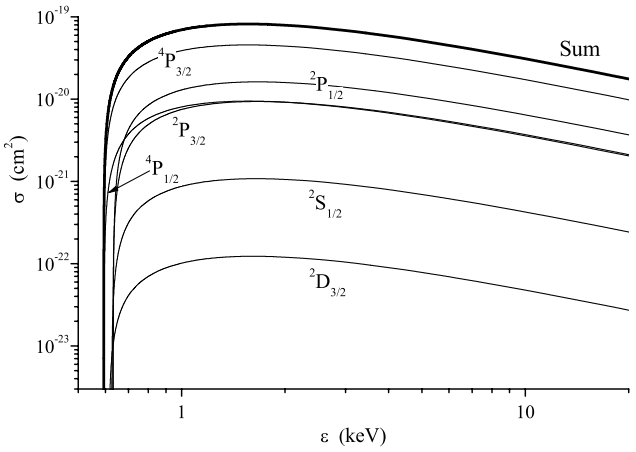

Figure 1. Thin curves show cross-sections corresponding to scheme (3). The labels denote final levels. The thick curve is the sum over the final levels (2).

$^2D_{5/2}$, cannot be obtained by removal of an s-electron from $1s^22s^22p^4\ ^3P_1$ level. Note that levels with $L'=0$ and $L'=2$ (namely, $^2S_{1/2}$ and $^2D_{3/2}$) are reached from the initial P-level by removal of an s-electron ($l=0$); these transitions are possible due to the changes in the orbital momentum of the $2p^4$ subshell. Cross-sections, corresponding to these two final levels, are small relative to the cross-sections of $P \to P$ transitions. All level-to-level cross-sections throughout this paper are calculated using the relativistic distorted-wave (RDW) approach using Flexible Atomic Code [1]. The thick curve in figure 1 shows the sum of all (eight) level-to-level cross-sections, i.e., the total cross-section (2) for direct ionization of a 2s electron from the $Ar^{10+}(1s^22s^22p^4\ ^3P_1)$ level.

Each $\sigma_{S'L'J'}(\varepsilon)$ has a certain threshold energy, $I_{S'L'J'}$. For total cross-section, $\sigma(\varepsilon)$, the threshold energy, I, is *defined* here as the smallest $I_{S'L'J'}$ of all $S'L'J'$ levels, *except for* those with $\sigma_{S'L'J'}(\varepsilon)=0$. This definition secures natural requirements on I, which are $\sigma(\varepsilon \leqslant I)=0$ and $\sigma(\varepsilon > I) > 0$.

It is known (e.g., [2]) that $\sigma(\varepsilon)$ has general features in *common* for ionization from inner and outer subshells. These features are as follows. Firstly, in the vicinity of the ionization threshold $\sigma(\varepsilon)$ increases with ε as $C_1(\varepsilon - I)$; here C_1 is constant. Secondly, $\sigma(\varepsilon)$ has a maximum at $\varepsilon_{\max} \simeq 2.5I$. Thirdly, this maximal value, $\sigma_{\max}$, is proportional to kI^{-2}. Fourthly, the non-relativistic high-energy asymptote is

$$\sigma(\varepsilon \gg I) \sim \frac{C_2}{\varepsilon}\ln(\varepsilon/I) + \frac{C_3}{\varepsilon},$$

with C_2 and C_3 being constants.

Our consideration is restricted to non-relativistic projectiles. Then, *qualitatively*, $\sigma(\varepsilon)$ is described by the above four features. However, this knowledge is insufficient for *quantitative* estimates of the cross-sections because constants $\sigma_{\max}$, C_1, C_2, C_3 are unknown. In the present paper, we give a general quantitative solution of this problem in the framework of the RDW approach.

2. The dependence on N

To demonstrate the higher-subshells effect on direct ionization from the nl-subshell, we show in figure 2(a) five total cross-sections, which correspond to removal of a 2s electron from the ground state of Ag^{43+}, Ag^{37+}, Ag^{29+}, Ag^{19+} and Ag^{11+} ions. Relative to the $2s^2$ subshell, these ions have $N=0$, 6, 14, 24 and 32, respectively. The cross-sections are expressed in πa_0^2 units, where a_0 is the Bohr radius. One can see that the ionization threshold decreases with N, while $\sigma_{\max}$ increases. For quantitative analysis of these changes, we introduce the scaled energy of incident electrons, $x=\varepsilon/I$, and the *scaled* total cross-section

$$f(\varepsilon/I) = \frac{1}{\pi a_0^2 R^2 k}\sum_{S',L',J'} I^2_{S'L'J''}\sigma_{S'L'J'}(\varepsilon/I_{S'L'J'}).$$

Here R is the Rydberg unit of energy (13.606 eV). In figure 2(b), we display five scaled cross-sections, $f(x)$, corresponding to figure 2(a). The five $f(x)$ differ from each other but the difference is relatively small. This means that scaled cross-sections depend on N but the dependence is weak, in this particular example at least. The approximate equality of the scaled cross-sections, found in the sequence of *ionization stages*, resembles the $\sigma(\varepsilon/I) \sim I^{-2}$ scaling known for *isoelectronic* sequences (see, e.g., [2]). However, in each isoelectronic sequence N is constant, while in each sequence of ionization stages N is a variable.

Looking for stronger (than figure 2(b)) dependence on N, we considered four sequences of ionization stages ($m > 4$) for ionization from each of the lowest five nl-subshells. In each of these twenty sequences, scaled cross-sections $f(x)$ differ from each other by less than 20% for energies $1.4 < x < 8$ and by less than 50% for $x < 1.4$ and $8 < x < 100$. There are two more observations common for all sequences studied. Namely, with an increase in N, scaled cross-sections *decrease monotonically* for near-threshold energies ($x \approx 1$) and *increase monotonically* for high energies ($x \gtrsim 6$).

To analyse the scaling on a broader set of ions and states, we performed the calculations as follows. For each of the lowest five nl-subshells (1s to 3p), we calculated scaled cross-sections $f(x)$ for about a hundred transitions of type (1). Parameters A, m, k, and γSLJ are chosen arbitrarily, except for two criteria as follows. Firstly, we considered ions with $m > 4$; this condition ensures sufficient accuracy in the RDW calculations. Secondly, we restricted the calculations to ions with $I < 5$ keV; this condition is required for the non-relativistic asymptote of $\sigma_{S'L'J'}(\varepsilon \gg I_{S'L'J'})$, prescribed in the code [1], to be applicable up to $x = 100$ at least.

Figure 3 shows a bunch of scaled cross-sections that correspond to removal of a 1s electron. We considered the target-ion electron configurations $1s^k$, $1s^22s^w$, $1s^22s^22p^u$, $1s^22s^22p^63s^w$, and $1s^22s^22p^63s^23p^u$ with $k=1$ and 2, $w=1$ and 2, $u=4$ and 6. Ionization stages of the target ions range from $m=5$ to $m=20$. One can see that the bunch is rather tight, i.e., dependence of the scaled cross-sections on A, m, k, γSLJ and N is rather weak.

Calculations performed for 2s, 2p, 3s and 3p subshells also showed a tight bunch of scaled cross-sections for each nl. Two examples are displayed in figures 4 and 5. They relate to ionization from 2p and 3p subshells, respectively. In each

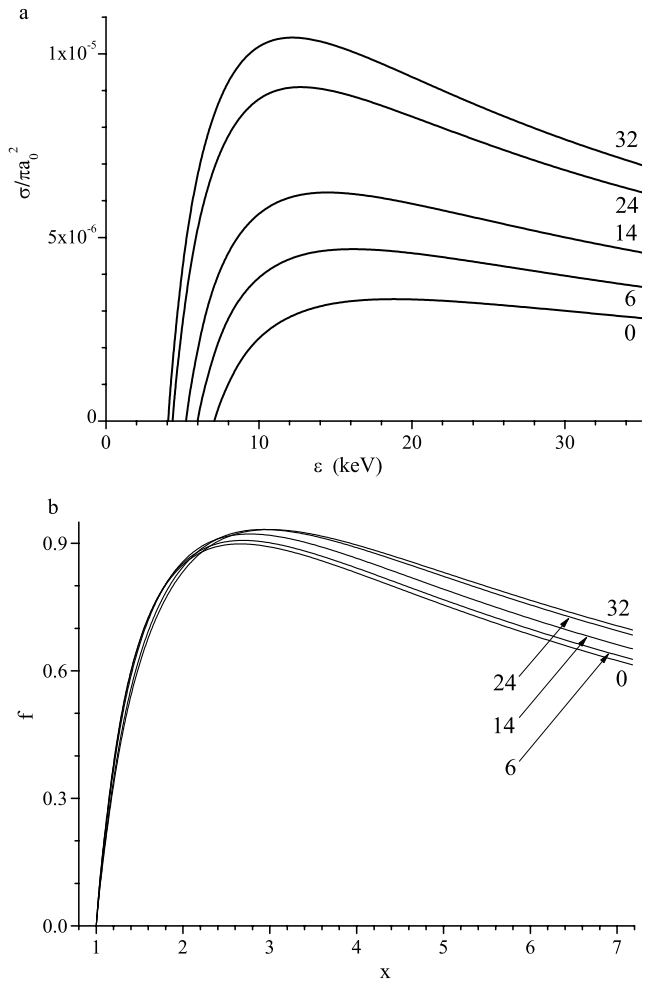

Figure 2. (a) Cross-sections for removal of a 2s electron from the ground states of Ag^{43+}, Ag^{37+}, Ag^{29+}, Ag^{19+} and Ag^{11+}. Numbers near the curves are the values of N. (b) Scaled cross-sections corresponding to panel (a). Numbers near the curves are the values of N.

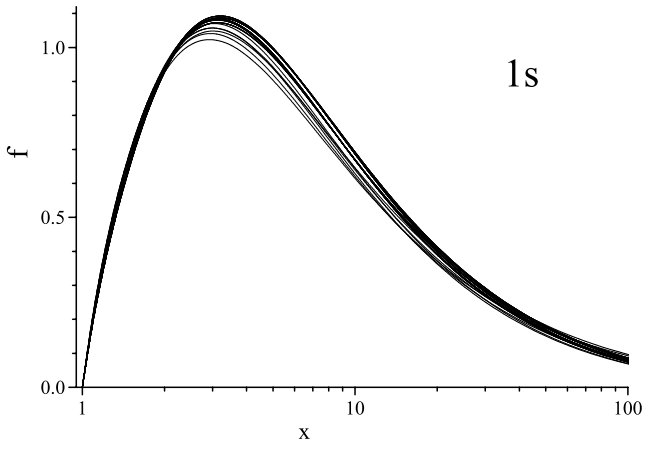

Figure 3. Scaled cross-sections calculated for ionization from the 1s subshell.

bunch there is an equal number of curves corresponding to 0, 1, 2, 3, 4 subshells in γ. All subshells, except for the outermost one, are completely filled. The outermost subshell is filled completely or partially, depending on the initial state selected.

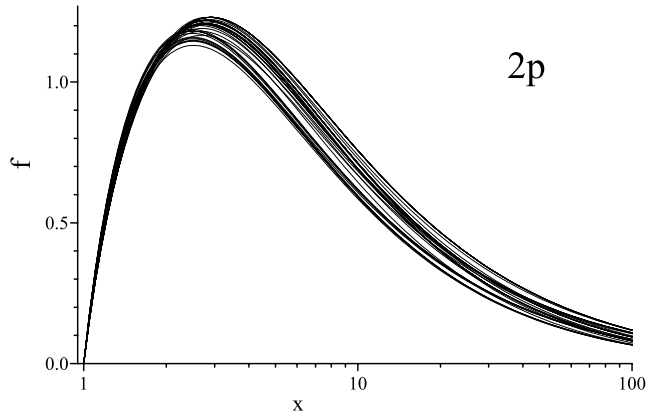

Figure 4. Scaled cross-sections calculated for ionization from the 2p subshell.

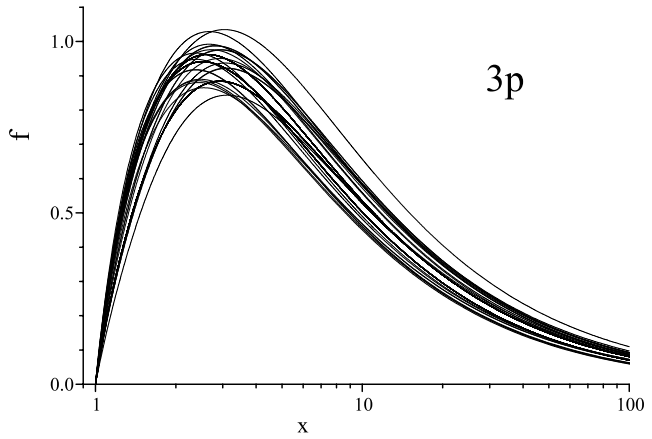

Figure 5. Scaled cross-sections calculated for ionization from the 3p subshell.

Table 1. Coefficients $H_{1,nl}$, $H_{2,nl}$, $H_{3,nl}$ and $H_{4,nl}$ for formula (4).

	H_1	H_2	H_3	H_4
1s	0.45	7.134	−3.771	5.833
2s	0.82	4.583	−1.353	3.113
2p	1.05	5.54	−1.554	4.267
3s	0.70	3.329	0.213	1.465
3p	1.126	3.106	−0.043	1.758

The calculations showed that in each of the five bunches all $f(x)$ curves at $x \leqslant 100$ are within ±40% of some median function $F_{nl}(x)$ of the bunch. We approximated each median function by the expression

$$F_{nl}(x) = H_{1,nl}\frac{\ln(x)}{x} + H_{2,nl}\frac{(x-1)^2}{x^3} + H_{3,nl}\frac{x-1}{x^3} + H_{4,nl}\frac{x-1}{x^4}. \quad (4)$$

proposed in [1]. Here $H_{1,nl}$, $H_{2,nl}$, $H_{3,nl}$ and $H_{4,nl}$ are nl-dependent coefficients found by minimizing

$$\sum \frac{|F_{nl}(x) - f(x)|}{f(x)},$$

within each bunch in the energy range $1 \leqslant x \leqslant 100$. The coefficients obtained are given in table 1.

3. Prediction formula for $\sigma(\varepsilon)$

Many users of inner-shell ionization cross-sections will appreciate a formula which is known to be accurate commonly to better than ±20% and never less than ±40%. For those users, we propose the prediction formula

$$\sigma^{\text{predict}}(\varepsilon) = \pi a_0^2 R^2 k I^{-2} F_{nl}(\varepsilon/I). \qquad (5)$$

The accuracy of this prediction is examined by comparison of cross-sections (5) with quantal calculations. Namely, we calculate the RDW cross-sections (2) for target ions that are *not* used in the determination of coefficients $H_{1,nl}$, $H_{2,nl}$, $H_{3,nl}$, $H_{4,nl}$. For this test the target ions and their initial states are chosen as follows. For removal of an electron from each nl subshell, we selected four chemical elements. The smallest atomic number, $A_{\min}$, corresponds to an element that has nl subshell as the *outermost* one of $A_{\min}^{5+}$. The largest atomic number, $A_{\max}$, corresponds to a chemical element that has $I \approx 5$ keV. Two more elements chosen are those with $A \approx A_{\min} + (A_{\max} - A_{\min})/3$ and $A \approx A_{\min} + 2(A_{\max} - A_{\min})/3$. Atoms of these four elements are ionized from the ionization stages $m = 5, 10, 15, \ldots, m_{\max}$. The largest value, $m_{\max}$, corresponds to an ion that has $N = 0$. If this selection leads to a target ion, A^{m+}, used for determination of $H_{1,nl} - H_{4,nl}$ coefficients, then the next chemical element is examined instead of A. Each of the selected ions is ionized from initial levels numbered 1, 6 and 11 in the NIST file [3]. Commonly levels 1, 6 and 11 differ in their electron configuration. If an A^{m+} ion is missing in the NIST database [3], then this ion is ionized from levels numbered 1, 6 and 11 in the eigenvalues list produced by Flexible Atomic Code [1]. Predicted cross-sections (5) and RDW cross-sections (2) are compared for nine values of the incident electron energy, namely for $\varepsilon_i = x_i I$ with $x_i = 1.3, 1.6, 2.4, 3.5, 5, 8, 15, 40, 100$.

Conclusions on the accuracy of prediction formula (5) may be derived from statistics of relative deviation of predicted cross-sections from calculated $\sigma(\varepsilon_i)$. The relative deviation is defined as

$$D_{nl}(\varepsilon_i) = \frac{\left|\sigma^{\text{predict}}(\varepsilon_i) - \sigma(\varepsilon_i)\right|}{\sigma(\varepsilon_i)}.$$

Table 2 shows a distribution of $D_{nl}(\varepsilon_i)$ values over three classes of accuracy. Class 1 is for $D_{nl}(\varepsilon_i) < 10\%$. Class 2 is for $10\% \leqslant D_{nl}(\varepsilon_i) < 20\%$ and class 3 is for $20\% \leqslant D_{nl}(\varepsilon_i) \leqslant 40\%$. One can see that class 3 is almost empty. This means that predicted cross-sections are accurate commonly to better than 20%. Contributions to class 3 are, almost exclusively, from fast projectiles ($x \simeq 100$) that have small ionization cross-sections.

Table 2. Distribution of $D_{nl}(\varepsilon_i)$ values over three classes of accuracy.

nl	Class 1 (%)	Class 2 (%)	Class 3 (%)
1s	90	9	1
2s	79	19	2
2p	84	15	1
3s	61	35	4
3p	72	22	6

4. Summary

We studied the effect of N on direct electron-impact ionization from inner subshells of ions ($m > 4$). It is found that scaled cross-sections depend on N but the dependence is rather weak. Namely, for removal of an electron from a definite nl-subshell of ions belonging to a sequence of ionization stages, the scaled cross-sections differ from each other by less than 20% in the energy range $1.4 < x < 8$ and by less than 50% for $x < 1.4$ and $8 < x < 100$. In each ionization sequence, with an increase in N the scaled cross-sections decrease monotonically for near-threshold energies ($x \approx 1$) and increase monotonically for high energies ($x > 6$).

For ionization from each nl-subshell, the scaled cross-sections corresponding to various A, m, N and γSLJ, are commonly within ±20% of the median function $F_{nl}(x)$ of the bunch at $1 \leqslant x \leqslant 100$. The deviations beyond ±20% take place almost exclusively at $x \simeq 100$. For practical use in applications, direct inner-shell ionization cross-sections are approximated by formula (5). It is important to remember that the threshold energy, I, is defined as the smallest $I_{S'L'J'}$ of all $S'L'J'$ levels, *except for* those with $\sigma_{S'L'J'}(\varepsilon) = 0$.

Acknowledgments

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