Nuclear Inst. and Methods in Physics Research B xxx (xxxx) xxx–xxx

Contents lists available at ScienceDirect

Nuclear Inst. and Methods in Physics Research B

journal homepage: www.elsevier.com/locate/nimb

Reprint of: Ionization probabilities of Ne, Ar, Kr, and Xe by proton impact for different initial states and impact energies☆

C.C. Montanari*, J.E. Miraglia

Instituto de Astronomía y Física del Espacio (CONICET and Universidad de Buenos Aires), Buenos Aires, Argentina
Universidad de Buenos Aires, Facultad de Ciencias Exactas y Naturales, Departamento de Física, 1428 Buenos Aires, Argentina

ARTICLE INFO

Keywords:
Ionization
Impact-parameter
Proton
Rare-gases
CDW-EIS
Born

ABSTRACT

In this contribution we present *ab initio* results for ionization total cross sections, probabilities at zero impact parameter, and impact parameter moments of order +1 and −1 of Ne, Ar, Kr, and Xe by proton impact in an extended energy range from 100 keV up to 10 MeV. The calculations were performed by using the continuum distorted wave eikonal initial state approximation (CDW-EIS) for energies up to 1 MeV, and using the first Born approximation for larger energies. The convergence of the CDW-EIS to the first Born above 1 MeV is clear in the present results. Our inner-shell ionization cross sections are compared with the available experimental data and with the ECPSSR results. We also include in this contribution the values of the ionization probabilities at the origin, and the impact parameter dependence. These values have been employed in multiple ionization calculations showing very good description of the experimental data. Tables of the ionization probabilities are presented, disaggregated for the different initial bound states, considering all the shells for Ne and Ar, the M-N shells of Kr and the N-O shells of Xe.

1. Introduction

Ionization data, involving experimental and theoretical values, has received great attention for a very long time ([1] and references therein). However, current progress of beam characterization methods, atomic analytical techniques such as the so-extended particle induced X-ray emission (PIXE) [2,3], and multiple-purpose simulations for the passage of particles through matter as the Geant4 [4], have aroused new interest and requirements of accurate data and reliable predictions. The probabilities as function of the impact parameter are the seeds to describe the total ionization cross sections of the different shells. But also, these probabilities are the inputs for the multiple ionization calculations in a multinomial combination of the impact parameter probabilities [5]. From the theoretical point of view, these probabilities represent a challenge and a test of the capability of a theory to describe wave functions and interaction potentials. Different approaches have been employed over the years, from the basic first Born approximation, to distorted wave methods, numerical solution of the Schrödinger equation or collective response models [6–11]. Moreover, in very recent works, the ionization probabilities by proton and antiproton impact have been the seeds to obtain multiple ionization cross sections of rare gases by electron and positron impact, with reasonably good results [12,13]. It is worth to note that multiple ionization cross sections are highly dependent on the inner-shell ionization probabilities, which contribute to the final values through Auger-type processes [8,12].

There are different compilations of experimental data for the total ionization cross sections of the K-shell [14,15] and the L-shell [1,16]. One of the most employed models for K and L-shell ionization cross sections is the ECPSSR by Brandt and Lapicki [17,18], of high efficiency and the usual input in PIXE codes [19]. Instead, reliable values of M-shell ionization are scarce [20,21]. This is related to the complexity of the M-X-ray spectra because of the existence of five sub-shells [22].

The goal of the present contribution is to make available *ab initio* CDW-EIS and first Born approximation results for proton impact ionization of different sub-shells of the heaviest rare gases. Presents results are calculated by rigorously solving the radial Schrödinger equation for different angular momenta for both the initial bound and the final continuum states. Thus, we can assure the proper description of the continuum wave function and its mathematical orthogonality to the bound state. These values have already been tested in total [23] and differential [24] ionization cross sections. Also the probabilities as function of the impact parameter have been employed in multiple ionization calculations [9,12,13,25] with good agreement with the

☆ This article is a reprint of a previously published article. For citation purposes, please use the original publication details; Nuclear Inst. and Methods in Physics Research, B Volume 407, September 2017, Pages 236–243.

* Corresponding author at: Universidad de Buenos Aires, Facultad de Ciencias Exactas y Naturales, Departamento de Física, 1428 Buenos Aires, Argentina.
E-mail address: mclaudia@iafe.uba.ar (C.C. Montanari).

https://doi.org/10.1016/j.nimb.2017.11.007
Received 20 June 2017; Accepted 2 July 2017

Table 1
Total ionization cross sections σ_{nlm} of the different sub-shells of Neon and Argon by impact of (0.1–10 MeV) protons. The cross sections for the different *nlm* sub-shells are given by Eq. (1), calculated with the CDW-EIS, Eq. (3), for impact energies 0.1–1 MeV; and with the first Born, Eq. (2), for impact energies 1–10 MeV. To save space, throughout these tables the subindex n replaces the 10^n factor. Units: the energy is in MeV and the cross sections in atomic units.

	Ne												
	CDW-EIS							Born					
E	0.1	0.2	0.3	0.4	0.5	0.7	1	1	2	3	5	7	10
σ_{2p1}	8.17_{-1}	7.96_{-1}	6.86_{-1}	5.95_{-1}	5.25_{-1}	4.26_{-1}	3.36_{-1}	3.41_{-1}	2.04_{-1}	1.49_{-1}	9.93_{-2}	7.55_{-2}	5.63_{-2}
σ_{2p0}	8.79_{-1}	9.03_{-1}	7.72_{-1}	6.59_{-1}	5.71_{-1}	4.52_{-1}	3.46_{-1}	3.44_{-1}	1.99_{-1}	1.43_{-1}	9.35_{-2}	7.09_{-2}	5.19_{-2}
σ_{2s}	2.49_{-1}	2.86_{-1}	2.40_{-1}	2.00_{-1}	1.69_{-1}	1.30_{-1}	9.62_{-2}	9.46_{-2}	5.30_{-2}	3.74_{-2}	2.40_{-2}	1.78_{-2}	1.30_{-2}
σ_{1s}	2.04_{-5}	1.44_{-4}	3.29_{-4}	5.20_{-4}	6.99_{-4}	9.92_{-4}	1.29_{-3}	1.34_{-3}	1.58_{-3}	1.50_{-3}	1.25_{-3}	1.04_{-3}	8.35_{-4}
	Ar												
	CDW-EIS							Born					
E	0.1	0.2	0.3	0.4	0.5	0.7	1	1	2	3	5	7	10
σ_{3p1}	2.86	2.31	1.84	1.53	1.32	1.08	7.85_{-1}	7.98_{-1}	4.54_{-1}	3.24_{-1}	2.21_{-1}	1.56_{-1}	1.16_{-1}
σ_{3p0}	3.52	2.68	2.04	1.65	1.38	1.10	7.79_{-1}	7.85_{-1}	4.32_{-1}	3.04_{-1}	1.94_{-1}	1.52_{-1}	1.05_{-1}
σ_{3s}	6.62_{-1}	5.09_{-1}	3.77_{-1}	2.98_{-1}	2.47_{-1}	1.85_{-1}	1.35_{-1}	1.36_{-1}	7.27_{-2}	5.01_{-2}	3.16_{-2}	2.28_{-2}	1.66_{-2}
σ_{2p1}	2.73_{-3}	7.71_{-3}	1.11_{-2}	1.32_{-2}	1.44_{-2}	1.54_{-2}	1.51_{-2}	1.61_{-2}	1.24_{-2}	9.96_{-3}	7.33_{-3}	5.71_{-3}	4.41_{-3}
σ_{2p0}	2.14_{-3}	6.98_{-3}	1.18_{-2}	1.41_{-2}	1.58_{-2}	1.73_{-2}	1.73_{-2}	1.71_{-2}	1.36_{-2}	1.08_{-2}	7.68_{-3}	5.98_{-3}	4.53_{-3}
σ_{2s}	1.16_{-3}	4.91_{-3}	7.49_{-3}	8.93_{-3}	9.69_{-3}	1.01_{-2}	9.69_{-3}	1.04_{-2}	7.40_{-3}	5.67_{-3}	3.91_{-3}	3.01_{-3}	2.27_{-3}
σ_{1s}	2.08_{-8}	3.52_{-7}	1.41_{-6}	3.35_{-6}	6.07_{-6}	1.33_{-5}	2.62_{-5}	2.73_{-5}	6.86_{-5}	9.58_{-5}	1.20_{-4}	1.24_{-4}	1.19_{-4}

Table 2
Total ionization cross sections σ_{nlm} of Krypton L, M and N shells by 0.1–10 MeV protons. Explanation as in Table 1.

	Kr												
	CDW-EIS							Born					
E	0.1	0.2	0.3	0.4	0.5	0.7	1	1	2	3	5	7	10
σ_{4p1}	3.36	2.51	1.94	1.58	1.35	1.04	7.77_{-1}	8.01_{-1}	4.38_{-1}	3.09_{-1}	1.98_{-1}	1.47_{-1}	1.07_{-1}
σ_{4p0}	4.48	2.91	2.12	1.76	1.38	1.03	7.53_{-1}	7.70_{-1}	4.24_{-1}	2.95_{-1}	1.79_{-1}	1.32_{-1}	9.52_{-2}
σ_{4s}	9.92_{-1}	7.03_{-1}	5.09_{-1}	3.96_{-1}	3.24_{-1}	2.38_{-1}	1.70_{-1}	1.71_{-1}	8.80_{-2}	5.95_{-2}	3.63_{-2}	2.62_{-2}	1.88_{-2}
σ_{3d2}	1.98_{-2}	3.53_{-2}	4.20_{-2}	4.45_{-2}	4.50_{-2}	4.37_{-2}	4.01_{-2}	4.25_{-2}	3.07_{-2}	2.43_{-2}	1.75_{-2}	1.39_{-2}	1.08_{-2}
σ_{3d1}	2.42_{-2}	4.13_{-2}	4.85_{-2}	5.14_{-2}	5.20_{-2}	5.04_{-2}	4.59_{-2}	4.65_{-2}	3.31_{-2}	2.57_{-2}	1.80_{-2}	1.40_{-2}	1.06_{-2}
σ_{3d0}	2.65_{-2}	4.81_{-2}	5.65_{-2}	5.88_{-2}	5.86_{-2}	5.54_{-2}	4.93_{-2}	4.79_{-2}	3.37_{-2}	2.61_{-2}	1.80_{-2}	1.39_{-2}	1.05_{-2}
σ_{3p1}	3.36_{-3}	9.02_{-3}	1.24_{-2}	1.42_{-2}	1.50_{-2}	1.52_{-2}	1.41_{-2}	1.51_{-2}	1.04_{-2}	7.96_{-3}	5.48_{-3}	4.23_{-3}	3.19_{-3}
σ_{3p0}	3.38_{-3}	9.92_{-3}	1.48_{-2}	1.70_{-2}	1.77_{-2}	1.74_{-2}	1.59_{-2}	1.63_{-2}	1.13_{-2}	8.46_{-3}	5.65_{-3}	4.28_{-3}	3.16_{-3}
σ_{3s}	1.40_{-3}	5.63_{-3}	8.22_{-3}	9.44_{-3}	1.00_{-2}	1.02_{-2}	9.62_{-3}	1.03_{-2}	7.10_{-3}	5.38_{-3}	3.65_{-3}	2.79_{-3}	2.09_{-3}
σ_{2p1}	5.88_{-7}	7.13_{-6}	2.28_{-5}	4.59_{-5}	7.36_{-5}	1.33_{-4}	2.14_{-4}	2.31_{-4}	3.71_{-4}	4.13_{-4}	4.13_{-4}	3.80_{-4}	3.31_{-4}
σ_{2p0}	1.80_{-6}	1.16_{-5}	2.72_{-5}	4.59_{-5}	6.54_{-5}	1.03_{-4}	1.58_{-4}	1.80_{-4}	3.28_{-4}	4.00_{-4}	4.33_{-4}	4.12_{-4}	3.64_{-4}
σ_{2s}	2.74_{-7}	1.40_{-6}	7.86_{-6}	2.21_{-5}	4.30_{-5}	9.70_{-5}	1.83_{-4}	1.90_{-4}	3.38_{-4}	3.73_{-4}	3.50_{-4}	3.09_{-4}	2.56_{-4}

experimental data, even for sextuple ionization of Kr (Xe), where L-shell (M-shell) contribution is decisive. In the following sections we compare the present inner-shell ionization cross sections with the available experimental data, and with the ECPSSR values [17], for the K-shell of Ne, K and L-shells of Ar, L and M-shells of Kr and M and N-shells of Xe. We make available our CDW-EIS values for proton impact energies 0.1–1 MeV, and also the first Born approximation results for proton energies 1–10 MeV, considering the ionization of different sub-shells: Ne (1s, 2s, 2p), Ar (1s,…, 3p), Kr (2s,…, 4p) and Xe (3s,…, 5p). We display tables of the present total ionization cross sections, probabilities at zero impact parameter, and impact parameter moments of order 1 and −1. Atomic units are used throughout this work, except when specifically mentioned.

2. Total ionization cross sections

The total ionization cross section of an electron initially in the *nlm* state, due to the interaction with a heavy projectile of charge Z_P (in this work $Z_P = 1$, proton impact) and impact velocity v, is given by the four-dimension integral

$$\sigma_{nlm} = \frac{(2\pi)^2}{v^2} \int d\vec{k} \int d\vec{\eta} \ |T_{\vec{k},nlm}(\vec{\eta})|^2 \tag{1}$$

where $T_{\vec{k},nlm}(\vec{\eta})$ is the transition matrix as a function of the momentum transferred $\vec{\eta}$ perpendicular to the incident velocity $\vec{v}$, and $\vec{k}$ is the momentum of the emitted electron. For heavy projectiles such as protons, the integration over $\vec{\eta}$ extends to infinity.

If we are interested in high energy collisions, we can resort to the first Born approximation. This is a perturbative method valid at large impact velocities and low projectile charges, with the initial and final wave functions being the unperturbed ones. The first Born transition matrix element is given by

$$T^{Born}_{\vec{k},nlm}(\vec{\eta}) = \frac{1}{(2\pi)^{3/2}} \widetilde{V}_P(p) \int d\vec{r} \ \varphi^{*}_{\vec{k}}(r) \exp(i\,\vec{p}\,.\,\vec{r})\varphi_{nlm}(r). \tag{2}$$

Here $\varphi_{\vec{k}}$ (φ_{nlm}) is the final (initial) continuum (bound) eigenfunction of the target hamiltonian; $\widetilde{V}_P(p) = -\sqrt{2/\pi}\ Z_P/p^2$ is the Fourier transform of the projectile-electron Coulomb potential, and $\vec{p} = \vec{K_i} - \vec{K_f}$ is the momentum transferred, with $\vec{K_i}$ ($\vec{K_f}$) being the initial (final) projectile momentum. The momentum transferred can also be expressed as