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Electron impact ionization cross sections of several ionization stages of Kr, Ar and Fe

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ABSTRACT

Direct electron impact ionization cross sections for all ionization stages of Kr were calculated with the modified relativistic binary encounter Bethe model (MRBEB), and excitation–autoionization cross sections were evaluated using the first order many body theory (FOMBT) for Kr^{+}, Kr^{5+}, Kr^{6+}, Kr^{10+}, Kr^{15+} and Kr^{17+}. Our results were compared to configuration-averaged distorted-wave (CADW) calculations, the widely used Lotz formula, and available experimental results. Comparison between direct ionization cross sections for the Ar and Fe isonuclear series was also done with the goal of assessing the versatility of the MRBEB model.

1. Introduction

Absolute cross sections for electron impact single and multiple ionization of atoms and ions are of great importance to model and diagnose astrophysical and laboratory plasmas, since one of the key steps in these studies is the knowledge of the charge state distribution [43,11,36,13,16]. Predicting the correct charge state distribution is critical for understanding radiation levels, energy deposition, energy balance, etc., of high- and low-temperature plasmas such as those generated in electron-cyclotron-resonance ion-sources (ECRIS). ECRIS plasmas have been recently used, coupled to a double-crystal-spectrometer, to provide absolute (reference-free) X-ray energies of electronic transitions in highly charged ions [1] and, given the accuracy of such devices, there is a rising need of correct diagnostics of all the plasma parameters. Considering the plasma diagnostics tools [36], a 20% or less uncertainty in the electron impact ionization cross section is enough for modeling the plasma's X-ray spectra so that the final error budget is not dominated by the cross section calculation.

The widely used Lotz expression [27], as well as other empirical theories such as the DM formalism [20], the XCVTS model [19] and the GKLV model [21], are not ideally suited for these studies since they often lead to different coefficients, or even expressions, for different elements, shells and/or charge states. Also, in some atomic systems, they show more than a 20% disagreement with experimental data.

In an earlier work, Guerra et al. [17] proposed the modified relativistic binary encounter Bethe model (MRBEB) expression for direct ionization cross sections of neutral atoms by electron impact, from the threshold to relativistic incident energy values. This simple analytical expression, which was recently implemented in a web page [37], is a function of the incident electron energy and requires only one atomic parameter, the binding energy of the electrons to be ionized. The MRBEB model was used to obtain the K-, L-, and M-shell ionization cross sections by electron impact for several atoms with Z from 6 to 83, between the threshold and several MeV, with an accuracy of ∼20%, or better [17].

The aim of this work is to study the applicability of the MRBEB model in obtaining electron impact cross sections from lowly to highly charged ions across the Z spectra. We have chosen the Kr, Ar, and Fe ions for this study because of their importance in fusion, astrophysical, and industrial plasmas [12,31,42]. For example, in magnetic confinement fusion, Kr, along with Ar, is a species of choice for the modification of edge conditions (via transport barriers, etc.) by radiative cooling and this has led to the decision by the fusion community to establish argon as a reference species [42]. In the astrophysical domain, high-resolution soft X-ray spectra of Fe from solar flares have been observed for many years by the SMM and YOKHOH satellites and, since 1999, by the CHANDRA X-ray observatory as well.

The results of our calculations for the direct ionization cross section are compared to the Lotz expression [15], the hydrogenic scaling (HS) model of Sampson et al. [15] and the distorted wave

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approximation (DWA) calculated with the GIPPER code of the Los Alamos National Laboratory [2], and to available experimental data.

This article is organized as follows: a brief outline of the underlying theory is presented in Section 2. The results are discussed and compared with available experimental and theoretical data in Section 3. The conclusions are presented in Section 4.

2. Theory

The processes that play a major role in electron impact ionization cross sections of krypton ions can be described by the following expressions

$$Kr^{q+} + e^- \longrightarrow Kr^{(q+1)+} + 2e^-, \tag{1}$$

$$Kr^{q+} + e^- \longrightarrow (Kr^{q+})^* + e^- \longrightarrow Kr^{(q+1)+} + 2e^-, \tag{2}$$

where q is the charge of the ion to be ionized. The first process is called direct ionization (DI), while the second corresponds to a process of excitation to a bound state followed by autoionization (EA). The later process can occur if the excitation energy is greater than the lowest ionization energy of the ion.

Therefore, for the purpose of comparing our calculations with experimental data for ionization of ions, one must compute not only the direct ionization cross sections, but also the contribution of the EA process to the ionization cross section and sum it to the direct ionization cross section values.

2.1. Direct ionization

The MRBEB cross section for direct ionization of a $n\,\ell\,j$ (n – principal quantum number, ℓ – orbital angular momentum, j – total angular momentum) bound electron with binding energy B in an atom in the initial state LS (L – total orbital angular momentum, S – total spin angular momentum S), by an electron with incident kinetic energy T is given by [17]

$$\sigma_{\mathrm{MRBEB},n\ell jLS} = \frac{4\pi a_0^2\alpha^4 N_{n\ell j}}{(\beta_t^2+\chi_{n\ell j}\beta_b^2)2b'}\left\{\frac{1}{2}\left[\ln\left(\frac{\beta_t^2}{1-\beta_t^2}\right)-\beta_t^2-\ln\left(2b'\right)\right]\right.$$
$$\left.\times\left(1-\frac{1}{t^2}\right)+1-\frac{1}{t}-\frac{\ln t}{t+1}\frac{1+2t'}{\left(1+t'/2\right)^2}+\frac{b'^2}{\left(1+t'/2\right)^2}\frac{t-1}{2}\right\} \tag{3}$$

where

$$\beta_t^2 = 1-\frac{1}{(1+t')^2} \qquad t' = \frac{T}{mc^2},$$
$$\beta_b^2 = 1-\frac{1}{(1+b')^2} \qquad b' = \frac{B}{mc^2}, \tag{4}$$
$$t = \frac{T}{B} \qquad \chi_{n\ell j} = \left(\frac{C_{n\ell j}}{B}\right)2R.$$

Here c is the speed of light in vacuum, m is the electron mass, $C_{n\ell j}$ is a scaling constant related to the potential energy of the incident electron in the ionization region, and R is the Rydberg energy (13.6 eV). In Eq. (3), α is the fine structure constant, $N_{n\ell j}$ is the subshell occupation number, and a_0 is the Bohr radius (5.29×10^{-11} m). The energy values should be in the same units and a_0 in meters.

The $C_{n\ell j}$ scaling factor is defined [17] as,

$$C_{n\ell j} = 0.3\frac{Z^2_{\mathrm{eff}_{n\ell j}}}{2n^2}+0.7\frac{Z^2_{\mathrm{eff}_{n'\ell' j'}}}{2n'^2}, \tag{5}$$

where $n'\,\ell'\,j'$ stands for next subshell after the subshell $n\,\ell\,j$. Considering that there are no values in the literature for the Z_{eff} of every subshell in every element or ion of the periodic table, we opted to use the number of electrons of all inner shells up to the subshell $n\,\ell\,j$ being ionized as screening of the primary electron, i.e.,

$$Z_{\mathrm{eff}_{n\ell j}} = Z-\sum_{i=1s1/2}^{n\ell j} N_i, \tag{6}$$

where Z is the target atomic number and N_i is the number of electrons of the subshell i. Since there is no occupied orbital lying above the valence subshell, for the last occupied subshell Eq. (5) must be changed to

$$C_{n\ell j_{\mathrm{last}}} = \frac{Z^2_{\mathrm{eff}_{n\ell j}}}{2n^2}. \tag{7}$$

This means that, in this model, we have considered that for outer subshells the penetration of the incident electron upon ionization is much higher than for inner-subshells.

2.2. Direct ionization for different ion final states

Eq. (3) concerns the ionization of a $n\,\ell\,j$ electron in an atom in a given initial state LS, and nothing is said about the final state L_fS_f after ionization. Because most of the experiments that measure total cross sections of atoms and ions do not distinguish the resulting ionic states, we have to weight the cross section calculated for a given ionized state with the corresponding statistical weight before we perform the summation to obtain the total ionization cross sections. Thus, the weighted MRBEB cross section for a given final state L_fS_f is given by

$$\sigma_{\mathrm{MRBEB},n\ell jLS,\mathrm{w}L_fS_f} = \frac{(2L_f+1)(2S_f+1)}{\sum_{L'_fS'_f}\left(2L'_f+1\right)\left(2S'_f+1\right)}\sigma_{\mathrm{MRBEB},n\ell jLS}, \tag{8}$$

where $\sigma_{\mathrm{MRBEB},n\ell jLS}$ is the cross section given by Eq. (3). The sum over L'_f and S'_f covers all final ionic states sharing the same electronic configuration.

Note that, with the use of Eq. (8), the parameter B no longer corresponds to the binding energy but to the ionization energy between the initial and final states. The adiabatic ionization energies from the ground levels and metastable levels of the Kr, Ar and Fe ions studied in this work are listed in Table 2.

The total direct electron impact ionization cross section, σ_{DI}, is obtained by summing $\sigma_{\mathrm{MRBEB},n\ell jLS,\mathrm{w}L_fS_f}$ over all occupied $n\,\ell\,jLS$ states, i.e.,

$$\sigma_{\mathrm{DI}} = \sum_{\mathrm{occupied}\ n\ell jLS}\sigma_{\mathrm{MRBEB},n\ell jLS,\mathrm{w}L_fS_f}. \tag{9}$$

To assess the importance of the several ionization channels on the direct ionization, we have performed, for every ion studied in this work, the cross section calculation using Eq. (3) with the adiabatic ionization energies listed in Table 2, as opposed to performing the calculation for every combination of initial and final states, through the use of Eq. (8). The relative difference between the results is less than 3 %. This is due to the fact that the weighted average of the ionization energies of every possible transition is not very different from the adiabatic ionization energy. Therefore, in the cases that involve many initial and final states, we may, as an approximation, simply use the ground states of the atom or ion to be ionized and the resulting cation, instead of going through the time consuming computation of the parameters necessary for Eq. (8). In these cases, the total direct electron impact ionization cross section is given by

$$\sigma_{\mathrm{DI}} = \sum_{\mathrm{occupied}\ n\ell jLS}\sigma_{\mathrm{MRBEB},n\ell jLS}. \tag{10}$$