Electron-impact ionization of Li, Be$^+$, B^{2+}, C^{3+}, N^{4+} and O^{5+}

A Yu Elizarov[1] and I I Tupitsyn[2]

[1] A. F. Ioffe Physico-Technical Institute, RAN, 194021, St. Petersburg, Russia
[2] Department of Physics, St. Petersburg State University, 198904, St. Petersburg, Russia

E-mail: a.elizarov@mail.ioffe.ru and tup@tup.usr.pu.ru

Abstract

A variant of the first Born approximation is used to calculate total electron-impact ionization cross-section. The calculations are performed for the lithium-like targets, Li, ..., O^{5+}. Wavefunction of the ejected electrons is presented by distorted wave. High-quality orthogonal initial- and final-state Hartree–Fock Slater orbitals are used to model the target wavefunctions. The wavefunctions of the initial and final states are calculated with allowance for relaxation effect. The one-electron wavefunction of the continuous spectrum for ejected electrons is obtained by using the single-configuration Hartree–Fock method. The present results are compared to available experimental measurements and theoretical calculations with the convergent close-coupling method.

1. Introduction

For many years there has been a significant amount of research into improving the theory of electron-impact ionization collision with atoms and ions. The first Born approximation calculations for electron-impact ionization had many variants over recent decades. This approximation differs by describing the wave of ejected continuum electrons (see, for example, [1, 2]) and the orbitals of the target and residual ions. In [3] high-quality Hartree–Fock Slater orbitals have been used for calculations of electron-impact total-ionization cross-sections for Ne, Ar, Kr, Xe, Fe, Cu, Ag, Si, Ge, Sn, P, As, Sb, S, Se and Te. Full orthogonalization of the continuum Coulomb wave to all occupied orbitals of the target atoms was made. Remarkable agreement with experiment for elastic, excitation and ionization processes by using the convergent close-coupled (CCC) [5] approach was obtained for targets such as hydrogen [4], sodium [6] and helium [7]. In [8] results were presented for electron-impact direct total ionization of lithium-like targets, Li, ..., O^{5+}, calculated using the CCC method. Agreement with experiment was obtained for targets such as Li, N^{4+} and O^{5+} targets. The existing discrepancy between theoretical predictions and experimental data [10–13] necessitates further investigation in this field.

The results reported in this paper were obtained by using plane wave first Born (PWB) approximation with a distorted wave to describe the ejected electrons and plane wave to construct incident and scattered electrons.

The wavefunctions of the target and residual ions were calculated by the multiconfiguration Hartree–Fock method accounting relaxation of energy levels of both the initial state to model the targets and residual ions (see [14] for a general discussion of this method). electron-impact ionization cross-section depends on the wavefunction of the continuous spectrum. In early works, this function did not take into account exchange interactions between an electron of the continuous spectrum and core-shell electrons and ignored off-diagonal Lagrange multipliers, which render the wavefunction of the continuous spectrum orthogonal to occupied single-electron final states. In this work, we take into account the effect of these factors.

In the following section, we outline the basic principles underlying the calculations of the total cross-sections of electron-impact ionization lithium-like targets Li, . . . , O^{5+}. Then, we give the comparison with experiments and CCC calculations.

Atomic units ($\hbar = e = m = 1$) are used throughout the paper.

2. Theory

2.1. The plane wave first Born approximation

In this paper we describe the ionization process

$$A_i^{q+} + e(\boldsymbol{k}_i) \rightarrow A_f^{q+1} + e(\boldsymbol{k}) + e_f(\boldsymbol{k}_f) \tag{1}$$

by using the following notations. (a) The momenta of the incident, scattered and ejected electrons are denote by $\boldsymbol{k}_i$, $\boldsymbol{k}_f$ and $\boldsymbol{k}$, respectively. (b) The states of both the target in initial states A_i^{q+} and residual ions A_f^{q+1} will be described by orbital and spin angular momentum quantum numbers L_i, M_i, S_i, M_{S_i} and $L_f M_f S_f M_{S_f}$, respectively. The present calculations assumed the target to be initially in the ground state. The ejected electrons are described by distorted wave. The targets and residual ions wavefunctions are evaluated by using the nonrelativistic multiconfigurational Hartree–Fock method. LS coupling will be assumed to apply throughout.

In the PWB approximation, the differential cross-section of the electron-impact ionization of a target A_i^{q+} can be written in the forms [15, 16]

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\varepsilon} = (2\pi)^4 \frac{k_f k}{k_i} \int \mathrm{d}\Omega_{\boldsymbol{k}_f} W_{L_i S_i, L_f S_f}(\boldsymbol{q}), \tag{2}$$

where σ is the total-ionization cross-section, ε is the incident electron energy, $\boldsymbol{q}$ is the momentum transfer ($\boldsymbol{q} = \boldsymbol{k}_i - \boldsymbol{k}_f$) and the magnitude $W_{L_i S_i, L_f S_f}(\boldsymbol{q})$ is given by the expression

$$W_{L_i S_i, L_f S_f}(\boldsymbol{q}) = \frac{1}{2L_i + 1} \frac{1}{2S_i + 1} \sum_{M_i, M_f} \sum_{M_{S_i}, M_{S_f}} \sum_{m_s} \int \mathrm{d}\Omega_{\boldsymbol{k}} |A_{i,f}(\boldsymbol{q}, \boldsymbol{k})|^2. \tag{3}$$

Here m_s is the spin projection of the ejected electron, $\mathrm{d}\Omega_{\boldsymbol{k}_f}$ and $\mathrm{d}\Omega_{\boldsymbol{k}}$ in equations (2, 3) are elements of a solid angle about the scattered and ejected electrons, respectively.

The scattering amplitude $A_{i,f}(\boldsymbol{q}, \boldsymbol{k})$ for the direct ionization process in the PWB approximation is introduced in the form

$$A_{i,f}(\boldsymbol{q}, \boldsymbol{k}) = \langle \Phi_f | V(\boldsymbol{q}) | \Phi_i \rangle, \tag{4}$$

where Φ_f and Φ_i are the total wavefunctions of the target final and initial states, respectively. The transition operator $V(q)$ is given by

$$V(q) = \frac{1}{2\pi^3} \int d\boldsymbol{r}\, e^{iqr} \left[\sum_{j=1}^{N} \frac{e^2}{|\boldsymbol{r}_j - \boldsymbol{r}|} - \frac{Z}{r} \right] = \frac{1}{2\pi^2 q^2} \sum_{j=1}^{N} \left[e^{iqr_j} - \frac{Z}{N} \right]. \tag{5}$$

Here N is the number of electrons in the target initial state and Z is the nuclear charge. Expanding plane wave in spherical harmonics we can rewrite equation (5) in the form

$$V(q) = \frac{2}{\pi q^2} \sum_{KQ} i^Q \hat{A}_{KQ} Y_{KQ}^*(\boldsymbol{k}), \tag{6}$$

where

$$\hat{A}_{KQ} = \sum_{j=1}^{N} \left[j_K(qr_j) Y_{KQ}(\boldsymbol{r}_j) - \delta_{K,0} \sqrt{\frac{1}{4\pi}} \frac{Z}{N} \right]. \tag{7}$$

Here Y_{KQ} is the spherical harmonic function and $j_K(qr)$—the spherical Bessel function. The initial and final N-electron wavefunctions can be written in the form

$$\Phi_i(x_1, x_2, \ldots, x_N) = \Psi_{L_i M_i, S_i M_{S_i}}(x_1, x_2, \ldots, x_N),$$
$$\Phi_f(x_1, x_2, \ldots, x_N) = \hat{A} \Psi_{L_f M_f, S_f M_{S_f}}(x_1, x_2, \ldots, x_{N-1}) \psi_{\boldsymbol{k}, m_s}^{(-)}(x_N), \tag{8}$$

where $\hat{A}$ is the antisymmetrizing operator, $\Psi_{L_i M_i, S_i M_{S_i}}$ is the bound state wavefunction of the target, $\Psi_{L_f M_f, S_f M_{S_f}}$ is the bound wavefunction of the residual ion and $\psi_{\boldsymbol{k}, m_s}^{(-)}$ is a continuum wavefunction of the ejecting electron. The distorted wave $\psi_{\boldsymbol{k}, m_s}^{(-)}$ can be presented in a partial wave expansion

$$\psi_{\boldsymbol{k}, m_s}^{(-)} = \frac{1}{\sqrt{k}} \sum_{lm} i^l\, e^{-i\delta_l} \frac{P_{\varepsilon l}(r)}{r} Y_{lm}(\boldsymbol{r}) Y_{lm}^*(\boldsymbol{k}) \chi_{m_s}, \tag{9}$$

where Y_{lm} is the spherical harmonic function, δ_l is the total phase, $P_{\varepsilon l}(r)$ is the radial part of the partial wave function $\psi_{\varepsilon l m}(\boldsymbol{r}) = P_{\varepsilon l}(r)/r Y_{lm}(\boldsymbol{r})$ and χ_{m_s} is the spin function of the ejected electron.

Inserting the partial wave expansion (9) in equation (3) and carrying out the integrations over Ω_k, we obtain

$$W_{L_i S_i, L_f S_f}(q) = \frac{1}{k} \frac{1}{\pi^3 q^4} \frac{1}{2L_i + 1} \frac{1}{2S_i + 1} \sum_{M_i, M_f} \sum_{M_{S_i}, M_{S_f}} \sum_{lmm_s} \sum_{KQ}$$

$$\times |\langle L_f M_f, S_f M_{S_f}, \varepsilon l m m_s | \hat{A}_{KQ} | L_i M_i S_i M_{S_i} \rangle|^2. \tag{10}$$

In this work the wavefunctions $\Psi_{L_i M_i, S_i M_{S_i}}$ and $\Psi_{L_f M_f, S_f M_{S_f}}$ were calculated for the fixed values of projections quantum numbers $\overline{M}_f$, $\overline{M}_{S_f}$, $\overline{M}_i$, $\overline{M}_{S_i}$ and $m_s = \overline{M}_{S_i} - \overline{M}_{S_f}$. To carry out the summation over other projections, we have to express the matrix elements for arbitrary projection quantum numbers $M_f M_{S_f}$, $M_i M_{S_i}$ in terms of the matrix elements with fixed projections. This can be done by using Wigner–Eckart theorem (see the appendix).

Finally, we note that the ionization differential cross-section is given as follows:

$$\frac{d\sigma}{d\varepsilon} = \frac{32\pi^2}{k_i^2} \sum_l \sum_I \int_{|k_f - k_i|}^{k_f + k_i} \frac{dq}{q^3} |\langle L_f S_f \varepsilon l \| \hat{T}_I(q) \| L_i S_i \rangle|^2. \tag{11}$$

The expressions for the reduced matrix element $\langle L_f S_f \varepsilon l \| \hat{T}_I(q) \| L_i S_i \rangle$ can be presented in the form [17]

$$\langle L_f S_f \varepsilon l \| \hat{T}_I(q) \| L_i S_i \rangle = \frac{1}{C_{S_f \overline{M}_{S_f}, \frac{1}{2} \overline{M}_{S_i} - \overline{M}_{S_f}}^{S_i \overline{M}_{S_i}} C_{L_f \overline{M}_f, I \overline{M}_I}^{L_i \overline{M}_i}}$$
$$\times \sum_{K,Q,m} C_{lm,KQ}^{I \overline{M}_I} \langle L_f \overline{M}_f, S_f \overline{M}_{S_f} \varepsilon l m | \hat{A}_{KQ} | L_i \overline{M}_i, S_i \overline{M}_{S_i} \rangle. \tag{12}$$

Here $C_{lm,l'm'}^{kq}$ are the Clebsch–Gordan coefficients, $\overline{M}_I = \overline{M}_i - \overline{M}_f$. The total cross-section is given by

$$\sigma(\varepsilon_i) = \int_0^{\varepsilon_{\max}} d\varepsilon \frac{d\sigma}{d\varepsilon}, \tag{13}$$

The energy conservation for this process can be presented in the form

$$\varepsilon_i = \varepsilon_f + \varepsilon + E_I, \qquad \varepsilon = \varepsilon_i - \varepsilon_f - E_I, \tag{14}$$

where E_I—the ionization energy (positive value). The incident and ejected electrons are identical particles but no allowance has been made for particle exchange. To compensate this omission, the upper integration limit of ε is taken to be $\varepsilon_{\max} = (\varepsilon_i - E_I)/2$, which is the energy of an electron ejected with half of the maximum possible energy. This approximation will always give better results when, as is usually the case, the effects of the exchange are to reduce the cross-section [18].

2.2. Calculation of the reduced matrix elements

The multiconfigurational Hartree–Fock (MCHF) method was used in all calculations of the wavefunctions of the target in the initial and final states. The many-electron wavefunction $\Psi(\gamma LM, S_{M_S})$ with quantum numbers γLM and SM_S is expanded in terms of a set of configuration state functions (CSFs) $\Theta_\alpha(LM, S_{M_S})$

$$\Psi(\gamma, LM, SM_S) = \sum_\alpha c_\alpha \Theta_\alpha(LM, SM_S). \tag{15}$$

The standard configuration-interaction (CI) method was used to find the coefficients c_α. The CSFs are the eigenfunctions of the $\hat{L}^2$ and $\hat{S}^2$ operators and they are constructed from the one-electron wavefunctions u_j as a linear combination of Slater determinants.

To generate the one-electron wavefunctions u_j, we employed the multiconfiguration HF method in the combined Hartree–Fock (HF) and the Hartree–Fock–Sturm (HFS) basis set $\{\varphi_n\}_{n=1}^M$

$$u_j = \sum_n C_{nj} \varphi_n. \tag{16}$$

Here the index n enumerates different occupied and vacant one-electron states. The coefficients C_{nj} were obtained by solving the MCHF matrix equations. For the occupied atomic shells, the orbitals φ_n with $n = 1, \ldots, M_0$ were generated by the restricted HF method, based on a numerical solution of the radial HF equations. The vacant orbitals φ_n with $n = M_0 + 1, \ldots, M$ were obtained by solving the Hartree–Fock–Sturm equations

$$[\hat{h}^{HF} - \varepsilon_{k_0}] \varphi_n = \xi_n W(r) \varphi_n, \tag{17}$$

which can be considered as a generalization of the method proposed in [19] to an arbitrary weight function $W(r)$. The parameter ξ_n in equation (17) can be considered as an eigenvalue

of the Sturmian operator. Obviously, for $\xi_n = 0$ the Sturmian function coincides with the reference HF orbital φ_{k_0}. If $W(r) \to 0$ at $r \to \infty$, all Sturmian functions φ_n have the same exponential asymptotics at $r \to \infty$. Therefore, the set of eigenfunctions of the Hartree–Fock–Sturm operator forms a discrete and complete basis set in the space of one-electron wavefunctions.

The widely used choice of the weight function is $W(r) = 1/r$, which leads to the well-known 'charge quantization'. In the relativistic case, however, this choice is not very suitable, since the behaviour of the Sturmian wavefunctions at the origin differs from that of the Dirac–Fock orbitals. In our nonrelativistic calculations we use the same weight function as in the relativistic case

$$W(r) = \frac{1 - \exp[-(\alpha r)^2]}{(\alpha r)^2}, \tag{18}$$

which, unlike $1/r$, is regular at the origin.

The set of one-electron wavefunctions u_j is orthonormal. However the basis set φ_n is not orthogonal in the usual sense, since the DFS orbitals are orthogonal with the weight $W(r)$.

The wavefunctions of the initial and final states in the electron-impact ionization process are usually calculated in the 'frozen' orbitals approximation. In this approximation the one-electron functions u_j of the initial and final states form the same set of orthonormal functions, which are optimized, for example, for the initial state. This computational method partially disregard the final-state electronic relaxations. Obviously, if the set of one-electron functions u_j and the set of CFS's are full (full CI), the disregarded part of electronic relaxations tends to zero.

For the finite set of u_j and restricted CI relaxations, effects of the final state should be considered. In this case we obtain two mutually nonorthogonal sets of orbitals. Let ϕ_j^i and ϕ_j^f denote the sets of one-electron functions of the final and initial states, respectively. The partial waves $\psi_{\varepsilon lm}$ of the continuum wavefunction $\psi_{\boldsymbol{k}, m_s}^{(-)}$ were included to the set of final-state orbitals.

The matrix elements were calculated with nonorthogonal orbitals. The N-electron wavefunctions Φ_i and Φ_f of the initial and final states, respectively (8) are expressed as a linear combination of the Slater determinants

$$\Phi_i = \sum_\alpha c_\alpha^i \det_\alpha\{\phi_j^i(x_k)\}, \qquad \Phi_f = \sum_\alpha c_\alpha^f \det_\alpha\{\phi_j^f(x_k)\}. \tag{19}$$

The reduced matrix elements (12) can be easily calculated if we introduce the first-order transition density matrix ρ^{if}, which are not dependent on the indices I, K, Q. The matrix elements of the operator $\hat{A}_{KQ}$ can be written in the form

$$\langle L_f \overline{M}_f, S_f \overline{M}_{S_f} \varepsilon lm | \hat{A}_{KQ} | L_i \overline{M}_i, S_i \overline{M}_{S_i} \rangle = \sum_{j,k=1}^{M} A_{jk}^{KQ} \rho_{jk}^{if}, \tag{20}$$

where $A_{jk}^{KQ} = \langle j | \hat{A}_{KQ} | k \rangle$ are one-electron matrix elements of the operator $\hat{A}_{KQ}$.

The matrix elements of the density matrix ρ^{if} for two mutually nonorthogonal sets of orbitals are given by [20]:

$$\rho_{jk}^{if} = \sum_{\alpha,\beta} c_\alpha^i c_\beta^f (D_{\alpha\alpha} D_{\beta\beta})^{-1/2} D_{\alpha\beta} (S^{\alpha,\beta})_{jk}^{-1}, \tag{21}$$

where $S_{jk}^{\alpha\beta}$ is the overlapping integral matrix $S_{jk}^{\alpha\beta} = \langle \phi_j^i | \phi_k^f \rangle$ between two groups of orbitals $\{\phi_j^i\}_\alpha$ and $\{\phi_k^f\}_\beta$ for two Slater determinants α and β, respectively and $D_{\alpha\beta} = \det|S^{\alpha\beta}|$ is

the determinant of the overlapping integral matrix $S^{\alpha\beta}$. For the initial state the set of orbitals $\phi_k^i(x)$ is orthonormal; therefore the determinants $D_{\alpha,\alpha}^i$ are equal to one. This is not so for the final state, where continuum wavefunctions $\psi_{\varepsilon lm}$ are orthogonal to the bound HF orbitals, but may not be orthogonal to the set of Sturmian basis functions.

2.3. Calculation of the distorted wavefunctions for the ejected electrons

The radial parts $P_{\varepsilon l}$ of the continuum wavefunctions were determined in the Hartree–Fock approximation by solving the equations

$$-\frac{1}{2}\frac{d^2}{dr^2}P_{\varepsilon l}(r) + \left[\frac{l(l+1)}{2r^2} + V_c(r)\right]P_{\varepsilon l}(r) + W_{ex}(r) = \varepsilon P_{\varepsilon l}(r) + \sum_{nl}\lambda_{\varepsilon l,nl}P_{nl}(r), \qquad (22)$$

where n and l are quantum numbers of occupied atomic shells of the residual ion in the final state, $\lambda_{\varepsilon l,nl}$ are off-diagonal Lagrange multipliers that render the continuous spectrum function $P_{\varepsilon l}$ orthogonal to the atomic radial functions P_{nl} of the same symmetry, $V_c(r)$ is the Coulomb potential, and W_{ex} is the result of action of the nonlocal exchange operator on the radial wavefunction of the continuum spectrum.

The radial wavefunction $P_{\varepsilon l}$ is normalized to the δ-function in terms of energy $\langle P_{\varepsilon l}|P_{\varepsilon'l}\rangle = \delta(\varepsilon - \varepsilon')$. It is convenient, therefore, to present the asymptotic of $P_{\varepsilon l}$ in the form

$$P_{\varepsilon l}(r) \simeq \sqrt{\frac{2}{\pi p}}\sin(\tau + \sigma_l), \qquad \tau = pr + \frac{Z}{p}\ln(2pr) - l\frac{\pi}{2}, \qquad (23)$$

where $p = \sqrt{2\varepsilon}$, Z is the target A_f^{q+1} charge and σ_l is scattering phase.

The normalized solution of equation (22) can be obtained by joining an arbitrary unnormalized solution $\tilde{P}_\varepsilon(r) = NP_\varepsilon(r)$ and its derivative $\tilde{P}'_{\varepsilon l}(r)$, which are regular at the origin, with the asymptotic function (23). However, to provide a high accuracy, this joining should be accomplished at a large distance, which is the order of 10 000–100 000 au. In this case the solution $\tilde{P}_{\varepsilon l}(r)$ should be found over a wide range of the radial variable r.
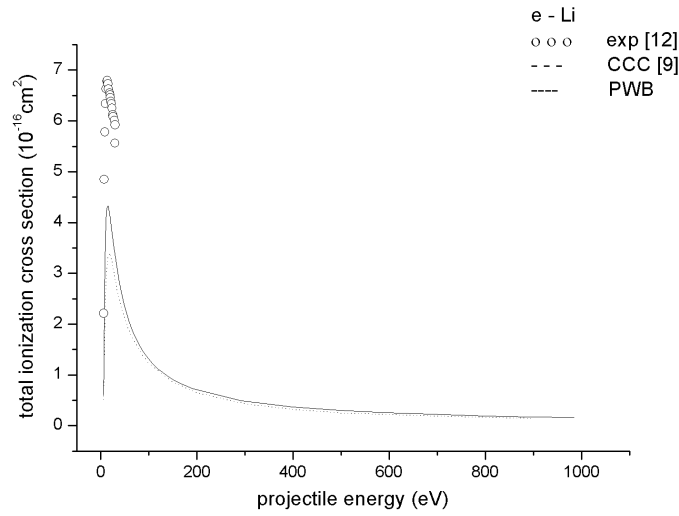
A much more efficient procedure is joining $\tilde{P}_{\varepsilon l}(r)$ and $\tilde{P}'_{\varepsilon l}(r)$ with a linear combination of Coulomb functions $F(r)$ and $G(r)$ that are, respectively, regular and irregular at the origin [21]:

$$\begin{cases} \tilde{P}_\varepsilon(R_a) = AF(R_a) + BG(R_a) \\ \tilde{P}'_\varepsilon(R_a) = AF'(R_a) + BG'(R_a) \end{cases}. \qquad (24)$$

Here, R_a is the joining point. The Coulomb functions F and G can be effectively calculated with the continued fraction technique [22].

The joining point R_a should be chosen in the region, where all radial bound wavefunctions are negligibly small and the atomic potential may be approximated by a point charge Coulomb potential with a high accuracy; that is $R_a \sim (20 \div 50)$ au. The normalized factor N and the phase σ_l are found from the coefficients A and B:

$$\begin{cases} \cos\sigma_l = \frac{1}{N}\left[A\cos\left(\sigma_l^0\right) - B\sin\left(\sigma_l^0\right)\right] \\ \sin\sigma_l = \frac{1}{N}\left[A\sin\left(\sigma_l^0\right) + B\cos\left(\sigma_l^0\right)\right], \end{cases} \qquad N = \sqrt{A^2 + B^2}, \qquad (25)$$

Figure 1. Total-ionization cross-section of Li by electron impact. The present calculations are performed for ejection of the 2s electrons and denoted by CCC for convergent close-coupling calculations and PWB for plane wave Born approximations, respectively.
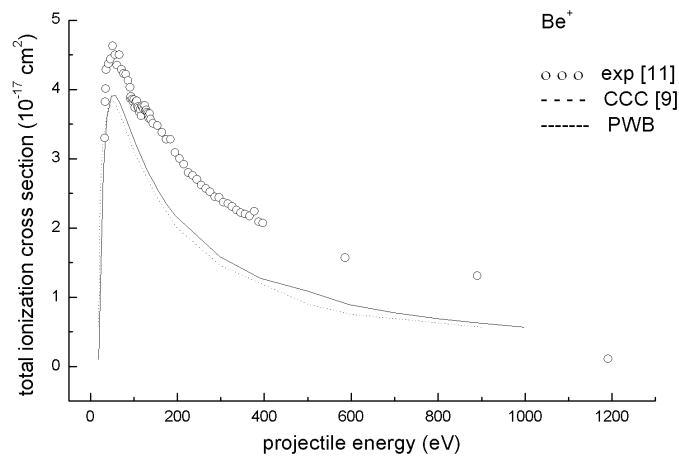
Figure 2. Total-ionization cross-section of Be$^+$ by electron impact. The present calculations are performed for ejection of the 2s electrons and denoted by CCC for convergent close-coupling calculations and PWB for plane wave Born approximations, respectively.

where σ_l^0 is the Coulomb phaseshift [21]

$$\sigma_l^0 = \arg\Gamma(l+1+i\eta), \qquad \eta = -\frac{Z}{\sqrt{2\varepsilon}}. \qquad (26)$$

2.4. Results for lithium-like targets

The results of our calculations for lithium-like targets Li, . . . , O^{5+} are given in figures 1–6. The results are plotted together with experimental data [10–13] and theoretical CCC-based calculations [8]. In figure 1, we present the PWB calculations of the total-ionization

Figure 3. Total-ionization cross-section of B^{2+} by electron impact. The present calculations are performed for ejection of the 2s electrons and denoted by CCC for convergent close-coupling calculations and PWB for plane wave Born approximations, respectively.
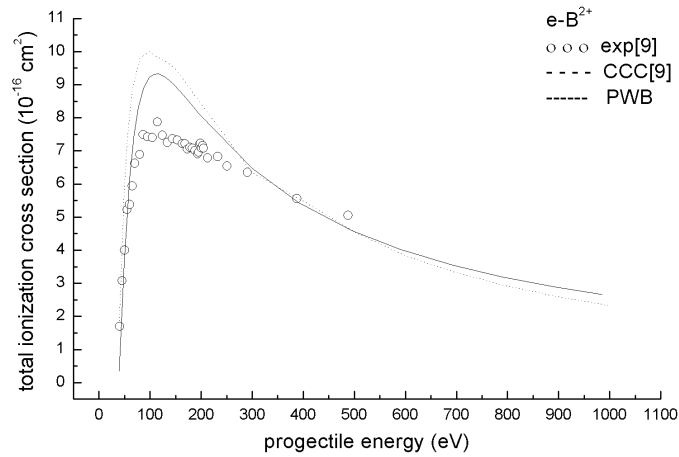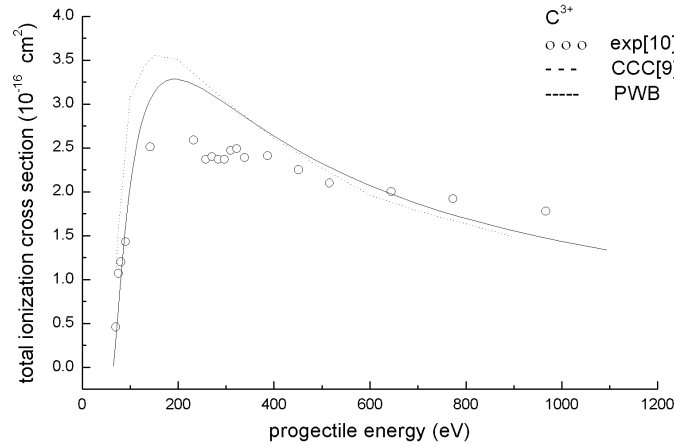

Figure 4. Total-ionization cross-section of C^{3+} by electron impact. The present calculations are performed for ejection of the 2s electrons and denoted by CCC for convergent close-coupling calculations and PWB for plane wave Born approximations, respectively.

cross-section for Li. The contributions of the 2s electrons to total-ionization cross-sections were compared with available experimental data at low energies (<50 eV) [13] and CCC calculations. This comparison indicates that the experimental procedure [13] suffered from experimental difficulties to measure the intensity of the atomic beam [8, 23]. The PWB calculation data are in remarkable agreement with both experiment [23] (not presented in figure 1) and the results of the CCC calculations at projectile energy more than 100 eV.

In our calculations, we took into account the exchange interaction (see W_{ex} in (22)) and orthogonalization the wavefunction of the partial ejected electron wave to the core wavefunction of the target in the final state due to the Lagrange multipliers. Our calculations of electron-impact ionization of Li are presented in table 1, where the state of residual ions is

Figure 5. Total-ionization cross-section of N^{4+} by electron impact. The present calculations are performed for ejection of the 2s electrons and denoted by CCC for convergent close-coupling calculations and PWB for plane wave Born approximations, respectively.
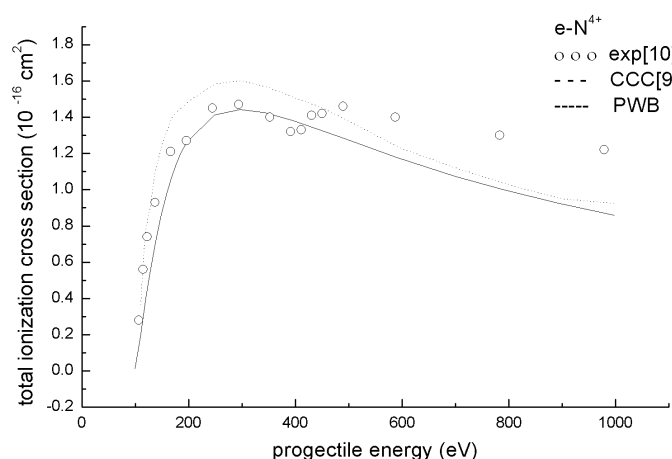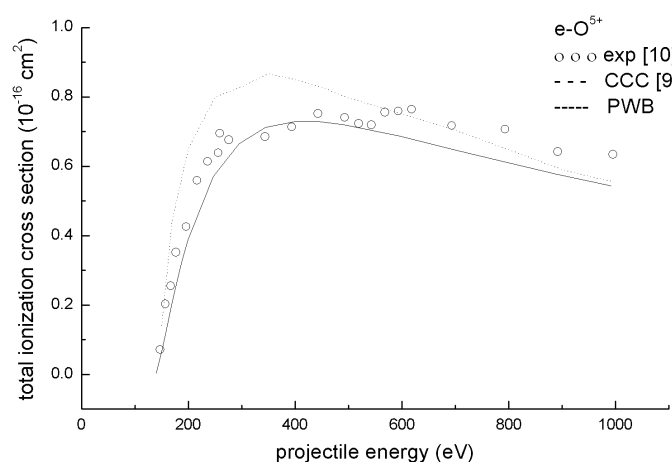

Figure 6. Total-ionization cross-section of O^{5+} by electron impact. The present calculations are performed for ejection of the 2s electrons and denoted by CCC for convergent close-coupling calculations and PWB for plane wave Born approximations, respectively.

$1s^{-1}2$ s. We shall see from this table that the values of cross-section greatly differ, depending on whether relaxation, orthogonalization and exchange were taken into account. For the $1s^2$ final state of the residual ions, the relaxation makes only a small effect on total cross-section of electron-impact ionization and the 'frozen '-core approximation can be successfully used for such calculations.

In figure 2, we present the total-ionization cross-sections for the electron-impact ionization of Be^+. It should be noticed here that results of our calculations are not in good agreement with experimental data. The results of our calculations are closer to those obtained by using the CCC method. Comparison of calculations for B^{2+}, C^{3+}, N^{4+} and O^{5+} gives much more satisfactory, presented in figures 3–6. These results are plotted together with the experimental

Table 1. Calculated total cross-sections (in a_0^2) for electron ionization of Li(1s^2) (residual ion Li^{+*}(1s2s)) are calculated in the 'frozen'-core approximation, σ^-; σ^+ are calculated with allowance for relaxation; σ_{00}, orthogonalization and exchange are disregarded; σ_{01} the calculations with exchange; and σ_{11}, both orthogonalization and exchange are unclouded.

E (eV)	σ_{00}^-	σ_{01}^-	σ_{11}^-	σ_{00}^+	σ_{01}^+	σ_{11}^+
110	0.007	0.006	0.005	0.022	0.018	0.015
120	0.019	0.018	0.016	0.059	0.050	0.044
130	0.035	0.032	0.031	0.101	0.088	0.080
140	0.049	0.046	0.044	0.137	0.121	0.111
150	0.064	0.060	0.059	0.175	0.156	0.145
160	0.081	0.076	0.074	0.212	0.191	0.179
170	0.091	0.086	0.084	0.236	0.213	0.201
180	0.107	0.100	0.099	0.269	0.244	0.231
190	0.116	0.109	0.108	0.289	0.262	0.250
200	0.125	0.118	0.116	0.307	0.279	0.266
300	0.161	0.151	0.150	0.371	0.338	0.327
400	0.157	0.147	0.147	0.352	0.321	0.312
500	0.145	0.136	0.136	0.320	0.291	0.284
700	0.122	0.114	0.115	0.261	0.237	0.232
800	0.113	0.105	0.106	0.236	0.215	0.209
900	0.105	0.098	0.099	0.216	0.197	0.192
1000	0.099	0.092	0.093	0.201	0.183	0.179

Table 2. Calculated total cross-sections (in a_0^2) for the ionization process e$^-$ + A(1s^2) $\rightarrow$ A^{+*}(3s) as functions of the incident electron energy.

E(eV)	$\sigma_{\text{Li}^{+*}}$	$\sigma_{\text{Be}^{+*}}$	$\sigma_{\text{B}^{2+*}}$	$\sigma_{\text{C}^{3+*}}$	$\sigma_{\text{N}^{4+*}}$	$\sigma_{\text{O}^{5*}}$
90	0.001 484 67					
80	0.006 108 18					
100	0.010 904 02					
120	0.015 030 63					
130	0.019 302 52					
140	0.023 465 81					
150	0.027 319 51					
160	0.029 645 96	0.000 01				
170	0.031 746 69	0.000 12				
180	0.033 607 09	0.000 29				
190	0.035 221 73	0.000 44				
200	0.036 592 75	0.000 69				
250	0.037 189 21	0.001 49				
300	0.040 045 57	0.002 13	0.000 03			
350	0.040 343 45	0.002 58	0.000 12			
400	0.039 531 81	0.002 82	0.000 20			
450	0.038 117 27	0.002 98	0.000 28	0.000 005		
500	0.036 669 41	0.003 06	0.000 33	0.000 020		
550	0.035 093 16	0.003 10	0.000 38	0.000 035		
600	0.033 791 35	0.003 10	0.000 42	0.000 048	0.000 0001	
700	0.032 483 61	0.003 05	0.000 47	0.000 073	0.000 0055	
800	0.029 923 68	0.002 95	0.000 50	0.000 093	0.000 0127	0.000 000
900	0.027 509 99	0.002 84	0.000 51	0.000 106	0.000 0191	0.000 001
1000	0.025 551 32	0.002 72	0.000 51	0.000 115	0.000 0244	0.000 003

Table 3. Calculated total cross-sections (in a_0^2) for the ionization process $e^- + A(1s^2) \rightarrow A^{+*}(2s)$ as functions of the incident electron energy.

E (eV)	$\sigma_{Li^{+*}}$	$\sigma_{Be^{+*}}$	$\sigma_{B^{+2*}}$	$\sigma_{C^{+3*}}$	$\sigma_{N^{+4*}}$	$\sigma_{O^{+5*}}$
70	0.007					
80	0.031					
90	0.055					
100	0.075					
110	0.096					
120	0.116					
130	0.134					
130	0.144	0.0002				
150	0.153	0.0022				
160	0.161	0.0053				
170	0.168	0.0089				
180	0.175	0.0143				
200	0.179	0.0179				
250	0.184	0.0299	0.0004			
300	0.181	0.0376	0.0034			
350	0.174	0.0424	0.0065			
400	0.165	0.0452	0.0093	0.0004		
450	0.157	0.0463	0.0113	0.0012		
500	0.151	0.0467	0.0128	0.0021		
550	0.142	0.0465	0.0138	0.0030	0.0001	
600	0.136	0.0459	0.0147	0.0037	0.0003	
700	0.124	0.0443	0.0156	0.0049	0.0010	
800	0.114	0.0423	0.0159	0.0057	0.0016	0.000 19
900	0.105	0.0403	0.0159	0.0061	0.0020	0.000 45
1000	0.097	0.0382	0.0158	0.0065	0.0024	0.000 70

data and CCC calculations and yet the total cross-sections are in reasonable agreement. These results were obtained with nine terms in the partial wave expansion (9) of the ejected electron wavefunction.

3. Conclusions

The plane wave first Born approximation presented in section 2 provides consistently good results for all elements studied. We demonstrated that the use of the multiconfigurational Hartree–Fock wavefunctions will improve the agreement between calculations and experimental total-ionization cross-sections. The exchange effect and orthogonalization of the atomic radial functions to ejected electron wavefunctions have been taken into account. It has been shown that the relaxation of core orbitals of the ground state of the residual ion produces a slight effect on the total-ionization cross-section, and the 'frozen'-core approximation can be successfully used. The relaxation effect noticeably modifies the value of the total cross-section, in cases where the residual ion is in the excited state ($1s^{-1}$ 2s).

For Li-like targets good agreement was obtained with experimental data for N^{4+} and O^{5+}; the PWB approximation and (CCC) results for C^{3+} are larger than those for the experiment by an amount increasing from threshold to about 12% (23%) cross-section at peak. We also present in tables 2–4 the computed total cross-sections results for excited (3s, 2s and 2p) final state of the target. Availability of the experimental data for ionization by electron impact

Table 4. Calculated total cross-sections (in a_0^2) for the ionization process $e^- + A(1s^2) \rightarrow A^{+*}(2p)$ as functions of the incident electron energy.

E (eV)	$\sigma_{Li^{+*}}$	$\sigma_{Be^{+*}}$	$\sigma_{B^{2+*}}$	$\sigma_{C^{3+*}}$	$\sigma_{N^{4+*}}$	$\sigma_{O^{5+*}}$
80	0.000 005					
90	0.000 020					
100	0.000 054					
110	0.000 098					
120	0.000 137					
130	0.000 212					
140	0.000 273					
150	0.000 342	0.000 0001				
160	0.000 458	0.000 0004				
165	0.000 500	0.000 0011				
175	0.000 587	0.000 0027				
190	0.000 679	0.000 0047				
200	0.000 774	0.000 0066				
250	0.001 116	0.000 0264				
300	0.001 445	0.000 0513	0.000 0005			
350	0.001 699	0.000 0788	0.000 0020			
400	0.001 884	0.000 1048	0.000 0043			
450	0.002 073	0.000 1316	0.000 0073	0.000 0001		
500	0.002 179	0.000 1536	0.000 0105	0.000 0003		
550	0.002 291	0.000 1748	0.000 0141	0.000 0007		
600	0.002 364	0.000 1947	0.000 0175	0.000 0011	0.000 000 01	
700	0.002 473	0.000 2233	0.000 0245	0.000 0023	0.000 000 11	
800	0.002 534	0.000 2476	0.000 0301	0.000 0036	0.000 000 30	
900	0.002 568	0.000 2652	0.000 0355	0.000 0049	0.000 000 57	0.000 000 03
1000	0.002 581	0.000 2796	0.000 0399	0.000 0062	0.000 000 86	0.000 000 08

of the lithium-like targets with simultaneous excitations of residual ions can benefit further theoretical studies.

Acknowledgments

Appendix

The matrix element of the operator $\hat{A}_{KQ}$ can be written in the form

$$\langle L_f M_f lm|\hat{A}_{KQ}|L_i M_i\rangle = \sum_{LM} C^{LM}_{L_f M_f, lm}\langle (L_f l)LM|\hat{A}_{KQ}|L_i M_i\rangle \tag{A.1}$$

Using the Wigner–Eckart theorem, we obtain

$$\langle L_f M_f lm|\hat{A}_{KQ}|L_i M_i\rangle = \sum_{LM} C^{LM}_{L_f M_f, lm} C^{LM}_{L_i M_i, KQ} \frac{\langle (L_f l)L\|\hat{A}_K\|L_i\rangle}{\sqrt{2L+1}}. \tag{A.2}$$

Taking into account the following relation for the Clebsh–Gordan coefficients [24]

$$C^{LM}_{L_f M_f, lm} C^{LM}_{L_i M_i, KQ} = \sum_{IM_I} (-1)^{l+L+L_f+K-Q} \frac{(2L+1)\sqrt{2I+1}}{\sqrt{2L_i+1}}$$

$$\times C^{IM_I}_{lm,K-Q} C^{L_i M_i}_{L_f M_f, IM_I} \begin{Bmatrix} K & l & I \\ L_i & L_f & L \end{Bmatrix}, \tag{A.3}$$

we obtain

$$\langle L_f M_f lm | \hat{A}_{KQ} | L_i M_i \rangle = \sum_{IM_I} (-1)^{K-Q} C^{IM_I}_{lm,K-Q} C^{L_i M_i}_{L_f M_f, IM_I} \langle L_f l \| \hat{T}^K_I \| L_i \rangle, \tag{A.4}$$

where

$$\langle L_f l \| \hat{T}^K_I \| L_i \rangle = \sum_L (-1)^{l+L+L_f} \frac{\sqrt{(2L+1)(2I+1)}}{\sqrt{2L_i+1}} \begin{Bmatrix} K & l & I \\ L_i & L_f & L \end{Bmatrix} \langle (L_f l) L \| \hat{A}_K \| L_i \rangle. \tag{A.5}$$

Multiplying both parts of equation (A.4) on C^{lm}_{KQ, IM_I} and summing over m and Q, one can obtain

$$\langle L_f l \| \hat{T}^K_I \| L_i \rangle = \frac{1}{C^{L_i M_i}_{L_f M_f, IM_I}} \sum_{mQ} (-1)^{K-Q} C^{IM_I}_{lm,K-Q} \langle L_f M_f lm | \hat{A}_{KQ} | L_i M_i \rangle. \tag{A.6}$$

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