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ELECTRON IMPACT DOUBLE IONIZATION OF HELIUM-LIKE IONS IN THE METASTABLE STATES

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ABSTRACT. For the first time total cross sections for double ionization of two-electron atomic systems He, Li^{+}, Be^{2+}, B^{3+} and C^{4+} being in the 2^1S and 2^3S metastable states are calculated within the framework of the shake-off model. Only radial correlation between the target electrons is taken into account and repulsion between the ejected electrons is ignored.

1. INTRODUCTION

Double ionization of helium and helium-like ions has been a subject of intensive theoretical and experimental studies for recent years. The reason is that the consideration of the simplest atomic systems ─ the members of the helium isoelectronic sequence ─ is the most effective tool for exploring the dynamics of double ionization and, in this way, to study the role of electron-electron correlation in atoms and ions.

In the experimental studies of ionization processes, the crossing beam technique is generally used [1]. For helium, the target beam is formed at room or even lower temperatures [2]. Therefore, one may suppose that all the helium atoms of the parent beam are kept in the ground state. However, for ion beams, the situation is quite different: depending on the method of formation of the parent beam, the population of long-lived excited states in it can be significant. Ions formed in metastable states are frequently observed in various plasmas and, in particular, in ion sources [3,4]. Due to their large lifetime, such particles can easily survive along the path from the source to the collision region and contribute to the ionization signal. As a consequence, it is easily understood that the population of the excited metastable states may play an important role in many collision

experiments. This role was observed in single ionization experiments, in particular for electron energies below the ground state ionization threshold [5]. These observations were confirmed by the theory [6]. It was also found that ions being in the metastable states might play a remarkable role in double ionization experiments [7].

It is worth noting that the same situation arises when an He^+ ion beam passes through a gas target in order to form an He atom beam by charge exchange [8,9]. Consequently, in order to interpret the experimental results correctly one needs to take into account all the states (ground and excited) presented in the parent beam. In order to estimate the respective role of these states in the double ionization (DI) process, it is necessary to know the corresponding cross sections.

In a series of three recent papers, within the framework of shake-off mechanism the first order contribution was analyzed in the case of electron impact DI of two-electron atomic systems, assuming that these systems are in their ground state. In the first paper [10] the fully (eightfold) differential cross section was calculated using plane waves for the incident and scattered electrons, the Hylleraas-type wavefunction (with radial correlation only) for the bound electrons and the Coulomb double-continuum wavefunction for the ejected electrons. The use of relatively simple wavefunctions allowed us to calculate the eightfold and fourfold differential cross sections analytically. The further integration of the fourfold differential cross section has been performed numerically and the total cross sections (TCS) were obtained for the members of helium isoelectronic sequence from $H^-(Z = 1)$ to $N^{5+}(Z = 7)$ [11]. The calculated values of TCS are found to be in fair agreement with the available experimental data for He and Li^+. In the third paper [12] the coefficients of the asymptotic formula for the TCS in the Bethe-Born approximation are determined.

In the present paper the scheme developed for the ground state two-electron systems is extended to both the 2^1S and 2^3S excited metastable states. To the best of the author's knowledge, the Born approximation has not been applied to the calculation of total DI cross section for any atom or ion in excited states. (In their recent paper Muktavat and Srivastava [13] calculated the fully differential cross

sections for DI of helium being in the 2^1S and 2^3S metastable states.) Again, only radial correlation between the bound electrons is taken into account in the present calculation. The fully differential cross section is obtained in an analytical form and it is integrated numerically in order to obtain the TCS.

The paper is organized as follows. After determining the goal of the present study (section 1), we give briefly the theory of double ionization process for helium-like ions in the metastable states (section 2). In section 3 we present the result of calculations and discuss the obtained cross sections. Atomic units (e = m = ħ = 1) will be used throughout this paper.

2. THEORY

The eightfold differential cross section (8DCS) for double ionization of helium-like ions is given as

$$\frac{d^8\sigma^{(\pm)}}{d\Omega_s d\Omega_1 d\Omega_2 d(k_1^2/2) d(k_2^2/2)} = \frac{(2\pi)^4 k_s k_1 k_2}{k_i} \left| T_{fi}^{(\pm)} \right|^2 . \qquad (1)$$

Here $\vec{k}_i, \vec{k}_s, \vec{k}_1, \vec{k}_2$ are the wavevectors of the incident, scattered and ejected electrons respectively, $d\Omega$ denotes the element of solid angle surrounding the corresponding wavevector, $T_{fi}^{(\pm)}$ represents the matrix element given by

$$T_{fi}^{(\pm)} = \int \Psi_f^{(\pm)^*} V_i \Psi_i^{(\pm)} d\vec{r} d\vec{r}_1 d\vec{r}_2 , \qquad (2)$$

where $\Psi_i^{(\pm)}$ and $\Psi_f^{(\pm)}$ are the wavefunctions of the colliding system in the initial and final states, respectively; V_i describes the interaction between the incident electron and a target

$$V_i = -\frac{Z}{r} + \frac{1}{|\vec{r} - \vec{r}_1|} + \frac{1}{|\vec{r} - \vec{r}_2|}. \qquad (3)$$

In (1) and (2) the unlike signs $(\pm)$ indicate that the total spin of the two bound electrons is zero or one, i.e. the target is in the 2^1S or 2^3S metastable states, respectively.

As noted above our scheme is based on an analytical calculation of the 8DCS. For this we employ the relatively simple wavefunctions. Namely, we describe the initial and final states of the colliding system by the following wavefunctions:

$$\Psi_i^{(\pm)}(\vec{r}, \vec{r}_1, \vec{r}_2) = \varphi_{\vec{k}_i}(\vec{r})\Phi_i^{(\pm)}(\vec{r}_1, \vec{r}_2) \qquad (4)$$

$$\Psi_f^{(\pm)}(\vec{r}, \vec{r}_1, \vec{r}_2) = \varphi_{\vec{k}_s}(\vec{r})\left[\Phi_f^{(\pm)}(\vec{r}_1, \vec{r}_2) - S^{(\pm)}\Phi_i^{(\pm)}(\vec{r}_1, \vec{r}_2)\right]. \qquad (5)$$

Here $\varphi_{\vec{k}_i} = e^{i\vec{k}_i\vec{r}}/(2\pi)^{3/2}$ and $\varphi_{\vec{k}_s} = e^{i\vec{k}_s\vec{r}}/(2\pi)^{3/2}$ are the plane waves describing the incident and scattered electrons, respectively, $\Phi_i^{(\pm)}(\vec{r}_1, \vec{r}_2)$ is the wavefunction of the bound electrons in the target, $\Phi_f^{(\pm)}$ is the wavefunction of the ejected electrons and $S^{(\pm)} = \left\langle \Phi_i^{(\pm)} \middle| \Phi_f^{(\pm)} \right\rangle$ is the overlap integral, which provides the orthogonalization of the double-continuum wavefunction $\Phi_f^{(\pm)}$ with respect to the target wavefunction $\Phi_i^{(\pm)}$.

The bound state wavefunctions $\Phi_i^{(+)}(\vec{r}_1, \vec{r}_2)$ and $\Phi_i^{(-)}(\vec{r}_1, \vec{r}_2)$ representing the initial target states and describing the metastable singlet state 2^1S and the metastable triplet state 2^3S, respectively, are chosen in the form:

$$\Phi^{(\pm)}(\vec{r}_1, \vec{r}_2) = C_i^{(\pm)}\left[e^{-\alpha r_1}e^{-\beta r_2}(1 - \gamma r_2) \pm e^{-\alpha r_2}e^{-\beta r_1}(1 - \gamma r_1)\right]. \qquad (6)$$

Here $C_i^{(\pm)}$ is a normalization constant; α, β, γ are the variational parameters, which have been calculated following the procedure suggested by Hylleraas and Undheim [14]. For the 2^1S and 2^3S metastable states of He, Li^+, Be^{2+}, B^{3+} and C^{4+} the obtained values of α, β, γ parameters together with the corresponding DI energies are presented in Table 1.

Table 1. Variational parameters and DI energies for 2^1S and 2^3S metastable and 1^1S ground states of He, Li^+, Be^{2+}, B^{3+} and C^{4+}

		α	**β**	**γ**	$\mathbf{I_{theor}}$	$\mathbf{I_{exp}}$
He (Z=2)	2^1S	1.997	0.558	0.682	2.1429	2.1460
	2^3S	2.003	0.633	1.429	2.1742	2.1752
	1^1S	2.214	1.442	-0.396	2.8762	2.9036
Li^+ (Z=3)	2^1S	2.985	1.061	1.192	5.0347	5.0408
	2^3S	3.005	1.142	1.881	5.1094	5.1104
	1^1S	3.332	2.399	-0.454	7.2492	7.2798
Be^{2+}(Z=4)	2^1S	3.977	1.566	1.698	9.1768	9.1842
	2^3S	4.006	1.645	2.370	9.2956	9.2965
	1^1S	4.429	3.351	-0.492	13.6233	13.6560
B^{3+} (Z=5)	2^1S	4.971	2.070	2.203	14.5691	14.5777
	2^3S	5.007	2.146	2.866	14.7322	14.7350
	1^1S	5.515	4.305	-0.524	21.9978	22.0325

	2^1S	5.96	2.57	2.705	21.2117	21.2211
$C^{4+}(Z=6)$	2^3S	7	3	3.364	21.4128	21.4203
	1^1S	6.00	2.64	-0.549	32.3725	32.4089
		7	7			
		6.59	5.26			
		1	0			

The wavefunction $\Phi_f^{(\pm)}$ describing the ejected electrons in the final state is taken in the following form:

$$\Phi_f^{(\pm)}(\vec{r}_1,\vec{r}_2)=\frac{1}{\sqrt{2}}\left[f_{k_1}^{\vec{r}}(\vec{r}_1)f_{k_2}^{\vec{r}}(\vec{r}_2)\pm f_{k_1}^{\vec{r}}(\vec{r}_2)f_{k_2}^{\vec{r}}(\vec{r}_1)\right], \tag{7}$$

where $f_k^{\vec{r}}(\vec{r})$ is the Coulomb continuum wavefunction normalized to a delta function in momentum space.

Substituting wavefunctions of the initial and final states (4-7) into (2) and performing the integration over $\vec{r},\vec{r}_1,\vec{r}_2$ the matrix element can be written as

$$T_{fi}^{(\pm)}=\frac{C_i^{(\pm)}}{\sqrt{2}\pi^2q^2}\left\{I_\alpha^{(0)}(\vec{k}_1)\left[J_\beta^{(0)}(k_2)-\gamma\, J_\beta^{(1)}(k_2)\right]\pm\right.$$
$$\left.\pm\left[I_\beta^{(0)}(\vec{k}_1)-\gamma\, I_\beta^{(1)}(\vec{k}_1)\right]J_\alpha^{(0)}(k_2)\right\}\pm\vec{k}_1\Leftrightarrow\vec{k}_2, \tag{8}$$

where

$$I_\mu^{(n)}(\vec{k}_j)=\int f_{k_j}^{*}(\vec{r})\left(e^{i\vec{q}\vec{r}}-\frac{1}{2}G^{(\pm)}\right)e^{-\mu r}r^n d\vec{r}=$$

$$=\frac{1}{(2\pi)^{3/2}}\Gamma\left(1-iZ/k_j\right)e^{\pi Z/2k_j}A_\mu^{(n)}(\vec{k}_j) \tag{9}$$

$$J_\nu^{(n)}(k_j) = \int f_{k_j}^{\vec{r}\,*}(\vec{r}) e^{-\nu r} r^n d\vec{r} = \frac{1}{(2\pi)^{3/2}} \Gamma\left(1 - iZ/k_j\right) e^{\pi Z/2k_j} B_\gamma^{(n)}(\vec{k}_j)$$

$$G^{(\pm)} = \int \Phi_i^{(\pm)*}(\vec{r}_1, \vec{r}_2)(e^{i\vec{q}\vec{r}_1} + e^{i\vec{q}\vec{r}_2}) \Phi_i^{(\pm)}(\vec{r}_1, \vec{r}_2) d\vec{r}_1 d\vec{r}_2$$

and $\vec{q} = \vec{k}_i - \vec{k}_s$ is the momentum transfer. The explicit expressions for $A_\mu^{(n)}(\vec{k}_j), B_\nu^{(n)}(\vec{k}_j)$ (n = 0,1) and $G^{(\pm)}, C_i^{(\pm)}$ are given in appendix.

Formula (8) shows that, when only radial correlation between target electrons is taken into account, the matrix element $T_{fi}^{(\pm)}$ may be represented as a sum of four terms, each of them being the product of two factors $I_\mu(\vec{k}_j)$ and $J_\nu(k_j)$. Here $I_\mu(\vec{k}_j)$ describes the direct ejection of a bound electron by the incident electron and $J_\nu(k_j)$ describes ionization of the second target electron due to the sudden change in potential. Now substituting (8) into (1) and taking into consideration (9) we obtain for the 8DCS corresponding to DI of helium-like ions in the 2^1S and 2^3S metastable states

$$\frac{d^8\sigma^{(\pm)}}{d\Omega_s d\Omega_1 d\Omega_2 d(k_1^2/2) d(k_2^2/2)} =$$

$$= \frac{Z^2 \left[C_i^{(\pm)}\right]^2 N(k_1, k_2) k_s}{2\pi^4 q^4 k_i} \left[M_I^{(\pm)} + M_{II}^{(\pm)} + M_{int}^{(\pm)}\right], \qquad (10)$$

where

$$N(k_1, k_2) = \left[\left(1 - e^{-2\pi Z/k_1}\right)\left(1 - e^{-2\pi Z/k_2}\right)\right]^{-1} \qquad (11)$$

$$M_{I}^{(\pm)} = \left|A_{\alpha}^{(0)}(\vec{k}_1)\right|^2 \left(B_{\beta}^{(0)}(k_2) - \gamma B_{\beta}^{(1)}(k_2)\right)^2 \pm \mathrm{Re}\left[A_{\alpha}^{(0)}(\vec{k}_1) A_{\alpha}^{(0)*}(\vec{k}_2)\right] \times$$

$$\times \left(B_{\beta}^{(0)}(k_1) - \gamma B_{\beta}^{(1)}(k_1)\right)\left(B_{\beta}^{(0)}(k_2) - \gamma B_{\beta}^{(1)}(k_2)\right) + \vec{k}_1 \Leftrightarrow \vec{k}_2$$

$$M_{II}^{(\pm)} = \left|A_{\beta}^{(0)}(\vec{k}_1) - \gamma A_{\beta}^{(1)}(\vec{k}_1)\right|^2 \left(B_{\alpha}^{(0)}(k_2)\right)^2 \pm$$

$$\pm \mathrm{Re}\left[\left(A_{\beta}^{(0)}(\vec{k}_1) - \gamma A_{\alpha}^{(1)}(\vec{k}_1)\right)\left(A_{\beta}^{(0)}(\vec{k}_2) - \gamma A_{\alpha}^{(1)}(\vec{k}_2)\right)^*\right] \times$$

$$\times B_{\alpha}^{(0)}(k_1) B_{\alpha}^{(0)}(k_2) + \vec{k}_1 \Leftrightarrow \vec{k}_2 \qquad (12)$$

$$M_{\mathrm{int}}^{(\pm)} = 2\,\mathrm{Re}\left[A_{\alpha}^{(0)}(\vec{k}_1)\left(A_{\beta}^{(0)}(\vec{k}_2) - \gamma A_{\beta}^{(1)}(\vec{k}_2)\right)^*\right] \times$$

$$\times B_{\alpha}^{(0)}(k_1)\left(B_{\beta}^{(0)}(k_2) - \gamma B_{\beta}^{(1)}(k_2)\right) \pm$$

$$\pm 2\,\mathrm{Re}\left[A_{\alpha}^{(0)}(\vec{k}_1)\left(A_{\beta}^{(0)}(\vec{k}_1) - \gamma A_{\beta}^{(1)}(\vec{k}_1)\right)^*\right] \times$$

$$\times B_{\alpha}^{(0)}(k_2)\left(B_{\beta}^{(0)}(k_2) - \gamma B_{\beta}^{(1)}(k_2)\right) + \vec{k}_1 \Leftrightarrow \vec{k}_2$$

In (10) the first term corresponds to direct ejection of an electron from inner-shell (1s) and the subsequent ejection of outer-shell (2s) electron due to the sudden change in potential (process I). The second term corresponds to direct ejection of an electron from outer-shell (2s) followed by ejection of the electron from inner-shell (1s) (process II). The third term in (10) describes the interference between these two processes.

The total DI cross section can be obtained by integrating the 8DCS over the solid angles $\Omega_1, \Omega_2, \Omega_s$ and the ejection energies $\varepsilon_1 = k_1^2/2$ and $\varepsilon_2 = k_2^2/2$

$$\sigma^{(\pm)}(E_i) = \frac{Z^2\left[C_i^{(\pm)}\right]^2}{2\pi^4 k_i} \int_0^{\varepsilon_{1max}} \int_0^{\varepsilon_{2max}} N(k_1 k_2) k_s \times$$

$$\times \iint \left[M_I^{(\pm)} + M_{II}^{(\pm)} + M_{int}^{(\pm)}\right] d\Omega_1 d\Omega_2 \frac{d\Omega_s}{q^4} d\varepsilon_1 d\varepsilon_2 \qquad (13)$$

Here $\varepsilon_{1max} = \left(E_i - I^{(\pm)}\right)/2$ and $\varepsilon_{2max} = \left(E_i - I^{(\pm)}\right)/2 - \varepsilon_1$, where $E_i = k_1^2/2$ and $I^{(\pm)}$ is the DI potential of electrons in helium-like ions. About the choice of the upper limits of integration in (full curves) see comment in [11].

3. RESULTS AND DISCUSSION

Using formulae (11-13) we have calculated the total DI cross section for two-electron atomic systems from He (Z = 2) to C^{4+} (Z = 6) being in the 2^1S and 2^3S metastable states. The calculations have been carried out for incident energies extending up to a maximum 150 times the DI threshold. The results for He, Li^+ and C^{4+} are presented in Figures 1, 2 and 3 (full curves).

Before analysing the obtained cross section let us estimate the contributions of process I and process II to double-electron ejection. From the explicit expressions for the matrix elements (formulae {A1} and {A2} in appendix) it is clear that

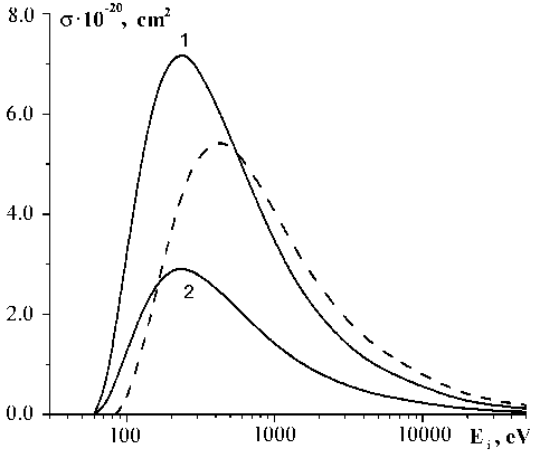

Fig.1. The total cross sections for DI of helium atoms by electrons. Curves 1 and 2 correspond to 2^1S and 2^3S metastable states, respectively. The dashed curve corresponds to the ground state.

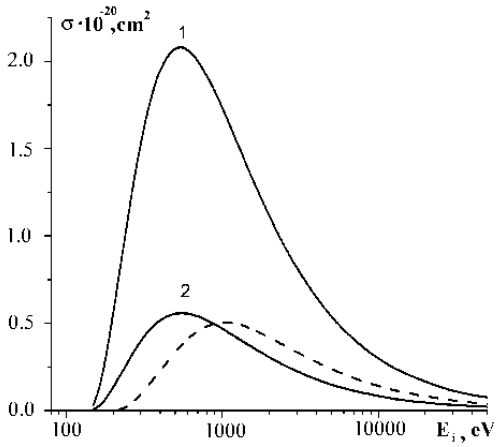

Fig.2. The total cross sections for DI of Li^+ ions by electrons. Curves 1 and 2 correspond to 2^1S and 2^3S metastable states, respectively.

The dashed curve corresponds to the ground state.

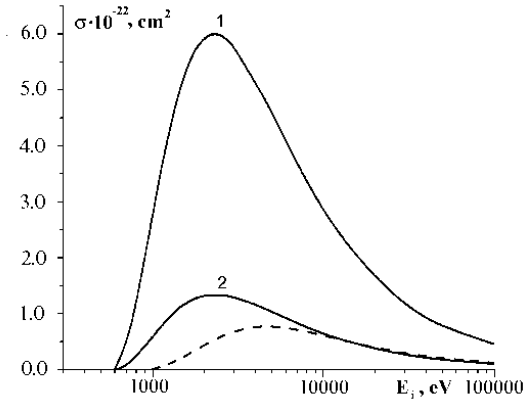

Fig.3. The total cross sections for DI of C^{4+} ions by electrons. Curves 1 and 2 correspond to 2^1S and 2^3S metastable states, respectively. The dashed curve corresponds to the ground state.

$$B_{\alpha}^{(0)}(k_j) \sim (Z-\alpha) \tag{14}$$

$$B_{\beta}^{(0)}(k_j) - \gamma B_{\beta}^{(1)}(k_j) \sim \left\{ \frac{Z-\beta-\gamma}{Z-\beta} + 2\gamma \frac{(Z-2\beta)}{\beta^2 + k_j^2} \right\} \tag{15}$$

It means that after direct ejection of one of the bound electron the probability of a second ionization is proportional to $(Z-\alpha)^2$ for the inner-shell electron and to the square of expression in curly brackets in (15) for the outer-shell electron. Taking into consideration that $\alpha \cong Z$ (see Table1) one can easily determine that the probability of relaxation to continuum is much less for the inner-shell electron than for the outer-shell one. This fact allows us to draw the conclusion that though direct ejection is more probable for the outer-shell electron

than for the inner-shell one, nevertheless process I plays dominant role. The numerical calculations confirm this conclusion. For instance, in the case of He the contribution of process I is nearly three order of magnitude larger than the contribution of process II for both the singlet and the triplet states. Therefore we can neglect process II in the further analysis.

It is worth to note that when $\beta = \gamma = Z/2$, the expression in curly brackets in (15) is equal to zero and process I does not occur as it should be. Indeed, in this case the outer-shell electron is described by the non-correlated hydrogen-like 2S wavefunction (see formula (6)), therefore the probability of the relaxation of this electron to the continuum equals zero. Similarly, when $\alpha = Z$, the inner-shell electron is described by the non-correlated hydrogen-like 1S wavefunction and, accordingly, process II fails.

It is clear from Figures 1-3 that the total cross section corresponding to the singlet state is larger in magnitude than the TCS corresponding to the triplet state. The difference between the maximum values of TCS increases from 2.5 for He to 4.5 for C^{4+}. Because the values of α parameters for the singlet and triplet states are close the probabilities of direct ejection of the inner-shell electron are almost the same for the both states. It means that the difference between the TCS is completely determined by the difference between the probabilities of relaxation of the outer-shell electron to the continuum. The latter is less for the triplet states than for the singlet state. This statement can be easily shown by analyzing the expression in curly brackets in (15). Indeed, in (15) the second term is of the order of one for the both states. As for the first term it is of the order of one for the singlet state, while owing to the closeness of the sum $\beta + \gamma$ to Z (see Table 1) it is very small for the triplet state.

The method suggested by Hylleraas and Undheim [14] allows us to calculate simultaneously the wavefunction of the 1^1S ground state and the wavefunction of the 2^1S metastable states. (The lowest root of the equation for energy gives the variational parameters for the ground state, while the next root corresponds to the metastable state.) Results obtained for α, β, γ and DI energies are presented in Table 1 for He, Li^+,...C^{4+}. As it can be seen in Table 1 parameter γ is negative

for all the targets being in the ground state. Accordingly the relevant wavefunctions are nodeless as it should be. We emphasize that such a procedure for constructing the wavefunctions ensures the mutual orthogonality of the wavefunctions corresponding to the ground and 2^1S metastable states.

The total DI cross section calculated for He, Li^+, C^{4+} being in the ground state are also shown in Figures 1,2 and 3 (dashed curves). It is clear from the figures that for all targets except helium maximum values of the TCS corresponding to the ground state are less than those corresponding to the metastable states. For helium the ground state maximum is between the two maxima corresponding to the singlet and triplet metastable states.

Recently the total DI cross section has been measured for C^{4+} ions in the keV energy region [7]. The experiment has been carried out at an electron-ion crossed-beam set-up using an electron-cyclotron-resonance ion source. An appreciable fraction of the ion beam was found to be in the 2^3S metastable state (about 8%) owing to the small lifetime of the 2^1S metastable state.

Assuming that the population of the ground state and of the 2^3S metastable state are 0.92 and 0.08, respectively, and using the calculated values for the cross sections corresponding to each component in the ion beam we obtain for the apparent cross section $\sigma_{app} = 0.6\times10^{-23}cm^2$ at 1000 eV incident electron energy. The experimentally measured value at that energy is $\sigma_{app} = 2.6\times10^{-23}\ cm^2$. Taking in the view that the region of validity of the first Born approximation is far away from the above mentioned energy (which only a little exceeds the DI potential for the ground state) one can conclude that there is satisfactory agreement between theory and experiment.

Thus, in order to check the reliability of results obtained in the present study it is necessary to carry out the systematic measurements of total DI cross sections for helium-like ions in the medium and especially in the high energy region.

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APPENDIX

The explicit analytical expressions for $B_\mu^{(n)}(k_j)$ and $A_\mu^{(n)}(\vec{k}_j)$ (n = 0, 1) are

$$B_\mu^{(0)}(k_j) = -8\pi \frac{Z-\nu}{\left(\mu^2+k_j^2\right)^2} e^{-\frac{Z}{k_j}\operatorname{arctg}\frac{2\mu k_j}{\mu^2-k_j^2}}, \tag{A.1}$$

$$B_\mu^{(1)}(k_j) = \left[\frac{1}{Z-\mu} - \frac{2(Z-2\mu)}{\mu^2+k_j^2}\right] B_\mu^{(0)}(k_j), \tag{A.2}$$

$$A_\mu^{(n)}(\vec{k}_j) = \left[\frac{a_\mu(q,k_j)}{\left(\mu^2+q^2+k_j^2-2qk_jx_j\right)^2} d_\mu^{(n)}(x_j) - \frac{1}{2} G^{(\pm)}(q) B_\mu^{(n)}(k_j)\right] +$$

$$+i\left[\frac{a_\mu(q,k_j)}{\left(\mu^2+q^2+k_j^2-2qk_jx_j\right)^2} h_\mu^{(n)}(x_j)\right]. \tag{A3}$$

In the formulae given above $x_j = \cos\vartheta_j$, where ϑ_j is the angle between $\vec{q}$ and the wavevector $\vec{k}_j$.

The functions $a_\mu(q,k_j)$, end $d_\mu^{(n)}(x_j), h_\mu^{(n)}(x_j)$ in (A.3) are determined as follows:

$$a_\mu(q,k_j) = -\frac{8\pi}{\left[\mu^2 + \left(q+k_j\right)^2\right]\left[\mu^2 + \left(q-k_j\right)^2\right]} e^{-\frac{Z}{k_j}\operatorname{arctg}\frac{2\mu k_j}{\mu^2+q^2-k_j^2}},$$

(A.4)

$$d_\mu^{(0)}(x_j) = \left[\left(\mu^2+q^2-k_j^2\right)w_\mu^{(1)}(x_j) - 4\mu^2 k_j w_\mu^{(2)}(x_j)\right]\cos\chi_\mu(x_j) -$$

$$-2\mu\left[\left(\mu^2+q^2-k_j^2\right)w_\mu^{(2)}(x_j) + k_j w_\mu^{(1)}(x_j)\right]\sin\chi_\mu(x_j), \qquad \text{(A.5)}$$

$$h_\mu^{(0)}\left(x_j\right) = \left[\left(\mu^2+q^2-k_j^2\right)w_\mu^{(1)}(x_j) - 4\mu^2 k_j w_\mu^{(2)}(x_j)\right]\sin\chi_\mu(x_j) +$$

$$+2\mu\left[\left(\mu^2+q^2-k_j^2\right)w_\mu^{(2)}(x_j) + k_j w_\mu^{(1)}(x_j)\right]\cos\chi_\mu(x_j), \qquad \text{(A.6)}$$

where

$$w_\mu^{(1)}(x_j) = 2Zqk_jx_j - q^2(Z+\mu) + (Z-\mu)(\mu^2-k_j^2),$$
$$w_\mu^{(2)}(x_j) = Zqx_j - (Z-\mu)k_j,$$

$$\chi_\mu(x_j) = \frac{Z}{k_j}\ln\frac{\mu^2+q^2+k_j^2-2qk_jx_j}{\sqrt{\left(\mu^2+q^2-k_j^2\right)^2+\left(2\mu k_j\right)^2}},$$

and

$$d_{\mu}^{(1)}(x_j)=\left[\frac{2Z\left(q^2-k_j^2-\mu^2\right)+4\mu\left(\mu^2+q^2+k_j^2\right)}{\left(\mu^2+\left(q+k_j\right)^2\right)\left(\mu^2+\left(q-k_j\right)^2\right)}+\right.$$

$$\left.+\frac{4\mu}{\mu^2+q^2+k_j^2-2qk_jx_j}\right]d_{\mu}^{(0)}(x_j)+$$

$$+\frac{2\mu Z}{k_j}\left[\frac{1}{\mu^2+q^2+k_j^2-2qk_jx_j}-\frac{\mu^2+q^2+k_j^2}{\left(\mu^2+\left(q+k_j\right)^2\right)\left(\mu^2+\left(q-k_j\right)^2\right)}\right]\times$$

$$\times h_{\mu}^{(0)}(x_j)+Q_{\mu}(x_j)\sin\chi_{\mu}(x_j)-R_{\mu}(x_j)\cos\chi_{\mu}(x_j), \qquad (A.7)$$

$$h_{\mu}^{(1)}(x_j)=\left[\frac{2Z\left(q^2-k_j^2-\mu^2\right)+4\mu\left(\mu^2+q^2+k_j^2\right)}{\left(\mu^2+\left(q+k_j\right)^2\right)\left(\mu^2+\left(q-k_j\right)^2\right)}+\right.$$

$$\left.+\frac{4\mu}{\mu^2+q^2+k_j^2-2qk_jx_j}\right]h_{\mu}^{(0)}(x_j)-\frac{2\mu Z}{k_j}\times$$

$$\times\left[\frac{1}{\mu^2+q^2+k_j^2-2qk_jx_j}-\frac{\mu^2+q^2+k_j^2}{\left(\mu^2+\left(q+k_j\right)^2\right)\left(\mu^2+\left(q-k_j\right)^2\right)}\right]d_{\mu}^{(0)}(x_j)$$

$$-R_{\mu}(x_j)\sin\chi_{\mu}(x_j)-Q_{\mu}(x_j)\cos\chi_{\mu}(x_j), \qquad (A.8)$$

$$Q_\mu(x_j) = 2Zqx_j\left(3\mu^2 + q^2 + k_j^2\right) - 4Zk_jq^2,$$

$$R_\mu(x_j) = -4Zq\mu k_j x_j + 4\mu Z\left(\mu^2 + k_j^2\right) - 4\mu^2\left(\mu^2 + k_j^2 + q^2\right) -$$

$$-\left(\mu^2 + \left(q + k_j\right)^2\right)\left(\mu^2 + \left(q - k_j\right)^2\right). \qquad (A.9)$$

The expressions for $C_i^{(\pm)}$ end $G^{(\pm)}$ are:

$$C_i^{(\pm)} = \frac{1}{4\pi}\left\{\frac{\beta^2 - 3\gamma\beta + 3\gamma^2}{8\alpha^3\beta^5} \pm \frac{8(\alpha + \beta - 3\gamma)^2}{(\alpha + \beta)^8}\right\}^{-\frac{1}{2}}, \qquad (A.10)$$

$$G^{(\pm)}(q) = 32\pi^2(C_i^{(\pm)})^2\left\{\frac{\alpha(\beta^2 - 3\gamma\beta + 3\gamma^2)}{\beta^5(4\alpha^2 + q^2)^2} + \right.$$

$$+\frac{1}{\alpha^3(4\beta^2 + q^2)^2}\left[\beta - \frac{\gamma(12\beta^2 - q^2)}{4\beta^2 + q^2} + \frac{12\beta\gamma^2(4\beta^2 - q^2)}{(4\beta^2 + q^2)^2}\right] \pm$$

$$\left. \pm\frac{8(\alpha + \beta - 3\gamma)}{(\alpha + \beta)^4((\alpha + \beta)^2 + q^2)^2}\left[\alpha + \beta - \frac{2\gamma(3(\alpha + \beta)^2 - q^2)}{(\alpha + \beta)^2 + q^2}\right]\right\}. \qquad (A.11)$$

REFERENCES

1. K. Dolder. In: Atomic Processes in Electron-Ion and Ion-Ion Collisions. 1986.
2. M. B. Shah, D. S. Elliott, P. McCallion, H. B. Gilbody. J. Phys. B: At..Mol. Phys**. 21,** 1988, 2751.

3. M. Zamkov, M. Benis, P. Richard, H. Tawara, T. J. M. Zouros. 2001 Proc. 22th Int. Conf. on Photonic, Electronic and Atomic Collisions (Santa Fe, 18-24 July 2001) ed: S. Datz, M.E.Bannister, H. F. Krause, L. H. Saddiq, D. Schultz, C. R. Vane. Abstracts of contributed papers, 356.
4. A. Müller, C. Boehme, J. Jacobi, H. Knopp, S. Schippers. 2001a Proc. 22th Int. Conf. on Photonic, Electronic and Atomic Collisions (Santa Fe, 18-24 July 2001) ed: S.Datz, M.E.Bannister, H. F. Krause, L. H. Saddiq, D. Schultz, C. R. Vane. Abstracts of contributed papers, 322.
5. S. Rachafi, M. Zambra, Hui.Zhang, M. Duponchelle, J. Jureta, P. Defrance. Physica Scripta**, 28,** 1989, 12.
6. Y. Attaourti, P.Defrance, A. Makhoute, C. J. Joachain. Physica Scripta, **43,** 1991, 578.
7. A. Müller, C. Boehme, J. Jacobi, H. Knopp, K. Ariki, S. Schippers. 2001b Proc. 22th Int. Conf. on Photonic, Electronic and Atomic Collisions (Santa Fe, 18-24 July 2001) ed: S. Datz, M.E. Bannister, H. F. Krause, L. H. Saddiq, D. Schultz, C. R. Vane. Abstracts of contributed papers, 321.
8. A. J. Dixon, M. F. A. Harrison, A. C. H. Smith. J. Phys. B: At.Mol. Phys. **9,** 1976, 2617.
9. E. Brook, M. F. A. Harrison, A. C. H. Smith. J. Phys. B: At.Mol. Phys. **17,** 1978, 3115.
10. P. Defrance, T. M. Kereselidze, Z. S. Machavariani, J.V. Mebonia. J. Phys. B: At.Mol.Opt. Phys. **32,** 1999, 2227.
11. P. Defrance, T. M. Kereselidze, Z. S. Machavariani, I. L. Noselidze. J. Phys. B: At.Mol.Opt. Phys**. 33,** 2000, 4323
12. P. Defrance, T. M. Kereselidze, Z. S. Machavariani, I. L. Noselidze. J. Phys. B: At.Mol.Opt. Phys. **34,** 2001, 4957.
13. K. Muktavat, M. K. Srivastava. Pramana J. Phys. **58,** 2002, 39.
14. E. A. Hylleraas, B.Undheim. Zs. f. Phys. **65,** 1930, 759.

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დასკვნა

გამოთვლილია მეტასტაბილურ 2^1S და 2^3S მდგომარეობაში მყოფი ორელექტრონიანი ატომური სისტემების He, $Li^{+,}$ $Be^{2+,}$ B^{3+} და C^{4+} ორჯერადი იონიზაციის სრული განივკვეთები, რისთვისაც გამოყენებულია ე.წ. შენჯღრევის მექანიზმი. სამიზნის ტალღურ ფუნქციაში მხოლოდ რადიალური კორელაციის შესაბამისი წევრია გათვალისწინებული.