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Computation of triple differential cross-sections with the inclusion of exchange effects in atomic K-shell ionization by relativistic electrons for symmetric geometry

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Abstract. The triple differential cross-section for K-shell ionization of silver and copper atoms by relativistic electrons have been computed in the coplanar symmetric geometry with the inclusion of exchange effects following the multiple scattering theory of Das and Seal [1] multiplied by suitable spinors. Present computed results are marginally improved in some cases from the previous computed results [2]. Present results are compared with measured values [3] and with previous computation results [2]. Some other theoretical computational results are also presented here for comparison.

Keywords. Cross-section; exchange effects; relativistic electrons; scattering.

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1. Introduction

Triple differential cross-section (TDCS) of K-shell ionization of medium to heavy atoms by relativistic electrons have been studied using fully relativistic distorted wave Born approximation [4,5], fully relativistic first Born approximation of Keller *et al* [6] and semi-relativistic Coulomb–Born computations of Jakubassa-Amundsen [7,8] and also experimentally [3,9–11]. For symmetric scattering it appears that the results of semi-relativistic computations of Jakubassa-Amundsen [7,8] agree better with experimental results [3], compared with those of fully relativistic first-order Born computation of Keller *et al* [6]. Jakubassa-Amundsen [7,8] systematically studied the influence of various combinations of approximate bound state and ejected electron wave functions and they found that the inclusion of lowest order relativistic corrections for the wave functions improve the first Born results for the heaviest target system considered. However, the computational results are still not satisfactory. It is also known that a non-relativistic description of the final electron is important. Das and Seal [1] have developed a wave function for electrons moving in Coulomb field which gives very interesting computational results for various kinematical conditions for both coplanar symmetric and asymmetric geometry in ionization of hydrogen atoms from 1S and 2S state for non-relativistic energies [12–15]. Recently, using the present theory of Das and Seal [1], multiplied with some spinors and without exchange term of Das [16], we computed the energy spectrum of scattered electrons in K-shell ionization of medium heavy atoms by relativistic electrons [17] which agree nicely with the experiment [11]. Energy spectrum of scattered particles in K-shell ionization of medium heavy atoms by relativistic electrons and positrons with exchange effects have been computed (to be communicated) which gives better results than the results in the asymmetric geometry of Das and Dhar [17].

Recently, we have computed triple differential cross-sections (TDCS) for K-shell ionization of silver and copper atoms by relativistic electrons [2] in the coplanar symmetric geometry using the earlier method [1,17]. In the present study, we have also computed TDCS for K-shell ionization of medium heavy atoms by relativistic electrons in the coplanar symmetric geometry with the exchange effect term of Das [16] using the previous method [1,2]. Inclusion of exchange effects gives still better results for both asymmetric (to be communicated) and symmetric scattering using the method described in [1].

2. Theory

The T-matrix element for the ionization of hydrogenic atoms by relativistic electrons [16] may be written as

$$T_{\mathrm{fi}} = T^{(\mathrm{d})} + T^{(\mathrm{ex})} + T^{(\mathrm{tr})}. \tag{1}$$

Here, $T^{(\mathrm{d})}$ is the direct scattering amplitude, $T^{(\mathrm{ex})}$ is the exchange amplitude and $T^{(\mathrm{tr})}$ is the transverse field contribution. In the present study we considered direct term $T^{(\mathrm{d})}$ and exchange effect term $T^{(\mathrm{ex})}$. $T^{(\mathrm{tr})}$ may give a contribution of the order of 10–20%, whereas higher order effects may be more important. So $T^{(\mathrm{tr})}$ is neglected here. In the present case the direct T-matrix element [1,17] is given by

$$T^{(\mathrm{d})} = \langle \phi_{\mathrm{f}}^{(-)}(\mathbf{r}_1, \mathbf{r}_2, \sigma_1', \sigma_2') | V_{\mathrm{i}}(\mathbf{r}_1, \mathbf{r}_2) | \phi_{\mathrm{i}}(\mathbf{r}_1, \mathbf{r}_2, \sigma_1, \sigma_2) \rangle. \tag{2}$$

Here, $\mathbf{r}_1$ and $\mathbf{r}_2$ represent the coordinates of the atomic active electron and the incident electron, (σ_1, σ_2) and (σ_1', σ_2') are the spin coordinates in the initial and final states of the two electrons. $(\mathbf{p}_1, \mathbf{p}_2)$ and (E_1, E_2) are the momenta and energies of the final two electrons and $(\mathbf{P}_{\mathrm{i}}, E_{\mathrm{i}})$ are the momentum and energy of the incident electron.

For initial channel unperturbed wave function $\phi_{\mathrm{i}}(\mathbf{r}_1, \mathbf{r}_2, \sigma_1, \sigma_2)$ we choose the wave function

$$\phi_{\mathrm{i}}(\mathbf{r}_1, \mathbf{r}_2, \sigma_1, \sigma_2) = \frac{1}{2\sqrt{2}\pi^2} \lambda_1^{3/2} \exp(i\mathbf{p}_{\mathrm{i}} \cdot \mathbf{r}_2) \exp(-\lambda_1 r_1) u_{\sigma_1}(0) u_{\sigma_2}(\mathbf{p}_{\mathrm{i}}), \tag{3}$$

where $\lambda_1 = \alpha_o Z_{\rm eff}$, α_o is the fine structure constant and $Z_{\rm eff}$ is the effective nuclear charge. For K-shell ionization, $Z_{\rm eff}$ = nuclear charge $(Z) - 0.3$. For the final state we choose a multiple scattering state wave function [1,17].

$$\begin{aligned}\phi_{\rm f}^{(-)}(\mathbf{r}_1,\mathbf{r}_2,\sigma_1',\sigma_2') = N(\mathbf{p}_1,\mathbf{p}_2) &\\ \times\{\varphi_{\rm p_1}^{(-)}(\mathbf{r}_1)\exp(i\mathbf{p}_2\cdot\mathbf{r}_2) + \varphi_{\rm p_2}^{(-)}(r_2)\exp(i\mathbf{p}_1\cdot\mathbf{r}_1)&\\ +\varphi_{\rm p}^{(-)}(\mathbf{r})\exp(i\mathbf{P}\cdot\mathbf{R}) - 2\exp(i\mathbf{p}_1\cdot\mathbf{r}_1)&\\ \times\exp i(\mathbf{p}_2\cdot\mathbf{r}_2)\}u_{\sigma_1'}(\mathbf{p}_1)u_{\sigma_2'}(\mathbf{p}_2)/(2\pi)^3,& \qquad (4)\end{aligned}$$

where

$$\mathbf{r} = \frac{(\mathbf{r}_2-\mathbf{r}_1)}{2},\quad \mathbf{R} = \frac{(\mathbf{r}_2+\mathbf{r}_1)}{2}$$
$$\mathbf{p} = (\mathbf{p}_2-\mathbf{p}_1),\quad \mathbf{P} = (\mathbf{p}_1+\mathbf{p}_2)$$

and $\varphi_{\rm q}^{(-)}(\mathbf{r})$ is the non-relativistic Coulomb wave function given by

$$\varphi_{\rm q}^{(-)}(\mathbf{r}) = \exp(\pi\alpha/2)\Gamma(1+i\alpha)\exp(i\mathbf{q}\cdot\mathbf{r})\ {}_1F_1(-i\alpha,1,-i(qr+\mathbf{q}\cdot\mathbf{r})). \qquad (5)$$

In the present case of electron impact ionization, the parameters α_1, α_2 and α are given below.

$$\alpha_1 = \alpha_o Z_{\rm eff}/p_1 \quad \text{for} \quad \mathbf{q} = \mathbf{p}_1$$
$$\alpha_2 = \alpha_o Z_{\rm eff}/p_2 \quad \text{for} \quad \mathbf{q} = \mathbf{p}_2$$

and

$$\alpha = -\alpha_o/p \quad \text{for} \quad \mathbf{q} = \mathbf{p}. \qquad (5a)$$

The perturbation potential $V_{\rm i}(\mathbf{r}_1,\mathbf{r}_2)$ is given by

$$V_i(\mathbf{r}_1,\mathbf{r}_2) = \frac{\alpha_o}{r_{12}} - \frac{\alpha_o Z_{\rm eff}}{r_2} \qquad (6)$$

and $u(\mathbf{p})$ represent Dirac free particle spinors.

The normalization constant $N(\mathbf{p}_1,\mathbf{p}_2)$ is calculated using the following expression from Das and Seal [1]:

$$\begin{aligned}|N(\mathbf{p}_1,\mathbf{p}_2)|^{-2} = \Bigg|7 - 2[\mu_1+\mu_2+\mu_3] - \left[\frac{2}{\mu_1}+\frac{2}{\mu_2}+\frac{2}{\mu_3}\right]&\\ + \left[\frac{\mu_1}{\mu_2}+\frac{\mu_1}{\mu_3}+\frac{\mu_2}{\mu_1}+\frac{\mu_2}{\mu_3}+\frac{\mu_3}{\mu_1}+\frac{\mu_3}{\mu_2}\right]\Bigg|,& \qquad (7)\end{aligned}$$

where

$$\mu_1 = \exp\left(\frac{\pi\alpha_1}{2}\right)\Gamma(1 - i\alpha_1),$$
$$\mu_2 = \exp\left(\frac{\pi\alpha_2}{2}\right)\Gamma(1 - i\alpha_2),$$
$$\mu_3 = \exp\left(\frac{\pi\alpha}{2}\right)\Gamma(1 - i\alpha). \tag{7a}$$

Here the parameters α_1, α_2 and α follow eq. (5a).

Now, the expression for the direct T-matrix element may be written as

$$T^{(\mathrm{d})} = u^+_{\sigma'_1}(\mathbf{p}_1)u_{\sigma_1}(0)u^+_{\sigma'_2}(\mathbf{p}_2)u_{\sigma_2}(\mathbf{p}_\mathrm{i})t(\mathbf{p}_1, \mathbf{p}_2), \tag{8}$$

where the matrix element $t(\mathbf{p}_1, \mathbf{p}_2)$ for the direct term $T^{(\mathrm{d})}(\mathbf{p}_1, \mathbf{p}_2)$ have been computed in the previous studies [2].

Now taking sum over final spin states and an average over initial states

$$\overline{|T^{(\mathrm{d})}|}^2 = (1/4)\sum |u^+_{\sigma'_1}(\mathbf{p}_1)u_{\sigma_1}(0)|^2 \sum |u^+_{\sigma'_2}(\mathbf{p}_2)u_{\sigma_2}(\mathbf{p}_\mathrm{i})|^2 |t(\mathbf{p}_1, \mathbf{p}_2)|^2. \tag{9}$$

Now the spin sums can be easily done giving

$$\sum |u^+_{\sigma'_1}(\mathbf{p}_1)u_{\sigma_1}(0)|^2 = \frac{(E_1 + 1)}{E_1}$$

and

$$\sum |u^+_{\sigma'_2}(\mathbf{p}_2)u_{\sigma_2}(\mathbf{p}_\mathrm{i})|^2 = \frac{(E_\mathrm{i}E_2 + 1 + \mathbf{p}_\mathrm{i}\cdot\mathbf{p}_2)}{E_1E_2}.$$

So

$$\overline{|T^{(\mathrm{d})}|^2} = (E_\mathrm{i}E_2 + 1 + \mathbf{p}_\mathrm{i}\cdot\mathbf{p}_2)(E_1 + 1)[t^2_\mathrm{R}(\mathbf{p}_1, \mathbf{p}_2) + t^2_\mathrm{I}(\mathbf{p}_1, \mathbf{p}_2)]/4E_1E_2E_\mathrm{i}, \tag{10}$$

where $t_\mathrm{R}(\mathbf{p}_1, \mathbf{p}_2)$ and $t_\mathrm{I}(\mathbf{p}_1, \mathbf{p}_2)$ are real and imaginary parts of the direct T-matrix element.

We have the exchange T-matrix elements

$$T^{\mathrm{ex}}(\mathbf{p}_1, \mathbf{p}_2) = T^{(\mathrm{d})}(\mathbf{p}_2, \mathbf{p}_1). \tag{11}$$

From eq. (8) we may write

$$T^{(\mathrm{ex})}(\mathbf{p}_1, \mathbf{p}_2) = u^+_{\sigma'_2}(\mathbf{p}_2)u_{\sigma_1}(0)u^+_{\sigma'_1}(\mathbf{p}_1)u_{\alpha_2}(\mathbf{p}_\mathrm{i})t(\mathbf{p}_2, \mathbf{p}_1). \tag{12}$$

Then

$$\overline{|T^{(\mathrm{ex})}|}^2 = \frac{1}{4}\sum |u^+_{\sigma'_2}(\mathbf{p}_2)u_{\sigma_1}(0)|^2 \sum |u^+_{\sigma'_1}(\mathbf{p}_1)u_{\sigma_2}(\mathbf{p}_\mathrm{i})|^2 |t(\mathbf{p}_2, \mathbf{p}_1)|^2. \tag{13}$$

After spin sum we have

$$\overline{|T^{(\mathrm{ex})}|}^2 = \frac{(E_\mathrm{i}E_1 + 1 + \mathbf{p}_\mathrm{i}\cdot\mathbf{p}_1)(E_2 + 1)[t^2_\mathrm{R}(\mathbf{p}_2, \mathbf{p}_1) + t^2_\mathrm{I}(\mathbf{p}_2, \mathbf{p}_1)]}{4E_1E_2E_\mathrm{i}}, \tag{14}$$

where $t_\mathrm{R}(\mathbf{p}_2, \mathbf{p}_1)$ and $t_\mathrm{I}(\mathbf{p}_2, \mathbf{p}_1)$ are real and imaginary parts of the exchange T-matrix element.

Also by eqs (8) and (12), we have

$$\begin{aligned}\overline{T^{(\mathrm{d})*}T^{(\mathrm{ex})}} &= \left(\frac{1}{4}\right)\sum u^{+}_{\sigma_1}(0)u_{\sigma'_1}(\mathbf{p}_1)u^{+}_{\sigma_2}(\mathbf{p}_\mathrm{i})u_{\sigma'_2}(\mathbf{p}_2)u_{\sigma_1}(\mathbf{0})\\ &\quad\times u_{\sigma'_1}(\mathbf{p}_1)u_{\sigma_2}(\mathbf{p}_\mathrm{i})[t^*(\mathbf{p}_1,\mathbf{p}_2)t(\mathbf{p}_2,\mathbf{p}_1)] \qquad (15)\\ &= \left(\frac{1}{16}E_1E_2E_\mathrm{i}\right)[(1+E_1+E_2+E_\mathrm{i})+(E_1E_\mathrm{i}+E_2E_\mathrm{i}+E_1E_2)\\ &\quad+E_1E_2E_\mathrm{i}+(\mathbf{p}_\mathrm{i}\cdot\mathbf{p}_2)E_1+(\mathbf{p}_\mathrm{i}\cdot\mathbf{p}_1)E_2\\ &\quad+(\mathbf{p}_1\cdot\mathbf{p}_2)E_\mathrm{i}+(\mathbf{p}_\mathrm{i}\cdot\mathbf{p}_1+\mathbf{p}_2\cdot\mathbf{p}_\mathrm{i}-\mathbf{p}_1\cdot\mathbf{p}_2)\\ &\quad\times[t^*(\mathbf{p}_1,\mathbf{p}_2)t(\mathbf{p}_2,\mathbf{p}_1)]. \qquad (16)\end{aligned}$$

Therefore

$$\begin{aligned}\overline{|T^{(\mathrm{d})}-T^{(\mathrm{ex})}|}^2 &= \overline{|T^{(\mathrm{d})}|}^2+\overline{|T^{(\mathrm{ex})}|}^2-\left(\overline{T^{(\mathrm{d})*}T^{(\mathrm{ex})}}+\overline{T^{(\mathrm{ex})*}T^{(\mathrm{d})}}\right) \qquad (17)\\ &= \frac{(E_\mathrm{i}E_2+1+\mathbf{p}_\mathrm{i}\cdot\mathbf{p}_2)(E_1+1)\{t^2_\mathrm{R}(\mathbf{p}_1,\mathbf{p}_2)+t^2_\mathrm{I}(\mathbf{p}_1,\mathbf{p}_2)\}}{4E_1E_2E_\mathrm{i}}\\ &\quad+\frac{(E_\mathrm{i}E_1+1+\mathbf{p}_\mathrm{i}\cdot\mathbf{p}_1)(E_2+1)\{t^2_\mathrm{R}(\mathbf{p}_2,\mathbf{p}_1)+t^2_\mathrm{R}(\mathbf{p}_2,\mathbf{p}_1)\}}{4E_1E_2E_\mathrm{i}}\\ &\quad-\left(\frac{1}{8}E_1E_2E_\mathrm{i}\right)\{(1+E_1+E_2+E_\mathrm{i})+(E_1E_\mathrm{i}+E_2E_\mathrm{i}+E_1E_2)\\ &\quad+E_1E_2E_\mathrm{i}+(\mathbf{p}_\mathrm{i}\cdot\mathbf{p}_2)E_1+(\mathbf{p}_\mathrm{i}\cdot\mathbf{p}_1)E_2+(\mathbf{p}_1\cdot\mathbf{p}_2)E_\mathrm{i}\}\\ &\quad+(\mathbf{p}_\mathrm{i}\cdot\mathbf{p}_1+\mathbf{p}_2\cdot\mathbf{p}_\mathrm{i}-\mathbf{p}_\mathrm{i}\cdot\mathbf{p}_2)\}\\ &\quad\times\{t_\mathrm{R}(\mathbf{p}_1,\mathbf{p}_2)t_\mathrm{R}(\mathbf{p}_2,\mathbf{p}_1)+t_\mathrm{I}(\mathbf{p}_1,\mathbf{p}_2)t_\mathrm{I}(\mathbf{p}_2,\mathbf{p}_1)\}]. \qquad (18)\end{aligned}$$

These are numerically evaluated using the Gaussian quadrature formula. The triple differential cross-section with the inclusion of exchange effects is finally given by

$$\frac{\mathrm{d}^3\sigma}{\mathrm{d}\Omega_1\,\mathrm{d}\Omega_2\,\mathrm{d}E_2} = \frac{r_0^2p_1p_2E_1E_2E_\mathrm{i}}{p_\mathrm{i}(2\pi)^3\alpha_0^2}\overline{|T^{(\mathrm{d})}-T^{(\mathrm{ex})}|}^2 \qquad (19)$$

for relativistic case.

Here r_o is the radius of the electron. Therefore, in our present calculation we have computed the TDCS with the exchange amplitude given by eq. (19).

In our present symmetric scattering calculations, energies of the two outgoing electrons are the same, that is $E_1 = E_2$ and also the two scattering angles are equal, that is $\theta_1 = \theta_2$ (with $\varphi_2 = 0$ and $\varphi_1 = \pi$), the scattering taking place in plane.

3. Results and discussion

Results of the present computation together with the first Born results of our computation are presented in figures 1a and 1b. Figure 1a shows results for $Z = 29$ and $E_\mathrm{i} = 300$ keV, figure 1b shows those for $Z = 29$ and $E_\mathrm{i} = 500$ keV, figure 1c

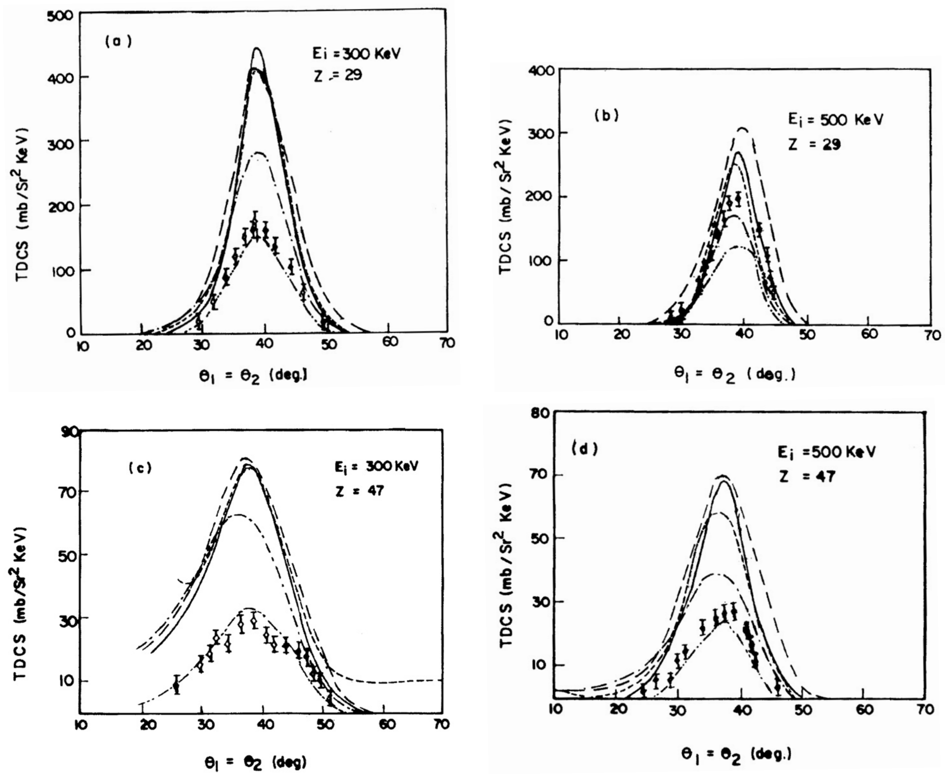

Figure 1. TDCS (in mbarn/srad^2 keV) for $IS_{1/2}$ state ionization as a function of θ_2 in coplanar symmetric geometries: (**a**) $E_i = 300$ keV, $Z = 29$, (**b**) $E_i = 500$ keV, $Z = 29$, (**c**) $E_i = 300$ keV, $Z = 47$ and (**d**) $E_i = 500$ keV, $Z = 47$. Theory: full curve: present results, small dashed curve: the results of Das and Dhar [2], long dashed curve: results of Keller *et al* [6], dashed and dotted curve: the present first Born results, dashed and double dotted curve: results of Coulomb–Born theory [8], symbols: experimental data of Bonfert *et al* [3].

shows those for $Z = 47$ and $E_i = 300$ keV and figure 1d shows those for $Z = 47$ and $E_i = 500$ keV. In these figures we exhibit the measured values of Bonfert *et al* [3], the computational results of Das and Dhar [2], the semi-relativistic Coulomb–Born computation results of Jakubassa-Amundsen [8] and the fully relativistic first-order Born approximation of Keller *et al* [6]. Firstly we note that our present exchange effect results are marginally improved than the previous results [2], comparison with the experimental data of Bonfert *et al* [3].

The present results generally lie in between the previous computational result [2] and the semi-relativistic Coulomb–Born computational results of Jakubassa-Amundsen [8] excepting some peak region. Here a point to note is that our results for 500 keV is in better agreement with the measured data [3], compared with 300 keV incident energy. Another point is that the first Born results for the present theory gradually improve as the incident energy increases. A conclusion is that our present multiple scattering computational results improve along with the increase in the incident energies. At very high incident energies the transverse field contribution will be needed. An important point to note here is that our present computation results for copper atom ($Z = 29$) at 500 keV incident energy give highly satisfactory agreement with the experimental results of Bonfert *et al* [3] and the results of Das and Dhar [2] (see figure 1b). This is as expected. At higher values of Z, our computational theory does not give satisfactory results. It is observed that the inclusion of exchange effects increases the peak in figures 1a and 1d by about 20% and in figures 1b and 1c by 10% and marginally improves the results beyond the peak angles.

The present case marginally improves the results in the peak angles and also some improvements are obtained in the small energy regions compared with the previous results of Das and Dhar [2]. In some circumstances one may need to include more relativistic effects (in particular, the effects of transverse term of T-matrix elements).

We hope by including the transverse terms the results will be better than the results obtained earlier by Jakabussa-Amundsen [8] and Keller *et al* [6]. Such complicated calculations will be reported in future.

For some cases our results agree better with the results of Keller *et al* [6]. But our present first Born results agree better with both the results of Coulomb–Born theory of Jakubassa-Amundsen [8] and the experimental data [3]. Finally, symmetric scattering results in the relativistic K-shall ionization of inclusion of exchange effects are generally good, particularly for lower charges and higher energies.

4. Conclusions

Presently no theory is in better agreement with experiment for symmetric K-shell ionization for silver and copper atoms by 300 and 500 keV incident energies. We note that our present result for the ionization of copper atom with incident energy 500 keV gives highly satisfactory result with experimental data. But in that case the other theories (see figure 1b) have poor agreement with experiment, whereas the theory of Jakubassa-Amundsen [8] is in good agreement with experimental results [3] for both silver and copper atomic K-shell ionization by other kinematical conditions (see figures 1a, 1c). The present results are very close to the theory of Keller *et al* [6]. In some other cases our present first Born results are close to the results of Jakubassa-Amundsen [8]. So new experimental results will be more interesting for such symmetric scattering problems.

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