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Calculation of triple differential cross-sections of K-shell ionization of medium-heavy atoms by electrons for symmetric geometry

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Abstract. Triple differential cross-section for K-shell ionization of medium-heavy atoms by relativistic electrons has been calculated for coplanar symmetric geometry. In this calculation the final state is described by a non-relativistic wave function of Das and Seal [*Phys. Rev.* **A47** (1993) 2978] multiplied with suitable spinors. Results of the present calculation are compared with the available experimental data and with other theoretical calculations.

Keywords. Cross-section; ionization; relativistic; electron; scattering.

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1. Introduction

The study of the differential cross-section for K-shell ionization by relativistic electrons has been done since early seventies both theoretically [1–4] and experimentally [5–8]. Recently some progress has been made through the use of fully relativistic distoded wave Born calculation (rDWBA [9–12]) and semi-relativistic Coulomb Born calculation [13–14]. For symmetric scattering it appears that the results of semi-relativistic calculations of Jakubassa–Amundsen [13–14] agree better with experimental results [15, 16] compared with those of rDWBA calculations of Keller *et al* [12]. It is also known that a non-relativistic description of the final ejected electron is very often quite satisfactory [5–8]. Moreover in such symmetric scattering correlation of the final electrons is important. Recently Das and Seal [17] have developed a wave function for electrons moving in a Coulomb field which gives very interesting results for various kinematical conditions and in particular for coplanar symmetric geometry in electron-atom ionization collisions for non-relativistic energies (Das and Seal [18]; Das and Dhar [19]). Recently using the present theory of Das and Seal [17], multiplied with some spinors, we calculated the energy spectrum of scattered electrons in K-shell ionization of medium to heavy atoms by relativistic electrons [4] which agree nicely with experiments. Inclusion of exchange effect gives still better results. So, it will be interesting to use similar wave functions in the study of symmetric scattering in K-shell ionization. Here we have done such a calculation.

2. Theory

The T-matrix element for the ionization of hydrogen atom by electrons may be written as (see Das [1])

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

where $T^{(\mathrm{d})}$ is the direct scattering amplitude, $T^{(\mathrm{ex})}$ is the exchange amplitude and $T^{(\mathrm{tr})}$ is the transverse field contribution. For the present kinematic conditions there are wide differences between results of different theories and with experiments [12]. Exchange and transverse field effects, here, may give atmost 20% to 25% additional contributions (see Das [1] and also elsewhere). So we neglect $T^{(\mathrm{ex})}$ and $T^{(\mathrm{tr})}$ to have some initial views. Here $T^{(\mathrm{d})}$ is given by

$$T^{(\mathrm{d})} = \langle \Phi_f^{(-)}(\mathbf{r}_1, \mathbf{r}_2, \sigma_1', \sigma_2') | V_i(\mathbf{r}_1, \mathbf{r}_2) | \Phi_i(\mathbf{r}_1, \mathbf{r}_2, \sigma_1, \sigma_2) \rangle \tag{2}$$

Here $\mathbf{r}_1$ and $\mathbf{r}_2$ represent the co-ordinates of the atomic active electron and the incident electron. (σ_1, σ_2) and (σ_1', σ_2') are the spin co-ordinates 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 electrons and $(\mathbf{p}_i, E_i)$ are the momentum and energy of the incident electron.

For Φ_i we choose the wave function

$$\Phi_i(\mathbf{r}_1, \mathbf{r}_2, \sigma_1, \sigma_2) = \frac{1}{\sqrt{\pi/a^3}} e^{-ar_1} e^{i\mathbf{p}_i\cdot\mathbf{r}_2} u_{\sigma_1}(0) u_{\sigma_2}(\mathbf{p}_i) \tag{3a}$$

where $a = \alpha_0 Z_{\mathrm{eff}}$, α_0 is the fine structure constant and effective nuclear charge $Z_{\mathrm{eff}} =$ nuclear charge $(Z) - 0.3$. The perturbation potential is given by

$$V_i(\mathbf{r}_1, \mathbf{r}_2) = \frac{\alpha_0}{r_{12}} - \frac{\alpha_0 Z_{\mathrm{eff}}}{r_2}. \tag{3b}$$

The final state is chosen as (Das and Seal [17])

$$\begin{aligned}\Phi_f^{(-)}(\mathbf{r}_1, \mathbf{r}_2, \sigma_1', \sigma_2') = {} & N(\mathbf{p}_1, \mathbf{p}_2)\{\phi_{\mathbf{p}_1}^{(-)}(\mathbf{r}_1) e^{i\mathbf{p}_2\cdot\mathbf{r}_2} + \phi\mathbf{p}_2^{(-)}(\mathbf{r}_2) e^{ip_1\cdot r_1} \\ & + \phi\mathbf{p}^{(-)}(\mathbf{r}) e^{i\mathbf{P}\cdot\mathbf{R}} - 2e^{i\mathbf{p}_1\cdot\mathbf{r}_1 + i\mathbf{p}_2\cdot\mathbf{r}_2}\} \times u_{\sigma_1'}(\mathbf{p}_1) u_{\sigma_2'}(\mathbf{p}_2)/(2\pi)^3\end{aligned} \tag{3c}$$

where

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

$u_\sigma(\mathbf{p})$ is the Dirac free particle spinor and $\phi_{\mathbf{q}}^{(-)}(\mathbf{r})$ is the non-relativistic Coulomb wave function given by

$$\phi_{\mathbf{q}}^{(-)}(\mathbf{r}) = e^{\pi\alpha/2}\Gamma(1 + i\alpha) e^{i\mathbf{q}\cdot\mathbf{r}}{}_1F_1(-i\alpha, 1, -i[qr + \mathbf{q}\cdot\mathbf{r}]) \tag{4}$$

where

$$\begin{aligned}\alpha &= \alpha_0 Z_{\mathrm{eff}}/p_1, \quad \text{for } \mathbf{q} = \mathbf{p}_1 \\ &= \alpha_0 Z_{\mathrm{eff}}/p_2, \quad \text{for } \mathbf{q} = \mathbf{p}_2 \\ &= -\alpha_0/p, \quad \text{for } \mathbf{q} = \mathbf{p}.\end{aligned} \tag{4a}$$

The normalization constant $N(\mathbf{p}_1, \mathbf{p}_2)$ is given by (see Das and Seal [17])

$$|N(\mathbf{p}_1, \mathbf{p}_2)|^{-2} = |7 - 2[\lambda_1 + \lambda_2 + \lambda_3] - [2/\lambda_1 + 2/\lambda_2 + 2/\lambda_3] + [\lambda_1/\lambda_2 + \lambda_1/\lambda_3 + \lambda_2/\lambda_1 + \lambda_2/\lambda_3 + \lambda_3/\lambda_1 + \lambda_3/\lambda_2]| \quad (5)$$

where

$$\begin{aligned} \lambda_1 &= e^{\pi\alpha_1/2}\Gamma(1 - i^{\alpha_1}), & \alpha_1 &= \alpha_0 Z_{\text{eff}}/p_1 \\ \lambda_2 &= e^{\pi\alpha_2/2}\Gamma(1 - i^{\alpha_2}), & \alpha_2 &= \alpha_0 Z_{\text{eff}}/p_2 \\ \lambda_3 &= e^{\pi\alpha/2}\Gamma(1 - i^{\alpha}), & \alpha &= -\alpha_0/p. \end{aligned} \quad (5a)$$

The above scattering state wave function (3c) consists of four parts and is correct everywhere to the first order in the potentials Z_{eff}/r_1, Z_{eff}/r_2 and $1/r_{12}$ as may be easily verified by direct substitution in the equation. It is particularly good in the asymptotic region as in the case of BBK wave function. Even then for short ranges, under certain kinematic conditions, there may arise considerable error. Another interesting point to note is that each term in the wave function may be physically interpreted and the corresponding term in the T-matrix element (after substitution in eq. (2)) may highlight the physical effect responsible for a particular feature observed in the scattering (see in this context Das and Seal [18]).

Finally the triple differential cross-section for each K-electron is given by

$$\frac{\mathrm{d}^3\sigma}{\mathrm{d}\Omega_1 \mathrm{d}\Omega_2 \mathrm{d}E_2} = r_0^2 \frac{p_1 p_2 E_1 E_2 E_i}{p_i (2\pi)^5} \cdot \frac{1}{\alpha_0^2} \overline{|T^{(\mathrm{d})}|^2} \quad (6)$$

where r_0 is the radius of the electron and the averaging is over spin states.

The calculation then proceeds as in Das and Seal [17]. Calculations were done for nuclear charge $Z = 29$ and 47 and for incident energies $E_i = 300$ keV and 500 keV for which experimental results exist [15, 16]. First Born results of the present calculations are also presented. In our present symmetric scattering calculations energies of the two outgoing electrons are the same i.e. $E_1 = E_2$ and also the two scattering angles are equal i.e. $\theta_1 = \theta_2$ (with $\phi_2 = 0, \phi_1 = \pi$), the scattering taking place in a plane.

3. Results and Discussion

Results of the present calculation together with the first Born results of our calculation are presented in figures 1(a–d). Figure 1(a) shows results for $Z = 29$ and $E_i = 300$ keV, figure 1(b) shows those for $Z = 29$, $E_i = 500$ keV, figure 1(c) shows those for $Z = 47$ and $E_i = 300$ keV and figure 1(d) shows those for $Z = 47$ and $E_i = 500$ keV. In these figures we present the experimental results of Nakel and collaborators [15–16] and the Coulomb Born theoretical results of Jakubassa–Amundsen [13–14] and rDWBA results of Keller *et al* [12]. Now, we note that our results generally lie in between the fully relativistic distorted wave Born approximation (rDWBA) calculation of Keller *et al* [12] and the semi-relativistic Coulomb Born calculation of Jakubassa–Amundsen [14]. Secondly, we note that the present results often are close to those of the theory of Keller *et al* [12]. Thirdly, we note that for 500 keV our results again agree better with experiment, compared with 300 keV energy, as is expected. For it is well known that in the Born theory the cross-section results improve as the energy increases. Moreover in the present multiple scattering calculation, the results improve rather more rapidly, mainly because the scattering state wave function (3c) is good in the asymptotic domain and that the main contribution to the scattering amplitude comes from the asymptotic domain for higher energies. Also the wave function is only correct to the first order in the potentials Z_{eff}/r_1, Z_{eff}/r_2 and $1/r_{12}$. So it is expected that smaller is the value of Z better will be the cross-section results. However at very high energies transverse field contribution and other relativistic effects must be taken into account properly. The fourth point to note is that our results for $Z = 29$, $E_i = 500$ keV agree very well with experiment [see figure 1(b)]. This is also expected. For heavy atoms approximations of the present paper do not hold. Thus with the increase of Z, the results of the present calculation deteriorates.

It is also observed that the inclusion of exchange increases the peak values in figures 1(a) and 1(d) by about 20% and in figure 1(b) by 12% and marginally improves the results beyond the peak angles (results with exchange included are not shown in the figures).

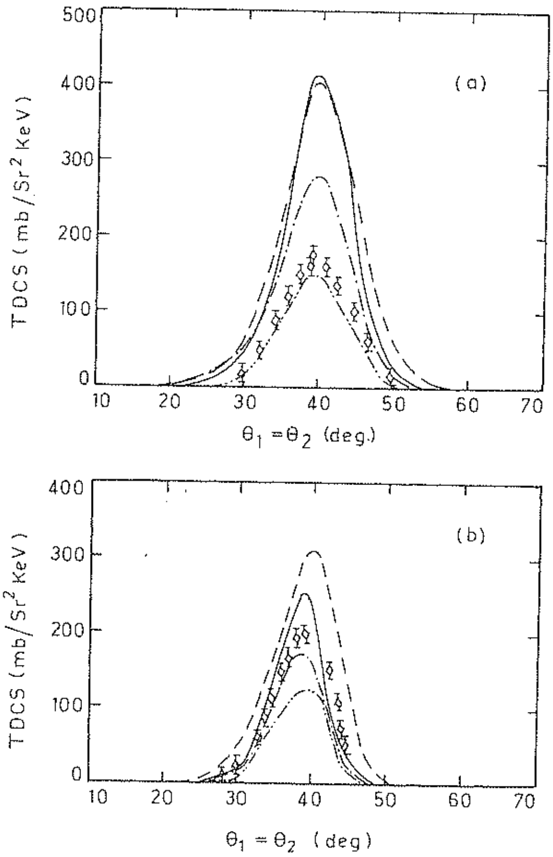

Figure 1(a–b). *(Continued)*

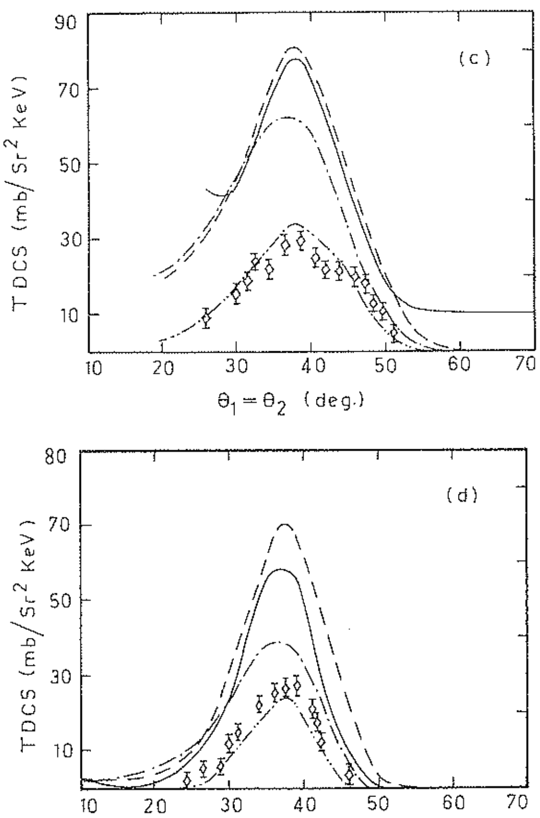

Figure 1a–c. TDCS (in mbarn/srad^2 keV) for $1S_{1/2}$state ionization as a function of θ_2 in coplanar symmetric geometries: **a**) $E_i = 300\,$keV, $Z = 29$, **b**) $E_i = 500\,$keV, $Z = 29$, **c**) $E_i = 300\,$keV, $Z = 47$ and (**d**) $E_i = 500\,$keV, $Z = 47$. Theory: full curve: present results, dashed curve: results of Keller *et al* [12], dashed and dotted curve: the first Born results, dashed and double dotted: resutls of Coulomb Born theory [14], symbols: experimental data [15].

4. Conclusions

It is clear that at present no theory is fully satisfactory in describing the symmetric K-shell ionization cross-section of medium-heavy atoms by relativistic electrons. Secondly, it is very interesting to note that the semi-relativistic Coulomb Born calculation often gives much better results compared to fully relativistic rDWBA calculations. It is also noted that the correlated wave function of Das and Seal [17] gives a better description of the final channel compared to that used in the Born calculation. Finally, it may be noted that the present theory for K-shell ionization of silver and copper atoms by relativistic electrons in the symmetric geometry shows wide differences from experimental data of Nakel *et al* [15–16] for lower incident energies (300 keV) and gives comparatively better results for higher (500 keV) energies. For the relativistic symmetric scattering case the results of the present theory lie between the Coulomb Born theory of

Jakubassa–Amundsen [13–14] and the relativistic distorted wave Born approximation theory of Keller *et al* [12]. Results of the present theory are often close to those of the theory of Keller *et al* [12]. So new experimental results will be interesting for such symmetric scattering problems also.

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