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Theoretical Triply Differential Cross Section of
Electron-Impact Ionization of Atoms

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ABSTRACT

The triply differential cross section of electron-impact ionization of atoms is given in a parameterized form, suitable for theoretical computations or for semi-empirical fittings. Application of the present formulation is demonstrated. Merits of coplanar measurements are discussed. It is also shown that the coplanar up-down asymmetry of the ejected electron is linear in the scattering angle, or the momentum transfer, of the incident electron for small momentum transfers.

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EXB

Impact ionization of atoms or ions by charged particles is important for diagnostics of high temperature plasmas as well as for fundamental understanding of the atomic structure. In recent years, the electron coincidence spectroscopy has become a powerful tool for testing dynamical theories of final states with two outgoing electrons.¹⁻⁴ To the author's knowledge, no theoretical kinematic analysis of the electron-impact ionization of atoms has been given. A complete kinematic analysis can provide an overall symmetry of the impact-ionization processes and facilitate the comparison between theory and experiment.

In this paper, we shall give the triply differential cross section in terms of angle-independent dynamical parameters. For low-energy ionization where only the first few partial waves contribute significantly, a small number of dynamical parameters are adequate to describe the full angular correlation between the incoming and outgoing electrons. The kinematic analysis which will be presented can apply to collision processes of the general type

$$a + A \rightarrow B + b + c, \quad (1)$$

where A and B are assumed to be sufficiently heavy such that they are stationary in the center of momentum frame. For definiteness, however, we shall consider specifically the electron-impact ionization of atoms.

Assume that the linear momentum and energy of the incident electron are denoted by $\vec{k}_1$ and E_1 , respectively. After collision with the atom, the two outgoing electrons are described by $(\vec{k}_1, E_1)$ and $(\vec{k}_2, E_2)$. The directions $\hat{k}_1$ and $\hat{k}_2$ of the outgoing electrons are specified by the polar-azimuthal angles (θ_1, ϕ_1) and (θ_2, ϕ_2) , respectively, relative to the incident direction $\hat{k}_1$. The electronic energies of the target before and after the collision are denoted by

E_0 and E_α , respectively. The energy conservation law requires

$$E_1 = E_1 + E_2 + E_\alpha - E_0, \quad (2)$$

where $E_\alpha - E_0$ includes the ionization energy and, possibly, the excitation energy of the target. If the excitation energy is zero or if there is a dominant excitation mode such that $E_\alpha - E_0$ is well-defined, the measurement of E_1 or E_2 determines completely the sharing of the available energy among the outgoing electrons. To give a specific result for the triply differential cross section, we assume that the atom is initially in an angular momentum eigenstate J_0 , and that after the collision the residual ion is in the eigenstate J_α . The partial waves of the incident and two outgoing electrons are specified in the relativistic notation by $\kappa_1 \equiv j_1 \ell_1$, $\kappa_1 \equiv j_1 \ell_1$, and $\kappa_2 \equiv j_2 \ell_2$, respectively. Because we are also interested in the fine structure of the atom and the spin polarization of the electrons, we shall start from the outset in the relativistic formulation. Details of derivation and spin polarization of the outgoing electrons will be reported. For the present purpose, we give only the triply differential cross section for the impact ionization of unpolarized atoms by unpolarized electrons.

The triply differential cross section for the impact ionization of unpolarized atoms by unpolarized electrons is obtained in atomic units as

$$\sigma(\theta_1 \phi_1 \theta_2 \phi_2) \equiv \frac{d^3 \sigma}{d\Omega_1 d\Omega_2 dE_1} = \frac{\sigma}{16\pi^2} F(\theta_1 \phi_1 \theta_2 \phi_2), \quad (3)$$

where σ is the total cross section per unit energy, and $F(\theta_1 \phi_1 \theta_2 \phi_2)$ is the angular distribution function. The total cross section has the form

$$\sigma = \frac{2\pi^3}{k_1^2 [J_0]^2} \bar{\sigma}, \quad (4)$$

where $[J_0] \equiv (2J_0 + 1)^{1/2}$ and

$$\bar{\sigma} = \sum_{\alpha} d_{\alpha}^2 \quad (5)$$

The transition amplitude d_{α} is defined by the reduced matrix element of the partial wave amplitude

$$i^{\ell_1 - (\ell_1 + \ell_2)} \exp[i(\sigma_{\kappa_1} + \sigma_{\kappa_2})] \langle \alpha^- [J_{\alpha}(j_1 j_2) j] J \| H_I \| (J_0 j_1) J \rangle \\ \equiv \exp(i\delta_{\alpha}) d_{\alpha}, \quad (6)$$

where σ_{κ_1} and σ_{κ_2} are Coulomb phase shifts of the two outgoing electrons. We note that antisymmetrizations of the initial and final states of the composite projectile-target system are assumed. Therefore both the so-called potential exchange and scattering exchange are treated on an equal footing and are included implicitly. The summation in (5) is over all possible channels, i.e.,

$$\sum_{\alpha} \equiv \sum_{\kappa_1 \kappa_2 j J}. \quad (7)$$

The angular distribution function in (3) is given as

$$F(\theta_1 \phi_1 \theta_2 \phi_2) = \sum_{L_1 L_2 K M=0} \beta_{L_1 L_2 K} \begin{pmatrix} L_1 L_2 K \\ M -M 0 \end{pmatrix} d_{0M}^{L_1}(\theta_1) d_{M0}^{L_2}(\theta_2) \cos M(\phi_1 - \phi_2). \quad (8)$$

where d_{mn}^{ℓ} are the standard d functions of rotation matrices.⁵ Here we note that the triply differential cross section for unpolarized targets depends only on

three angles θ_1 , θ_2 , and $|\phi_1 - \phi_2|$. The dynamical parameters $\beta_{L_1 L_2 K}$ in (8) is given as

$$\begin{aligned} \beta_{L_1 L_2 K} = & \bar{\sigma}^{-1} \sum_{\alpha' \alpha} \Pi(\ell'_1 \ell_1 L_1) \Pi(\ell'_2 \ell_2 L_2) \Pi(\ell'_1 \ell_1 K) \Pi(L_1 L_2 K) \\ & \times [j'_1 j'_2 j'_i J'] [j_1 j_2 j_i J] [L_1 L_2 K]^2 \\ & \times (-)^{J_0 - J_\alpha - 1/2} \begin{pmatrix} j'_1 & j_1 & L_1 \\ 1/2 & -1/2 & 0 \end{pmatrix} \begin{pmatrix} j'_2 & j_2 & L_2 \\ 1/2 & -1/2 & 0 \end{pmatrix} \begin{pmatrix} j'_i & j_i & K \\ 1/2 & -1/2 & 0 \end{pmatrix} \\ & \times \begin{Bmatrix} J' & J & K \\ j'_1 & j'_i & J_0 \end{Bmatrix} C_{L_1 L_2 K}, \end{aligned} \quad (9)$$

where the parity function is defined as

$$\Pi(\ell' \ell L) = \begin{cases} 1, & \ell' + \ell + L = \text{even}, \\ 0, & \ell' + \ell + L = \text{odd}, \end{cases} \quad (10)$$

and $C_{L_1 L_2 K}$ depends on the coupling scheme. Corresponding to the choice of coupling in (6), we have

$$\begin{aligned} C_{L_1 L_2 K} = & (-)^{j_1 + j_2 + j + K} [j' j] \begin{Bmatrix} J' & J & K \\ j & j' & J_\alpha \end{Bmatrix} \begin{Bmatrix} j'_1 & j_1 & L_1 \\ j'_2 & j_2 & L_2 \\ j' & j & K \end{Bmatrix} \\ & \times d_{\alpha'} d_{\alpha} \cos(\delta_{\alpha'} - \delta_{\alpha}). \end{aligned} \quad (11)$$

The expressions in different coupling schemes can easily be derived from (11).

For comparison with experiment, it is more convenient to write the triply differential cross section in the form

$$\sigma(\theta_1 \phi_1 \theta_2 \phi_2) = \sum_{L_1 L_2 M} b_{L_1 L_2 M} d_{0M}^{L_1}(\theta_1) d_{0M}^{L_2}(\theta_2) \cos M(\phi_1 - \phi_2). \quad (12)$$

where the dynamical parameters are

$$b_{L_1 L_2 M} = \frac{\sigma}{16\pi^2} \sum_K \beta_{L_1 L_2 K}^{(-)} \begin{pmatrix} M & L_1 L_2 & K \\ & M & -M & 0 \end{pmatrix}. \quad (13)$$

A complete measurement of triply differential cross section will yield all dynamical parameters $b_{L_1 L_2 M}$. Conversely, once the dynamical parameters $b_{L_1 L_2 M}$ are obtained, either semiempirically by fitting the functional form (12) to experimental data or theoretically by calculating the expression (13), the triply differential cross section at arbitrary angles θ_1 , ϕ_1 , θ_2 , and ϕ_2 can be constructed. Furthermore, quantities such as the magnitude and angular position of the binary or recoil peaks, and the spatial symmetry of the angular distribution of the outgoing electrons can easily be deduced.

The coplanar cross section, where we have $\phi_1 = \phi_2$, can be written as

$$\begin{aligned} \sigma(\theta_1 \theta_2) &\equiv \sigma(\theta_1 \phi_1 \theta_2 \phi_1) \\ &= \sum_{L_1 L_2 M} b_{L_1 L_2 M} d_{OM}^{L_1}(\theta_1) d_{OM}^{L_2}(\theta_2), \end{aligned} \quad (14)$$

where we have introduced the notation $\sigma(\theta_1 \theta_2)$. We can see from (14) that by studying only the coplanar angular distribution, we cannot obtain all the dynamical properties about the electron-impact ionization processes. This point will become obvious later. From (14), we can also prove that the up-down asymmetry is linear in θ_1 or θ_2 for small θ_1 or θ_2 , respectively; for example, $[\sigma(\theta_1 \theta_2) - \sigma(\theta_1 - \theta_2)] / [\sigma(\theta_1 \theta_2) + \sigma(\theta_1 - \theta_2)]$ is linear in θ_1 for $\theta_1 \ll 1$.

Another interesting special case is when $\phi_1 - \phi_2 = \pi/2$,

$$\sigma(\theta_1 \phi_1 \theta_2 \phi_1 - \pi/2) = \sum_{L_1 L_2 M}^{\text{even}} b_{L_1 L_2 M} (-)^{M/2} d_{0M}^{L_1}(\theta_1) d_{0M}^{L_2}(\theta_2). \quad (15)$$

We note however that this type of measurement in general yield less information about the collision processes than the coplanar measurement, although they complement each other.

To compare the full triply differential measurement with the coplanar measurement, we study the number of independent parameters in each case. Assume that, in (12), $b_{L_1 L_2 M}$ are negligible for L_1 or L_2 larger than L ; i.e., we have $L_1 \leq L$ and $L_2 \leq L$. Therefore, the number of independent parameters for the triply differential cross section is $N_L = (L+1)(L+2)(2L+3)/6$. For the coplanar cross section, the number of independent parameters is $N_L(\phi_1 = \phi_2) = 2L(L+1) + 1$, while $N_L(\phi_1 - \phi_2 = \pi/2) = (L+1)^2$. Consequently, we have the trivial case of spherical distribution for $L = 0$. For $L = 1$, we have

$$\begin{aligned} \sigma(\theta_1 \phi_1 \theta_2 \phi_2) = & b_{000} + b_{100} d_{00}^1(\theta_1) + b_{010} d_{00}^1(\theta_2) \\ & + b_{110} d_{00}^1(\theta_1) d_{00}^1(\theta_2) + b_{111} d_{01}^1(\theta_1) d_{01}^1(\theta_2) \cos \phi. \end{aligned} \quad (16)$$

To determine the triply differential cross section for $L_1, L_2 \leq 1$, it is sufficient to measure only the coplanar coincidence. For $L = 2$, the triply differential cross section is given by

$$\begin{aligned} \sigma(\theta_1 \phi_1 \theta_2 \phi_2) = & \sum_{L_1 L_2=0}^2 b_{L_1 L_2 0} d_{00}^{L_1}(\theta_1) d_{00}^{L_2}(\theta_2) \\ & + \sum_{L_1 L_2=1}^2 b_{L_1 L_2 1} d_{01}^{L_1}(\theta_1) d_{01}^{L_2}(\theta_2) \cos(\phi_1 - \phi_2) \end{aligned}$$

$$+ b_{222} d_{02}^2(\theta_1) d_{02}^2(\theta_2) \cos 2(\phi_1 - \phi_2). \quad (17)$$

Coplanar measurement can only determine thirteen of the fourteen unknown parameters for $L_1, L_2 \leq 2$. The additional parameter can be obtained, e.g., by making also measurements at $\phi_1 - \phi_2 = \pi/2$.

To apply the present formulation to analyze coplanar coincidence with $E_1 \gg E_2$, we rewrite (14) as

$$\sigma(\theta_1, \theta_2) = \sum_{\ell=0}^L \beta_{\ell}(\theta_1) d_{00}^{\ell}(\theta_2) + \sum_{\ell=1}^L \gamma_{\ell}(\theta_1) d_{01}^{\ell}(\theta_2), \quad (18)$$

where β_{ℓ} and γ_{ℓ} can be written as expansions in terms of dynamical parameters $b_{L_1 L_2 M}$. The first term on the right-hand side of (18) is even both in θ_1 and in θ_2 , and the second term is odd. Coplanar measurements can determine all $(2L + 1)$ functions, $\beta_{\ell}(\theta_1)$ and $\gamma_{\ell}(\theta_1)$. In contrast, a complete triply differential measurement would yield $\frac{1}{2}(L + 1)(L + 2)$ independent functions of θ_1 . For high energy E_1 , the functions $\beta_{\ell}(\theta_1)$ and $\gamma_{\ell}(\theta_1)$ are peaked in the forward direction $\theta_1 \lesssim (1/k_1 R)$, where R is the effective size of the atom. Because $\beta_{\ell}(\theta_1)$ and $\gamma_{\ell}(\theta_1)$ are even and odd functions, respectively, it is clear that the up-down asymmetry is linear in θ_1 for $\theta_1 \ll (1/k_1 R)$. We can also see that, as $\theta_1 \rightarrow 0$, the coplanar angular distribution (18) is symmetric about the incident direction, and two of the extrema of the distribution occur at $\theta_2 = 0$ and π .

As a demonstration, we fit the functional form (18) to the experimental data of electron-impact ionization of helium presented in Fig. 1 of ref. 4. The incident electron has an energy $E_1 = 500$ eV and is scattered at $\theta_1 = 3.5^\circ$. The ejected slow electron has an energy $E_2 = 5$ eV. We therefore include up to, say,

d waves of the ejected slow electron; i.e., we consider $L_2 < 4$. The semiempirical parameters obtained at $\theta_1 = 3.5^\circ$ are $\beta_0 = 2.288$, $\beta_1 = 0.306$, $\beta_2 = -0.943$, $\beta_3 = -0.906$, $\beta_4 = 0.095$, $\gamma_1 = -0.806$, $\gamma_2 = -2.530$, $\gamma_3 = 0.360$, and $\gamma_4 = 0.133$. The coplanar cross section constructed from these parameters are presented in Fig. 1, along with the experimental data of Ehrhardt et al.⁴ The dependence of these parameters on θ_1 can be obtained by fitting experimental data at different angles θ_1 . Because these parameters can also be calculated theoretically by using formulas presented here, summarizing experimental data in terms these parameters can facilitate the comparison between experiment and theory as well as between experiments with different scattering angles θ_1 .

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FIGURE CAPTION

Figure 1. The triply differential cross section (in a.u.) for the ionization of helium by electron impact. The dots are experimental data of Ehrhardt et al. (Ref. 4). The solid curve is obtained semiempirically with the function form (18).

Fig. 1