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A systematic study of relativistic (e, 2e) collisions in comparison with experiment

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Abstract. Triply-differential cross sections for K-shell ionization by fast electron impact are calculated within the first-order Coulomb Born approximation for the case of a coplanar *symmetric geometry*. Comparison is made with experimental data on 300 keV and 500 keV $e^- + Cu$, Ag and Au. For the two lighter targets, the binary peak region is reasonably well described by a theory which uses semirelativistic electronic eigenfunctions to the target field, provided spin-flip is included. For the gold target, the Coulomb Born approximation seriously overestimates the data, pointing to the necessity of a fully relativistic description of the electronic states.

Triply-differential cross sections for inner-shell ionization in electron–atom collisions provide a sensitive test for theoretical models since a coincident detection of the two momentum-analysed outgoing electrons allows for a complete determination of the collision kinematics (McCarthy and Weigold 1976, Ehrhardt *et al* 1986, Lahmam-Bennani 1991). For fast collisions where a first-order treatment of the electron–electron interaction should be appropriate and polarization effects may be neglected, the basic information to be extracted from (e, 2e) cross sections concerns thus the particulars of the electronic wavefunctions.

For low-energy electron scattering it has become standard to use a Hartree–Fock-type function for the bound target electron, and numerically generated scattering states to the static-exchange potential for the continuum electrons (Madison *et al* 1977). The multiple partial wave expansion required for the evaluation of the cross section becomes, however, prohibitive at high projectile energies, and such elaborate wavefunctions have up to now only been employed for energies of 150 keV and below (Pindzola and Buie 1988).

The (e, 2e) experiments have recently been extended to the relativistic regime with impact energies up to 500 keV (Schüle and Nakel 1982, Ruoff and Nakel 1987, Bonfert *et al* 1991, Walters *et al* 1991). Apart from the distorted-wave Born approximation of Pindzola and Buie (1988), the theoretical approaches for relativistic electron impact ionization are restricted to the plane-wave Born approximation (PWBA; Möller 1932), where the primary electron is described by Dirac plane waves, while the target field is accounted for in the states of the secondary electron (Das 1972, Davidovic *et al* 1978). Such a simple prescription works well for weak target fields and for asymmetric energy sharing between the two outgoing electrons (the secondary electron being much slower than the primary one). However, it has been shown that the plane-wave Born approximation overestimates experiments with a symmetric energy sharing, the more so, the heavier the target nucleus (Bonfert *et al* 1991). Therefore we have developed a theory, termed Coulomb Born approximation, which comprises the advantages of the PWBA and the distorted-wave theory: The target potential is considered in the states

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of the primary electron, but by choosing non-relativistic Coulomb waves multiplied by a Dirac spinor for all unbound electronic states, a partial wave expansion can be avoided (Jakubassa-Amundsen 1989).

Adopting the argumentation of Moiseiwitsch (1980) that spin-flip contributes little to total ionization cross sections at moderate relativistic impact energies, we had neglected spin-flip in our previous work. However, it has recently been shown by Walters *et al* (1991) within a PWBA treatment, that inclusion of spin-flip leads to a considerable enhancement of (e, 2e) cross sections for a symmetric energy sharing where the momenta of both outgoing electrons are large. In the present work, we therefore allow for spin-flip, but we also test the wavefunction effects by (i) replacing the Darwin K-shell function by a relativistic hydrogenic function, (ii) replacing the non-relativistic Coulomb wave for the secondary electron by a Darwin function (in our PWBA code), and (iii) accounting for the final-state interaction by a simple modification of the two-electron wavefunction. The importance of the non-perturbative treatment of the electron-electron interaction had been pointed out by Brauner *et al* (1989) for small relative momenta of the outgoing electrons.

A detailed description of the Coulomb Born theory has been given earlier (Jakubassa-Amundsen 1989). In short, the triply-differential cross section for ejecting a (secondary) electron from the target subshell i with occupation number N_i into the solid angle $d\Omega_{\kappa_f}$, while scattering the impinging (primary) electron into the solid angle $d\Omega_{k_f}$, is given by (in atomic units, $\hbar = m = e = 1$)

$$\frac{d^3\sigma}{dE_{\kappa_f}\, d\Omega_{\kappa_f}\, d\Omega_{k_f}} = \frac{N_i}{c^6 k_i}\, \kappa_f E_{\kappa_f} k_f E_{k_f} E_{k_i} \sum_{s_f\sigma_f s_i\sigma_i} |W^{\rm d}_{s_f\sigma_f s_i\sigma_i}(\boldsymbol{k}_f, \boldsymbol{\kappa}_f) - W^{\rm ex}_{s_f\sigma_f s_i\sigma_i}(\boldsymbol{k}_f, \boldsymbol{\kappa}_f)|^2 \qquad (1)$$

where i characterizes the initial and f the final state. The momenta and total energies of the primary and the secondary electron are denoted by $\boldsymbol{k}$, $\boldsymbol{\kappa}$ and E_k, E_κ, respectively, while their spin quantum numbers are termed s and σ, respectively. Spin-flip is included by summing over all 16 combinations of the four spins ($s, \sigma = \{+, -\}$). The exchange interaction is accounted for by subtracting from the direct term, $W^{\rm d}$, an exchange term, $W^{\rm ex}$, which is obtained from the direct term by exchanging momenta and spins of the two outgoing electrons according to $W^{\rm ex}_{s_f\sigma_f s_i\sigma_i}(\boldsymbol{k}_f, \boldsymbol{\kappa}_f) = W^{\rm d}_{\sigma_f s_f s_i\sigma_i}(\boldsymbol{\kappa}_f, \boldsymbol{k}_f)$. Since the wavefunctions of the primary and the secondary electron, $\psi_f^{(s_f)}$ and $\phi_f^{(\sigma_f)}$, have the same structure, being composed of a Coulomb wave ψ_{k_f}, ψ_{κ_f} times a Dirac spinor $a_{k_f}^{(s_f)}$, $a_{\kappa_f}^{(\sigma_f)}$ (times a normalization constant; for their definition see e.g. Bjorken and Drell 1964), respectively, the so obtained exchange term is—within the Coulomb Born approximation—exact. Taking for the bound-state function $\phi_i^{(\sigma_i)}$ a Darwin function, i.e. a spinor $a_i^{(\sigma_i)}$ acting on a hydrogenic 1s state, ψ_i, (where $a_i^{(\sigma_i)}$ is obtained from $a_{k_i}^{(\sigma_i)}$ by replacing $k_{i\lambda}$ by $-i\partial_\lambda$ ($\lambda = z, \pm$) where $k_\pm = k_x \pm ik_y$ and $\partial_\pm = \partial/\partial_x \pm i\partial/\partial_y$), the direct term which accounts for the electron-electron coupling to first order, is obtained from

$$W^{\rm d}_{s_f\sigma_f s_i\sigma_i}(\boldsymbol{k}_f, \boldsymbol{\kappa}_f)$$
$$= C_{fi} \int \frac{d\boldsymbol{q}}{q^2 - q_0^2 - i\varepsilon} [(a_{k_f}^{(s_f)+} a_{k_i}^{(s_i)})\langle\psi_{k_f}|e^{-i\boldsymbol{q}\boldsymbol{r}}|\psi_{k_i}\rangle\langle\psi_{\kappa_f}|e^{i\boldsymbol{q}\boldsymbol{r}}(a_{\kappa_f}^{(\sigma_f)+} a_i^{(\sigma_i)})|\psi_i\rangle$$
$$- (a_{k_f}^{(s_f)+} \boldsymbol{\alpha} a_{k_i}^{(s_i)})\langle\psi_{k_f}|e^{-i\boldsymbol{q}\boldsymbol{r}}|\psi_{k_i}\rangle\langle\psi_{\kappa_f}|e^{i\boldsymbol{q}\boldsymbol{r}}(a_{\kappa_f}^{(\sigma_f)+} \boldsymbol{\alpha} a_i^{(\sigma_i)})|\psi_i\rangle] \qquad (2)$$

$$C_{fi} = \left(\frac{E_{k_i} + mc^2}{2E_{k_i}} \frac{E_{k_f} + mc^2}{2E_{d_f}} \frac{E_{\kappa_f} + mc^2}{2E_{\kappa_f}} \frac{1}{1 + [Z_T c/(E_i + mc^2)]^2}\right)^{1/2} \qquad \varepsilon = +0$$

where E_i is the total bound-state energy, Z_T is the target charge and the matrices $\boldsymbol{\alpha} = (\alpha_x, \alpha_y, \alpha_z)$ are the (magnetic) Dirac matrices (Bjorken and Drell 1964). The fourth component of the momentum transfer $(\boldsymbol{q}, q_0)$ is $q_0 = (E_{k_i} - E_{k_f})/c$, and $\boldsymbol{r}$ is the coordinate of the respective electron in the target reference frame. From equation (2), the plane-wave Born approximation is easily obtained by replacing ψ_{k_i} and ψ_{k_f} by plane waves. Hence, $\langle \psi_{k_f} | \exp(-\mathrm{i}\boldsymbol{q}\boldsymbol{r}) | \psi_{k_i} \rangle = \delta(\boldsymbol{q} + \boldsymbol{k}_f - \boldsymbol{k}_i)$ such that the momentum transfer is fixed, $\boldsymbol{q} = \boldsymbol{k}_i - \boldsymbol{k}_f$.

In the following we restrict ourselves to a coplanar symmetric geometry where both electrons are ejected in-plane with the impinging electron, such that $k_f = \kappa_f$, $\vartheta_{k_f} = \vartheta_{\kappa_f}$ and $\varphi_{k_f} - \varphi_{\kappa_f} = \pi$ (where k, ϑ_k, φ_k are the spherical coordinates of $\boldsymbol{k}$ and the z axis is taken along $\boldsymbol{k}_i$). Since in this case one has the symmetry property, $W^{\mathrm{d}}_{s_f\sigma_f s_i\sigma_i}(\boldsymbol{k}_f, \boldsymbol{\kappa}_f) = W^{\mathrm{d}}_{s_f\sigma_f s_i\sigma_i}(\boldsymbol{\kappa}_f, \boldsymbol{k}_f)$, all terms with equal final spin quantum numbers, $s_f = \sigma_f$, do not contribute to the spin sum in (1). Defining $\hat{W}_{s_f\sigma_f s_i\sigma_i} \equiv W^{\mathrm{d}}_{s_f\sigma_f s_i\sigma_i}(\boldsymbol{k}_f, \boldsymbol{\kappa}_f)/C_{fi}$, one is left with a sum of eight terms which are pairwise identical

$$\begin{aligned}
&\frac{\mathrm{d}^3\sigma}{\mathrm{d}E_{\kappa_f}\,\mathrm{d}\Omega_{\kappa_f}\,\mathrm{d}\Omega_{k_f}} \\
&\quad = \frac{2N_i}{8c^6 k_i}\,\kappa_f k_f \Delta E_{k_i} \Delta E_{k_f} \Delta E_{\kappa_f}\,\frac{1}{1+(Z_T c/\Delta E_i)^2} \\
&\quad \times [\,|\hat{W}_{+-+-} - \hat{W}_{-++-}|^2 + |\hat{W}_{-+-+} - \hat{W}_{+--+}|^2 \\
&\quad + |\hat{W}_{+--+} - \hat{W}_{-++-}|^2 + |\hat{W}_{-+--} - \hat{W}_{+---}|^2\,]
\end{aligned} \tag{3}$$

where $\Delta E_p \equiv E_p + mc^2$ with $p = i$, k_i, k_f and κ_f. For the evaluation of (2), four integrals have to be calculated numerically with the techniques described in the earlier paper

$$I^{\mathrm{d}}_{\substack{0\\ \lambda}} = \int \frac{\mathrm{d}\boldsymbol{q}}{q^2 - q_0^2 - \mathrm{i}\varepsilon} \langle \psi_{k_f} | \mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}} | \psi_{k_i} \rangle \langle \psi_{\kappa_f} | \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}} | \psi_{\partial_\lambda \psi_i} \rangle \qquad \lambda = z, \pm \tag{4}$$

where I^{d}_0 and I^{d}_λ refer to ψ_i and $\partial_\lambda \psi_i$, respectively. With the help of the definitions $\beta_0 \equiv 1 + c^2 k_{fz} k_i/(\Delta E_{k_f} \Delta E_{k_i})$, $\gamma_0 \equiv c^2 k_i/(\Delta E_{k_f} \Delta E_{k_i} \Delta E_{\kappa_f})$, $\gamma_i \equiv \mathrm{i}c^2/\Delta E_i$ and $\delta_i \equiv \gamma_i(\beta_0 \kappa_{fz}/\Delta E_{\kappa_f} - k_i/\Delta E_{k_i} - k_{fz}/\Delta E_{kf})$, the contributions to (3) take the following form

$$\begin{aligned}
\hat{W}_{\substack{+-+-\\ -+-+}} &= I^{\mathrm{d}}_0 \left(\beta_0 - \frac{c^2 \kappa_{fz}}{\Delta E_{\kappa_f}} \left(\frac{k_i}{\Delta E_{k_i}} + \frac{k_{fz}}{\Delta E_{k_f}} \right) - \frac{2c^2 \kappa_{f\pm} k_{f\mp}}{\Delta E_{k_f} \Delta E_{\kappa_f}} \right) - I^{\mathrm{d}}_z \delta_i - I^{\mathrm{d}}_\mp \gamma_i \beta_0 \frac{\kappa_{f\pm}}{\Delta E_{\kappa_f}} \\
\hat{W}_{\substack{+-++\\ -+--}} &= \mp I^{\mathrm{d}}_0 \frac{c^2 \kappa_{f\pm}}{\Delta E_{\kappa_f}} \left(\frac{k_i}{\Delta E_{k_i}} + \frac{k_{fz}}{\Delta E_{k_f}} \right) \mp I^{\mathrm{d}}_z \gamma_i \beta_0 \frac{\kappa_{f\pm}}{\Delta E_{\kappa_f}} \pm I^{\mathrm{d}}_\pm \delta_i \\
\hat{W}_{\substack{-+++\\ +---}} &= \pm I^{\mathrm{d}}_0 \frac{c^2 k_{f\pm}}{\Delta E_{k_f}} \left(\frac{k_i}{\Delta E_{k_i}} - \frac{\kappa_{fz}}{\Delta E_{\kappa_f}} \right) \mp I^{\mathrm{d}}_z \gamma_i \left(\gamma_0 k_{f\pm} \kappa_{fz} - \frac{k_{f\pm}}{\Delta E_{k_f}} \right) \\
&\quad \mp I^{\mathrm{d}}_\pm \gamma_i \left(\gamma_0 k_{f\pm} \kappa_{f\mp} - \frac{2k_i}{\Delta E_{k_i}} + \frac{2k_{fz}}{\Delta E_{k_f}} \right) \\
\hat{W}_{\substack{-++-\\ +--+}} &= -I^{\mathrm{d}}_0 \left[\frac{2c^2 \kappa_{fz}}{\Delta E_{\kappa_f}} \left(\frac{k_i}{\Delta E_{k_i}} - \frac{k_{fz}}{\Delta E_{k_f}} \right) - \frac{c^2 k_{f\pm} \kappa_{f\mp}}{\Delta E_{k_f} \Delta E_{\kappa_f}} \right] + I^{\mathrm{d}}_z \gamma_i \left(\gamma_0 k_{f\pm} \kappa_{f\mp} - \frac{2k_i}{\Delta E_{k_i}} + \frac{2k_{fz}}{\Delta E_{k_f}} \right) \\
&\quad - I^{\mathrm{d}}_\mp \gamma_i \left(\gamma_0 k_{f\pm} \kappa_{fz} - \frac{k_{f\pm}}{\Delta E_{k_f}} \right)
\end{aligned} \tag{5}$$

where the upper and lower signs correspond to the upper and lower spin combination of $\hat{W}_{s_f\sigma_f s_i\sigma_i}$, respectively.

The triply-differential cross sections for the K-shell ionization of Cu, Ag and Au by 300 keV and 500 keV electrons as a function of the emission angle are shown in figure 1. The energy of the outgoing electrons is fixed by energy conservation, $E_{k_f} = E_{\kappa_f} = (E_{k_i} + E_i)/2$. In the data from Nakel and his group (Bonfert *et al* 1991, Walters *et al* 1991) the binary peak around $\vartheta_{\kappa_f} = 40°$ is clearly visible for the lighter targets. It appears when the momentum transfer $\boldsymbol{q}$ matches the momentum $\boldsymbol{\kappa}_f$ of the secondary electron, provided the ratio Z_T/k_i is sufficiently small. This means that only small intrinsic momenta of the bound-state electron are required, the peak shape being determined by the momentum distribution of the bound state.

Comparison is made with the Coulomb Born theory (using Slater-screened wavefunctions and experimental binding energies) with and without the inclusion of spin-flip. It is found that consideration of spin-flip gives a significant enhancement of the cross sections, leading to an improved agreement with the experimental data. The only exception concerns the heaviest (Au) target with large discrepancies between theory and experiment.

Plane-wave Born results with the same choice of wavefunctions $\phi_i^{(\sigma_i)}$ and $\phi_f^{(\sigma_f)}$ and the same prescription for the exchange term (which, however, is no longer exact) are included in figure 1. As has been shown by Walters *et al* (1991), these results lead to a considerable overprediction of the experimental data for the heavier targets, the more so, when spin-flip is included. However, due to the similar structure of the two theories, the spin-flip enhancement is very much the same as that found in the Coulomb Born theory. Quantifying this enhancement by the ratio $R = \mathrm{d}^3\sigma(\text{flip})/\mathrm{d}^3\sigma(\text{non-flip})$ of the cross sections with and without consideration of spin-flip, we have found a difference between the PWBA and the Coulomb Born results for R of at most 10%. Also, R is rather insensitive to the choice of the target species (R_{Cu}, R_{Ag} and R_{Au} differ from each other by less than 10%). However, the spin-flip enhancement depends strongly on angle and on the collision energy. The increase of R with E_{k_i} is shown in figure 2 for a Cu target within the PWBA. R reaches a factor of 2 in the binary peak maximum at a kinetic energy $E_{k_i} - mc^2 \sim 1$ MeV, and spin-flip even is the dominant mechanism at the higher energies. Since the momentum transfer $\boldsymbol{q} = \boldsymbol{k}_i - \boldsymbol{k}_f$ increases (for fixed E_{k_i}) with angle, so does R. At ultrarelativistic energies, the focusing of the two electrons into the forward direction leads, however, to the largest spin-flip enhancement at small angles.

Making use of the similarities between the Coulomb Born and the plane-wave Born approximation which led to the correct estimate of the spin-flip enhancement in the PWBA, we apply in the following this much simpler theory for the investigation of wavefunction effects. First of all, we have studied the importance of describing the initial target state by an improved wavefunction. To this aim, we have replaced the Darwin function by a hydrogenic relativistic function

$$\phi_i^{(\sigma_i)}(\boldsymbol{r}) = u_i^{(\sigma_i)}\varphi_i(r) \qquad \varphi_i(r) = \frac{1}{\sqrt{\pi}} Z_T^{3/2}\, \mathrm{e}^{-Z_T r}(2Z_T r)^{\gamma-1}\frac{1}{\sqrt{\Gamma(2\gamma+1)}}$$

$$u_i^{(+)} = \begin{pmatrix} \sqrt{1+\gamma} \\ 0 \\ \mathrm{i}\sqrt{1-\gamma}\cos\theta \\ \mathrm{i}\sqrt{1-\gamma}\sin\theta\,\mathrm{e}^{\mathrm{i}\varphi} \end{pmatrix} \qquad u_i^{(-)} = \begin{pmatrix} 0 \\ \sqrt{1+\gamma} \\ \mathrm{i}\sqrt{1-\gamma}\sin\theta\,\mathrm{e}^{-\mathrm{i}\varphi} \\ -\mathrm{i}\sqrt{1-\gamma}\cos\theta \end{pmatrix} \tag{6}$$

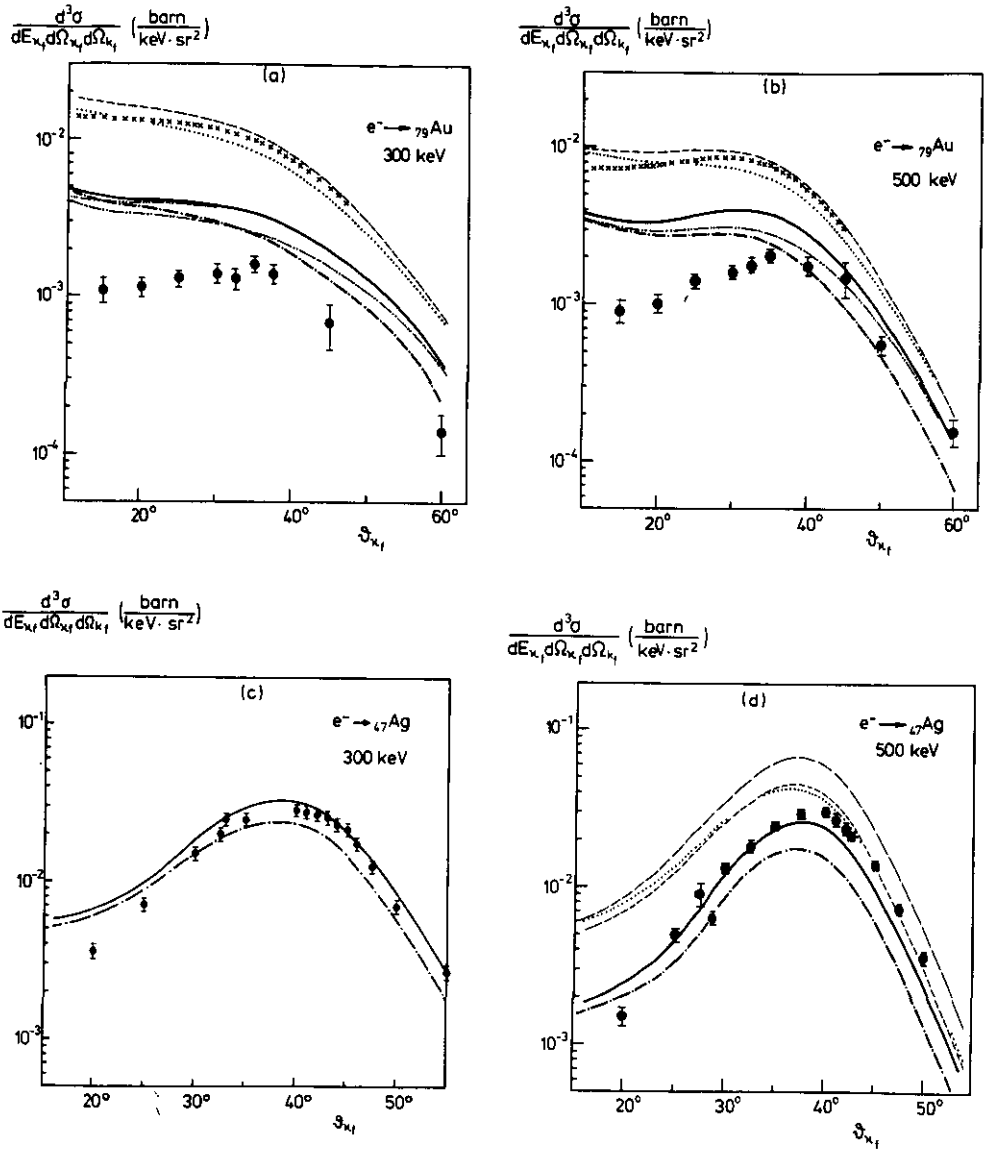

Figure 1. Triply-differential cross sections for K-shell ionization of Au (*a*), (*b*), Ag (*c*), (*d*) and Cu (*e*), (*f*) by 300 keV and 500 keV electrons in coplanar symmetric geometry as a function of emission angle ϑ_{x_f}. Shown are the data (●) from Bonfert *et al* (1991) and Walters *et al* (1991) in comparison with theory: Coulomb Born theory with spin-flip (——) and without spin-flip (—·—), plane-wave Born theory with (— —) and without (– – –) spin-flip, all theories with a Darwin K-shell function. Also shown is the PWBA without spin-flip, using a Dirac K-shell function (····), and using Darwin functions for the bound and free secondary electron (×××), as well as the spin-flip Coulomb Born theory with the correction factor F_i(—··—) and with the correction factor F_{ee} (—···—).

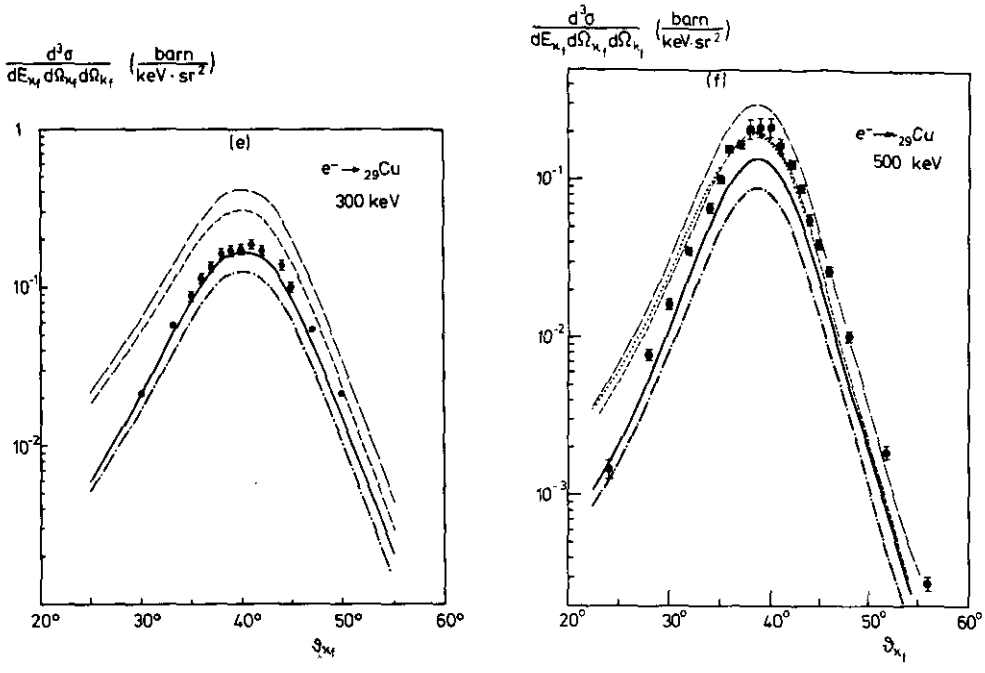

Figure 1. (continued)

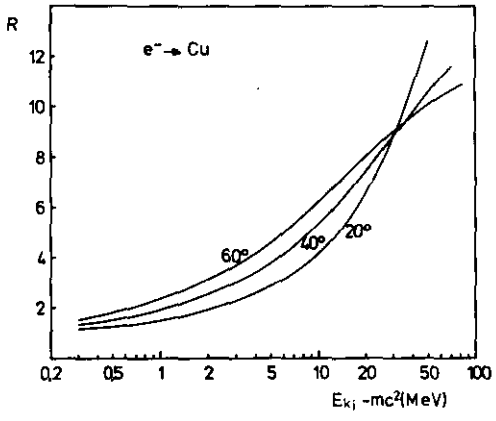

Figure 2. Ratio R between the triply-differential PWBA cross sections for K-shell ionization of Cu, calculated with and without inclusion of spin-flip, respectively, as a function of impact energy E_{k_i} for the emission angles $\vartheta_{\kappa_f} = 20°$, 40° and 60°.

where $\gamma = (1-(Z_T/c)^2)^{1/2}$ and r, θ, φ are the spherical coordinates of $\boldsymbol{r}$ with $\boldsymbol{k}_i$ as quantization axis. With this function, the target ionization matrix elements $\langle \phi_f^{(\sigma_f)}| \exp(i\boldsymbol{q}\boldsymbol{r})|\phi_i^{(\sigma_i)}\rangle$ and $\langle \phi_f^{(\sigma_f)}| \exp(i\boldsymbol{q}\boldsymbol{r})\boldsymbol{\alpha}|\phi_i^{(\sigma_i)}\rangle$ can no longer be given in closed form; however, the integral over the azimuthal angle can be evaluated analytically if the reference frame of $\boldsymbol{r}$ is rotated by $-\vartheta_{\kappa_f}$ such that the new quantization axis is aligned with $\boldsymbol{\kappa}_f$. Transforming $r\cos\theta$ and $r\sin\theta\exp(\pm i\varphi)$ occurring in $u_i^{(\sigma_i)}$ into the rotated frame and carrying out the spinor multiplications, one is left with a series of two-

dimensional integrals entering into $W^{\mathrm{d}}_{s_f\sigma_f s_i\sigma_i}$

$$\int \mathrm{d}\boldsymbol{r}\,\psi^*_{\kappa_f}(\boldsymbol{r})\,\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}}\,\varphi_i(r)\begin{pmatrix}1\\ x\\ \sqrt{1-x^2}\cos\varphi_r\\ \sqrt{1-x^2}\sin\varphi_r\end{pmatrix}$$

$$= 2\pi N_\kappa \int_0^\infty \mathrm{d}r \int_{-1}^{1} \mathrm{d}x \begin{pmatrix} J_0(y)\\ xJ_0(y)\\ \mathrm{i}\sqrt{1-x^2}\,J_1(y)\\ 0\end{pmatrix} r^{\gamma+1}\,\mathrm{e}^{-Z_{\mathrm{T}}r}$$

$$\times \mathrm{e}^{-\mathrm{i}\kappa_f rx}\,{}_1F_1(\mathrm{i}\eta_\kappa, 1, \mathrm{i}\kappa_f r(1+x))\,\mathrm{e}^{\mathrm{i}qrx\cos\vartheta_{q,\kappa_f}} \tag{7}$$

which have been written in vector form in (7). The normalization constant is $N_\kappa = \pi^{-2}(\Gamma(2\gamma+1))^{-1/2}2^{\gamma-5/2}Z_{\mathrm{T}}^{\gamma+1/2}\exp(\pi\eta_\kappa/2)\Gamma(1-\mathrm{i}\eta_\kappa)$ with $\eta_\kappa = Z_{\mathrm{T}}/\kappa_f$, $x = \cos\vartheta_r$ with ϑ_r, φ_r the angular coordinates of $\boldsymbol{r}$ in the rotated frame, and $y = qr(1-x^2)^{1/2}\sin\vartheta_{q,\kappa_f}$. The functions $J_0(y)$ and $J_1(y)$ are Bessel functions, and ${}_1F_1$ is a confluent hypergeometric function (for which it is necessary to use the asymptotic expansion for large arguments $\kappa_f r(1+x) \gtrsim 20$).

The results of a PWBA calculation with $\phi_i^{(\sigma_i)}$ from (6), excluding spin-flip, are also plotted in figure 1. For Cu (figure 1(*f*)) and to a somewhat lesser extent for Ag (figure 1(*d*)), the difference between the results using a Darwin function or the Dirac functtion (6) for the K-shell electron, respectively, is rather small. This difference is somewhat greater on the wings of the binary peak where the larger intrinsic momenta of the bound state are enhanced due to the r^γ contraction of the relativistic wavefunction.

In contrast to the lighter targets, the wavefunction effects are very large for the Au target. From figures 1(*a*), (*b*) it follows that the use of the relativistic function (6) reduces the cross section by ~30% near the binary peak maximum. Since the target ionization is described in terms of the same matrix elements both in PWBA and in the Coulomb Born theory, the wavefunction effects are presumably much alike in both theories. Hence, we have derived a correction factor F_i as the ratio between the non-flip PWBA results obtained with a Dirac and a Darwin function, respectively, and have multiplied the Coulomb Born spin-flip cross sections by F_i. As seen in figures 1(*a*), (*b*) this procedure provides an improved agreement with the data at angles above 30°.

As a next step in investigating wavefunction effects, we have used Darwin functions for both states, $\phi_f^{(\sigma_f)}$ and $\phi_i^{(\sigma_i)}$, of the secondary electron, as has been done in the PWBA calculations given in Bonfert *et al* (1991) or Jakubassa-Amundsen (1989). The effect of describing $\phi_f^{(\sigma_f)}$ by a Darwin function is readily seen in the PWBA results of Walters *et al* (1991) where this theory is compared with the one using Coulomb waves for $\phi_f^{(\sigma_f)}$ like in (2): While both theories nearly coincide for Cu and Ag, the cross sections are substantially reduced for the Au target when the improved (Darwin) function is used. For the sake of completeness, we have included the non-flip PWBA results with Darwin functions for $\phi_i^{(\sigma_i)}$ and $\phi_f^{(\sigma_f)}$ in figures 1(*a*), (*b*). Assuming tentatively that a similar reduction occurs when each of the states $\psi_f^{(s_f)}$ and $\psi_i^{(s_i)}$ of the primary electron is replaced by a Darwin function, and applying this estimate to the Coulomb Born theory, one expects to get a total reduction of about a factor of 2 at the smaller angles. This would bring the Au results to a reasonable agreement with the data for $\vartheta_{\kappa_f} \gtrsim 20°$.

So far, only the decrease of the Au data for angles below 20° remains unexplained, where theory provides increasing cross sections. In this context it should be noted that the first-order treatment of the electron-electron coupling in (2) breaks down for $\vartheta_{\kappa_f} \to 0$, because the two outgoing electrons will acquire the same momenta, $\kappa_f \to k_f$, with the result of a strong interelectronic repulsion. Brauner *et al* (1989) have considered the electron-electron interaction non-perturbatively by replacing the two-electron final state $|\psi_f^{(s_f)}\phi_f^{(\sigma_f)}\rangle$ by a distorted wave $|\psi_f^{(s_f)}\phi_f^{(\sigma_f)}\chi_f\rangle$ with $\chi_f = \exp(\pi\eta_{ee}/2)\Gamma(1+i\eta_{ee})\,{}_1F_1(-i\eta_{ee}, 1, -i(k_{ee}r + \boldsymbol{k}_{ee}\boldsymbol{r}))$ where $\eta_{ee} = -1/(2k_{ee})$, $\boldsymbol{r}$ is the interelectronic coordinate and $\boldsymbol{k}_{ee} = (\boldsymbol{\kappa}_f - \boldsymbol{k}_f)/2$ the relative momentum of the two outgoing electrons. Similar distorted-wave prescriptions are often simplified by using peaking approximations which reduce the effect of distortion simply to the normalization constant of χ_f (Garibotti and Miraglia 1980). Following this idea, we estimate the reduction of the (e, 2e) cross section by the interelectronic repulsion by scaling the Coulomb Born results with the correction factor F_{ee}

$$F_{ee} = e^{\pi\eta_{ee}}|\Gamma(1+i\eta_{ee})|^2 = \frac{2\pi|\eta_{ee}|}{e^{2\pi|\eta_{ee}|}-1}. \tag{8}$$

For 300 keV electron impact where the effect of F_{ee} is largest, one finds only a rather small reduction of the cross section ($\lesssim 10\%$) at angles above 10° (figure 1(*a*)), because the electronic momenta and hence k_{ee} are very large.

In conclusion, we have performed calculations of triply-differential electron emission cross sections in the Coulomb Born approximation, varying both impact velocity and target charge. We have found that this theory, when spin-flip is included, provides a reasonable explanation of the binary-peak data for the two lighter targets (Cu and Ag). Large discrepancies persist, however, for the heaviest (Au) target, particularly at small electron angles. The consideration of the electron-electron repulsion in an approximate non-perturbative way improves only marginally the agreement with experiment. The use of a more accurate (relativistic) wavefunction for the bound electron or for a continuum electron has a considerable effect on the cross section for the Au target, while leading only to small corrections for Cu or Ag. Clearly, the use of exact relativistic wavefunctions for all electronic states is required in order to give a better accord with the data on electron ejection from very heavy targets.

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