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Relativistic theory for *K*-shell ionisation by fast electrons

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The first-order Born approximation is applied for the calculation of the triply differential cross section for electron ejection from heavy target atoms. For the impinging electron, Coulomb waves as well as plane waves are used, and the exchange interaction is correctly accounted for. Two examples are considered, $e^- + \mathrm{Ag}$ and $e^- + \mathrm{Ta}$. While for Ag, reasonable agreement with the experimental spectra is obtained with plane waves, the much heavier Ta target requires the use of Coulomb waves for the continuum electronic states.

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1. Introduction

The formulation of a relativistic theory for electron impact ionisation dates back to the early thirties [1, 2], but a series of experiments on ionisation cross sections at relativistic collision energies [3–5] has called for a theoretical reinvestigation of that subject [6–9]. The various models account for the electron-electron interaction in a first-order approximation, including the relativistic current-current coupling. The projectile electron is described in terms of relativistic plane waves; the calculations differ, however, in the treatment of the active target electron. In the original Møller theory, Darwin functions are used [1, 6, 7]. These wavefunctions are based on a semirelativistic approximation and are accurate up to the order of $(Z_T/c)^2$ where Z_T is the target charge [10]. Later, the Darwin functions have been substituted by product functions consisting of nonrelativistic hydrogenic functions which are multiplied by a Dirac spinor [8]. An improvement upon these wavefunctions consists in the choice of a Sommerfeld-Maue function for the continuum state, which is a high-energy approximation to the relativistic Coulomb wave [9]. It has been shown, however, that the ionisation cross section is rather insensitive to these different continuum functions [7, 9], and the agreement with total cross section measurements is in general quite satisfactory [6, 8, 9].

A more stringent test of the theories has recently become available from experimental data on cross sections which are differential with respect to the momenta of the two outgoing electrons [11, 12]. The exchange interaction can no longer be neglected, but even if it is included via the Ochkur approximation [13], large discrepancies between theory and experiment have been found, which increase strongly with target charge [9, 11, 12]. Partly, these discrepancies are due to an insufficient treatment of the exchange interaction, as the Ochkur approximation implies a peaking approximation [14] which is highly inappropriate for large momenta of the ejected target electron. More importantly, for heavy targets the Sommerfeld parameter η is no longer small compared to $1/(2\pi)$ at near-relativistic impact velocities, which calls for a modification of the plane-wave description of the impinging electron.

In this work the theory is improved by preserving exchange symmetry which is most easily achieved if in addition, the target Coulomb field is accounted for in the wavefunctions of *both* electrons. A description in terms of relativistic target eigenfunctions has recently been carried out for collision energies up to 150 keV [15], but the exchange interaction has not been included exactly. Also, the partial-wave expansion applied in this calculation becomes prohibitive at much higher impact energies.

Therefore, an approximation to the electronic wavefunction is chosen which allows the coupling matrix elements to be represented by a closed expression. In the next section, the relativistic Born theory for ionisation is reformulated, and in Sect. 3, three approximations for the electronic wavefunctions are discussed, Dirac plane waves, Darwin functions as well

as product functions composed of nonrelativistic Coulomb waves and Dirac spinors. A comparison of the results with experimental data and with previous calculations is presented in Sect. 4 for the impact of 500 keV electrons on Ag and Ta. Concluding remarks follow (Sect. 5). Atomic units ($\hbar=m=e=1$) are used unless otherwise indicated.

2. Derivation of the ionisation cross section

When treating the ionisation of N-electron targets by low- to moderate-energy electrons it is common to use close-coupling electronic wavefunctions which provide an accurate representation of the full $(N+1)$ electron problem [16, 17]. Such elaborate wavefunctions are, however, only necessary in the case of inclusive cross sections where neither the initial nor the final electronic target states are specified. Already in this case a single-channel approximation may be sufficient if the relevant electronic configurations have a large energy spacing [17]. For the calculation of triply differential cross sections where the initial and final states of the electrons are fixed by the kinematical conditions (the target being finally in its ground state), an independent electron model can be used [18]. The restriction to only two electrons, the projectile electron as well as the active target electron, is especially suited for ionisation of the inner shells of heavy targets which are widely separated in energy from adjacent shells. Moreover, at relativistic velocities, the transferred energy is in general much larger than the correlation energy of the target electrons, and it is sufficient to consider the transition matrix element describing the relativistic coupling between the projectile and one target electron [19]

$$\begin{aligned} &S_{\mathrm{fi}}=S_{\mathrm{fi}}^{d}-S_{\mathrm{fi}}^{\mathrm{ex}} \\ &S_{\mathrm{fi}}^{d}=-i\,\mathrm{e}\int \mathrm{d}^4x_2\,\bar{\phi}_f^{(\sigma_f)}(x_2)\,\mathbb{A}(x_2)\,\phi_i^{(\sigma_i)}(x_2) \end{aligned} \tag{2.1}$$

where ϕ_i and ϕ_f are the initial and final wavefunctions of the target electron, the upper index denoting the spin degrees of freedom. $\mathbb{A}$ is the electromagnetic potential created by the projectile (in the Lorentz gauge)

$$\begin{aligned} \mathbb{A}(x_2)&=\sum_{\mu=0}^{3}\gamma_{2\mu}\int \mathrm{d}^4x_1\,D_F(x_2-x_1)\,J^{\mu}(x_1) \\ J^{\mu}(x)&=-\mathrm{e}\,\bar{\psi}_f^{(s_f)}(x)\,\gamma_1^{\mu}\,\psi_i^{(s_i)}(x) \\ D_F(x)&=-\frac{1}{2\pi^2 c}\frac{1}{\sqrt{2\pi}}\int\frac{\mathrm{d}^4q}{q^2+i\varepsilon}\,\mathrm{e}^{-iqx},\qquad \varepsilon\to 0 \end{aligned} \tag{2.2}$$

where J^{μ} is the transition matrix element of the projectile current from the initial state ψ_i to the final state ψ_f, γ_i^{μ} are Dirac matrices for particle i ($i=1$: projectile, $i=2$: target electron), and D_F is the photon propagator. The electron charge e is set equal to unity in the following. The exchange contribution $S_{\mathrm{fi}}^{\mathrm{ex}}$ is obtained from the direct term S_{fi}^{d} through an interchange of ϕ_f and ψ_f. Explicitly, one has with $\bar{\psi}=\psi^{+}\gamma^0$

$$\begin{aligned} S_{\mathrm{fi}}^{d}=&-\frac{i}{2\sqrt{2}\,\pi^{5/2}c}\int\frac{\mathrm{d}^4q}{q^2+i\varepsilon} \\ &\cdot\Big[\int \mathrm{d}^4x_1\,\psi_f^{(s_f)+}(x_1)\,\mathrm{e}^{\mathrm{i}qx_1}\,\psi_i^{(s_i)}(x_1) \\ &\cdot\int \mathrm{d}^4x_2\,\phi_f^{(\sigma_f)+}(x_2)\,\mathrm{e}^{-\mathrm{i}qx_2}\phi_i^{(\sigma_i)}(x_2) \\ &-\int \mathrm{d}^4x_1\,\psi_f^{(s_f)+}(x_1)\,\mathrm{e}^{\mathrm{i}qx_1}\,\boldsymbol{\alpha}_1\,\psi_i^{(s_i)}(x_1) \\ &\cdot\int \mathrm{d}^4x_2\,\phi_f^{(\sigma_f)+}(x_2)\,\mathrm{e}^{-\mathrm{i}qx_2}\,\boldsymbol{\alpha}_2\,\phi_i^{(\sigma_i)}(x_2)\Big] \end{aligned} \tag{2.3}$$

where $\boldsymbol{\alpha}_{1,2}$ are Dirac matrices and q is the transferred four-momentum.

Without further specification of the wavefunctions only the time integrals ($x^0=ct$) can be carried out. Using $qx=E_qt-\mathbf{qx}$ as well as the normalisation $\psi_{\mathbf{k}}(x)=(2\pi)^{-1/2}\psi_{\mathbf{k}}(\mathbf{x})\exp(-\mathrm{i}Et)$ for a continuum function where $\psi_{\mathbf{k}}(\mathbf{x})$ is δ-normalised in momentum $\mathbf{k}$, each of the four-dimensional integrals is reduced to a three-dimensional integral in space multiplied by an energy-conserving δ-function. This makes the integration over $q_0=E_q/c$ trivial, and the transition matrix element reduces to

$$\begin{aligned} S_{\mathrm{fi}}^{d}=&\frac{i}{2\pi^2}\,\delta(E_{k_f}-E_{k_i}+E_{\kappa_f}-E_i)\,W_{s_f\sigma_f s_i\sigma_i}(\mathbf{k}_f,\boldsymbol{\kappa}_f) \\ W_{s_f\sigma_f s_i\sigma_i}(\mathbf{k}_f,\boldsymbol{\kappa}_f)=&\int\frac{\mathrm{d}\,\mathbf{q}}{\mathbf{q}^2-q_0^2-i\varepsilon} \\ &\cdot\Big[\int \mathrm{d}\,\mathbf{x}_1\,\psi_f^{(s_f)+}(\mathbf{x}_1)\,\mathrm{e}^{-\mathrm{i}\mathbf{q}\mathbf{x}_1}\psi_i^{(s_i)}(\mathbf{x}_1) \\ &\cdot\int \mathrm{d}\,\mathbf{x}_2\,\phi_f^{(\sigma_f)+}(\mathbf{x}_2)\,\mathrm{e}^{\mathrm{i}\mathbf{q}\mathbf{x}_2}\,\phi_i^{(\sigma_i)}(\mathbf{x}_2) \\ &-\int \mathrm{d}\,\mathbf{x}_1\,\psi_f^{(s_f)+}(\mathbf{x}_1)\,\mathrm{e}^{-\mathrm{i}\mathbf{q}\mathbf{x}_1}\,\boldsymbol{\alpha}_1\,\psi_i^{(s_i)}(\mathbf{x}_1) \\ &\cdot\int \mathrm{d}\,\mathbf{x}_2\,\phi_f^{(\sigma_f)+}(\mathbf{x}_2)\,\mathrm{e}^{\mathrm{i}\mathbf{q}\mathbf{x}_2}\boldsymbol{\alpha}_2\,\phi_i^{(\sigma_i)}(\mathbf{x}_2)\Big] \end{aligned} \tag{2.4}$$

where $q_0=(E_{k_i}-E_{k_f})/c$ and E_{k_i} and E_{k_f} are the total energies of the impinging electron in the initial and final state, respectively, $\mathbf{k}_i$ and $\mathbf{k}_f$ being the corresponding momenta. Further, E_{κ_f} and E_i are the total energies of the target electron in its final and initial state, respectively, and $\boldsymbol{\kappa}_f$ is the final momentum.

The differential ionisation cross section in first order perturbation theory follows from the relativistic generalisation of the golden rule by means of summing over the final spins (s_f,σ_f) and averaging over the initial ones (s_i,σ_i) [19]

$$\begin{aligned} \mathrm{d}\sigma=&\frac{2\pi}{\hbar}\frac{1}{4}\sum_{\mathrm{spin}}|S_{\mathrm{fi}}|^2\,\delta(E_{k_f}-E_{k_i}+E_{\kappa_f}-E_i)^{-1} \\ &\cdot\mathrm{d}\,\mathbf{k}_f\,\mathrm{d}\,\boldsymbol{\kappa}_f\frac{(2\pi)^3\,E_{k_i}}{c^2\,k_i}. \end{aligned} \tag{2.5}$$

From this, the triply differential cross section for the ejection of N_i electrons from the shell i is easily obtained [2, 6]

$$\frac{\mathrm{d}\sigma}{\mathrm{d}E_{\kappa_f}\,\mathrm{d}\Omega_{\kappa_f}\,\mathrm{d}\Omega_{k_f}}=N_i\frac{1}{c^6\,k_i}\kappa_f\,E_{\kappa_f}\,k_f\,E_{k_f}\,E_{k_i}$$
$$\cdot\sum_{s_f\sigma_f s_i\sigma_i}|W_{s_f\sigma_f s_i\sigma_i}(\mathbf{k}_f,\boldsymbol{\kappa}_f)-W_{\sigma_f s_f s_i\sigma_i}(\boldsymbol{\kappa}_f,\mathbf{k}_f)|^2$$
$$E_{k_f}=E_{k_i}+E_i-E_{\kappa_f} \tag{2.6}$$

where Ω_{κ_f} and Ω_{k_f} are the solid angles of the two outgoing electrons.

3. Approximations

In order to specify the electronic wavefunctions we shall assume for reasons of simplicity that the target field is purely Coulombic, and that the effective charge is the same for all electronic states such that the mutual orthogonality and exchange symmetry can easily be accounted for. Still, the corresponding eigenfunctions, the relativistic Coulomb waves, do not exist in a closed form. We therefore have to resort to further approximations, even at the expense of orthogonality between bound and continuum electronic state. Like in the Møller theory, the bound target state is taken to be a Darwin function [7]

$$\phi_i^{(\sigma_i)}(\mathbf{x})=\left[1+\left(\frac{Z_T c}{E_i+mc^2}\right)^2\right]^{-1/2}a_i^{(\sigma_i)}\,\psi_i(\mathbf{x})$$

$$a_i^{(+)}=\begin{pmatrix}1\\0\\-ic\partial_z/(E_i+mc^2)\\-ic\partial_+/(E_i+mc^2)\end{pmatrix},\qquad a_i^{(-)}=\begin{pmatrix}0\\1\\-ic\partial_-/(E_i+mc^2)\\ic\partial_z/(E_i+mc^2)\end{pmatrix} \tag{3.1}$$

where the notation $\mathbf{x}=(x,y,z)$ has been introduced, $\partial_\pm=\partial/\partial x\pm i\partial/\partial y$, $\partial_z=\partial/\partial_z$, and ψ_i is a nonrelativistic bound hydrogenic function of the target with charge Z_T.

For the continuum states plane waves, Darwin functions as well as (nonrelativistic) Coulomb waves will be considered.

a) Plane wave – Coulomb approximation

For high collision energies, the Coulomb field is usually neglected for the projectile electron, such that its wavefunction reduces to a Dirac plane wave

$$\psi_{\mathbf{k}}^{(s)}(\mathbf{x})=(2\pi)^{-3/2}\sqrt{\frac{E_k+mc^2}{2E_k}}\,a_k^{(s)}\,\mathrm{e}^{\mathrm{i}\mathbf{k}\mathbf{x}}$$

$$a_k^{(+)}=\begin{pmatrix}1\\0\\ck_z/(E_k+mc^2)\\ck_+/(E_k+mc^2)\end{pmatrix},\qquad a_k^{(-)}=\begin{pmatrix}0\\1\\ck_-/(E_k+mc^2)\\ck_z/(E_k+mc^2)\end{pmatrix} \tag{3.2}$$

where $k_\pm=k_x\pm ik_y$.

With this approximation, the momentum integral in the direct term becomes trivial, such that one has

$$W_{s_f\sigma_f s_i\sigma_i}(\mathbf{k}_f,\boldsymbol{\kappa}_f)$$
$$=\frac{1}{\mathbf{q}^2-q_0^2-i\varepsilon}\sqrt{\frac{E_{k_f}+mc^2}{2E_{k_f}}}\sqrt{\frac{E_{k_i}+mc^2}{2E_{k_i}}}$$
$$\cdot\left[(a_{k_f}^{(s_f)+}a_{k_i}^{(s_i)})\int\mathrm{d}\,\mathbf{x}_2\,\phi_f^{(\sigma_f)+}(\mathbf{x}_2)\,\mathrm{e}^{\mathrm{i}\mathbf{q}\mathbf{x}_2}\,\phi_i^{(\sigma_i)}(\mathbf{x}_2)\right.$$
$$\left.-(a_{k_f}^{(s_f)+}\boldsymbol{\alpha}_1\,a_{k_i}^{(s_i)})\int\mathrm{d}\,\mathbf{x}_2\,\phi_f^{(\sigma_f)+}(\mathbf{x}_2)\,\mathrm{e}^{\mathrm{i}\mathbf{q}\mathbf{x}_2}\,\boldsymbol{\alpha}_2\,\phi_i^{(\sigma_i)}(\mathbf{x}_2)\right] \tag{3.3}$$

with fixed momentum transfer $\mathbf{q}=\mathbf{k}_i-\mathbf{k}_f$.

Like the bound electron, also the ejected target electron may be described by a Darwin function [6, 7, 9]; this choice together with (3.2) is, however, only consistent if its momentum κ_f is much smaller than the momentum k_f of the projectile electron:

$$\phi_f^{(\sigma_f)}(\mathbf{x})=\left[1+\left(\frac{\kappa_f c}{E_{\kappa_f}+mc^2}\right)^2\right]^{-1/2}a_f^{(\sigma_f)}\,\psi_{\boldsymbol{\kappa}_f}(\mathbf{x}). \tag{3.4}$$

The spinor $a_f^{(\sigma_f)}$ is obtained from $a_i^{(\sigma_i)}$ in (3.1) by replacing E_i with E_{κ_f}, while $\psi_{\boldsymbol{\kappa}_f}(\mathbf{x})$ is a nonrelativistic Coulomb wave. It is easily verified that the Darwin function (3.4) coincides for vanishing target charge (where $\psi_{\boldsymbol{\kappa}_f}$ reduces to a plane wave) with the Dirac plane wave (3.2).

If the derivatives contained in $a_f^{(\sigma_f)}$ only act on the plane wave part of ψ_{κ_f}, but not on the confluent hypergeometric function, a still simpler approximation to ϕ_f is found. In this case, ϕ_f factorises into a Dirac spinor times a Coulomb wave

$$\phi_f^{(\sigma_f)}(\mathbf{x}) \approx \sqrt{\frac{E_{\kappa_f}+mc^2}{2E_{\kappa_f}}}\, a_{\kappa_f}^{(\sigma_f)}\, \psi_{\kappa_f}(\mathbf{x}) \tag{3.5}$$

with $a_k^{(s)}$ from (3.2). For the systems presently investigated, the two approximations (3.4) and (3.5) lead to very similar results for the differential cross section (see Sect. 4).

If the wavefunctions (3.4) or (3.5) and (3.1) are inserted into the direct term, (2.4), the matrix element of $\exp(\mathrm{i}\,\mathbf{q}\mathbf{x}_2)$ does not vanish for $q=0$ because the Darwin functions are not orthogonal. This deficiency has to be compensated by the requirement that the other pair of functions, ψ_i and ψ_f, must be orthogonal such that the singularity from the propagator at small q is damped out. This requirement is fulfilled for the plane waves (3.2).

The situation is, however, different for the exchange term. There, ϕ_i is connected with ψ_f and ψ_i with ϕ_f, such that with the above choice of the wavefunctions, none of the two matrix elements will contain mutually orthogonal functions, which in turn will lead to a severe overestimation of the exchange contribution. We have, instead, retained orthogonality by approximating $\psi_f^{(s_f)}$ by a Darwin function or by a function of the type (3.5), but taking for $\phi_f^{(\sigma_f)}$ a Dirac plane wave, i.e. by using *different* wavefunctions than for the direct term. With this approximation, the exchange term follows as in the exact formulation (2.6), from the direct term by means of interchanging $\mathbf{k}_f$ with $\boldsymbol{\kappa}_f$ and s_f with σ_f, and the cross section reduces to an analytical expression. In this manner, exchange symmetry in the total transition amplitude is preserved, despite of the approximations necessary for its evaluation.

The calculation of the cross section is done in a similar way as indicated by Moiseiwitsch and coworkers [6, 7] where, however, exchange had been neglected as only total cross sections were considered. In contrast to that work we disregard spin-flip because it contributes at most 10% to the total cross sections at impact energies below a few MeV [6]. Then the spin sum is only composed of four direct terms and four exchange terms.

There occur two types of matrix elements if the approximation (3.5) is used for the continuum electronic state

$$\begin{aligned} F_{\mathrm{fi}}(\mathbf{q}) &= \langle \psi_{\kappa_f}(\mathbf{r}) \,|\, \mathrm{e}^{\mathrm{i}\,\mathbf{q}\mathbf{r}} \,|\, \psi_i(\mathbf{r})\rangle \\ A_{\mathrm{fi}}^{\tau}(\mathbf{q}) &= \langle \psi_{\kappa_f}(\mathbf{r}) | \mathrm{e}^{\mathrm{i}\,\mathbf{q}\mathbf{r}} | \,\partial_\tau \psi_i(\mathbf{r})\rangle. \qquad \tau = z, \pm. \end{aligned} \tag{3.6}$$

In case of a $1s$ initial state and hydrogenic wavefunctions, these matrix elements take the form

$$\begin{aligned} &F_{\mathrm{fi}}(\mathbf{q}) = N_0\, \tilde{F}_{\mathrm{fi}}(\mathbf{q}); \\ &\tilde{F}_{\mathrm{fi}}(\mathbf{q}) = (1+i\eta_\kappa)\frac{1}{A_1} + (1-i\eta_\kappa)\frac{1}{B_1} \\ &A_{\mathrm{fi}}^{\tau}(\mathbf{q}) = N_0\, \tilde{A}_{\mathrm{fi}}^{\tau}(\mathbf{q}); \\ &\tilde{A}_{\mathrm{fi}}^{\tau}(\mathbf{q}) = -i\left[i\eta_\kappa\, q_\tau \frac{1}{A_1} + (1-i\eta_\kappa)(q_\tau - \kappa_{f\tau})\frac{1}{B_1}\right] \\ &N_0 = \frac{2\sqrt{2}}{\pi} Z_T^{5/2}\, \mathrm{e}^{\pi\eta_\kappa/2}\, \Gamma(1-i\eta_\kappa)\, A_1^{-i\eta_\kappa}\, B_1^{-1+i\eta_\kappa} \end{aligned} \tag{3.7}$$

with $q_\pm = q_x \pm i q_y$ and the abbreviations

$$\begin{aligned} &A_1 = q^2 - (\kappa_f + iZ_T)^2, \qquad B_1 = Z_T^2 + (\mathbf{q}-\boldsymbol{\kappa}_f)^2, \\ &\eta_\kappa = Z_T/\kappa_f. \end{aligned} \tag{3.8}$$

The evaluation of the spinor parts of the transition amplitude is simple but tedious. Denoting by $M^d_{s_f\sigma_f s_i\sigma_i}$ the direct and by $M^{\mathrm{ex}}_{\sigma_f s_f s_i \sigma_i}$ the exchange contribution, the differential cross section for K-shell ionisation can be written in the following way

$$\begin{aligned} \frac{\mathrm{d}\sigma^{PC}}{\mathrm{d}E_{\kappa_f}\,\mathrm{d}\Omega_{\kappa_f}\,\mathrm{d}\Omega_{k_f}} &= N_{\mathrm{fi}}\big[|M^d_{++++}(\mathbf{q}) - M^{\mathrm{ex}}_{++++}(\mathbf{q})|^2 \\ &+ |M^{\mathrm{d}}_{----}(\mathbf{q}) - M^{\mathrm{ex}}_{----}(\mathbf{q})|^2 + |M^{\mathrm{d}}_{+--+}(\mathbf{q})|^2 \\ &+ |M^{\mathrm{d}}_{-++-}(\mathbf{q})|^2 + |M^{\mathrm{ex}}_{+--+}(\mathbf{q})|^2 + |M^{\mathrm{ex}}_{-++-}(\mathbf{q})|^2\big] \\ N_{\mathrm{fi}} &= \frac{2Z_T^5}{\pi^2 c^6 k_i}\, \kappa_f\, k_f \frac{1}{1+\left(\frac{Z_T c}{E_i+mc^2}\right)^2} (E_{k_i}+mc^2) \\ &\cdot (E_{k_f}+mc^2)(E_{\kappa_f}+mc^2) \end{aligned} \tag{3.9}$$

with $\mathbf{q} = \mathbf{k}_i - \mathbf{k}_f$. Taking the z-direction along $\mathbf{k}_i$ and introducing the following abbreviations

$$\begin{aligned} M^d_{s_f\sigma_f s_i\sigma_i}(\mathbf{q}) &= \frac{1}{\mathbf{q}^2 - q_0^2} \frac{A_1^{-i\eta_\kappa}}{B_1^{1-i\eta_\kappa}} \\ &\cdot \mathrm{e}^{\pi\eta_\kappa/2}\, \Gamma(1-i\eta_\kappa)\, \tilde{M}^d_{s_f\sigma_f s_i\sigma_i}(\mathbf{q}) \\ \tilde{M}_0(\mathbf{q}) &= \beta_0 \left(\tilde{F}_{\mathrm{fi}}(\mathbf{q}) - i\frac{c\kappa_{fz}}{E_{\kappa_f}+mc^2}\tilde{A}^z_{\mathrm{fi}}\frac{c}{E_i+mc^2}\right) \\ &+ i\left(\frac{ck_i}{E_{k_i}+mc^2} + \frac{ck_{fz}}{E_{k_f}+mc^2}\right) \\ &\cdot \left(\frac{c}{E_i+mc^2}\tilde{A}^z_{\mathrm{fi}} + i\frac{c\kappa_{fz}}{E_{\kappa_f}+mc^2}\tilde{F}_{\mathrm{fi}}\right) \\ \beta_0 &= 1 + \frac{ck_i}{E_{k_i}+mc^2}\frac{ck_{fz}}{E_{k_f}+mc^2} \end{aligned} \tag{3.10}$$

one finds

$$\tilde{M}^d_{++++}(\mathbf{q}) = \tilde{M}_0(\mathbf{q}) + \tilde{A}^+_{\mathrm{fi}} \frac{c}{E_i + mc^2}\left(-i\beta_0 \frac{c\kappa_{f-}}{E_{\kappa_f}+mc^2} + 2i\frac{ck_{f-}}{E_{k_f}+mc^2}\right)$$

$$\tilde{M}^d_{----}(\mathbf{q}) = \tilde{M}_0(\mathbf{q}) + \tilde{A}^-_{\mathrm{fi}} \frac{c}{E_i + mc^2}\left(-i\beta_0 \frac{c\kappa_{f+}}{E_{\kappa_f}+mc^2} + 2i\frac{ck_{f+}}{E_{k_f}+mc^2}\right)$$

$$\tilde{M}^d_{+-+-}(\mathbf{q}) = \tilde{M}_0(\mathbf{q}) - \frac{c\kappa_{f+}}{E_{\kappa_f}+mc^2}\left(i\beta_0 \tilde{A}^-_{\mathrm{fi}} \frac{c}{E_i+mc^2} + 2\frac{ck_{f-}}{E_{k_f}+mc^2}\tilde{F}_{\mathrm{fi}}\right)$$

$$\tilde{M}^d_{-+-+}(\mathbf{q}) = \tilde{M}_0(\mathbf{q}) - \frac{c\kappa_{f-}}{E_{\kappa_f}+mc^2}\left(i\beta_0 \tilde{A}^+_{\mathrm{fi}} \frac{c}{E_i+mc^2} + 2\frac{ck_{f+}}{E_{k_f}+mc^2}\tilde{F}_{fi}\right). \tag{3.11}$$

The exchange terms follow from the interchange of $\mathbf{k}_f$ and $\boldsymbol{\kappa}_f$. Because of the summation over spin in (3.9), spin interchange can be omitted.

b) Coulomb-Coulomb approximation

For very heavy targets the impinging electron will, even at rather high collision velocities, be strongly perturbed by the target field. Then, the plane-wave approximation (3.2) should be abandoned. Rather, the Coulomb approximation (3.5) may be chosen for all unbound electronic states entering into the transition matrix element (2.4), while the bound electron is still described by the Darwin function. The wavefunctions (3.5) are mutually orthogonal due to the properties of the Dirac spinors and Coulomb waves, and the choice of identical wavefunctions for all free electrons has the advantage of yielding a consistent exchange term.

If Coulomb waves are used, the momentum transfer $\mathbf{q}$ has no longer a fixed value. Instead, (3.9) has to be replaced by

$$\begin{aligned}
&\frac{\mathrm{d}\sigma^{CC}}{\mathrm{d}E_{\kappa_f}\,\mathrm{d}\Omega_{\kappa_f}\,\mathrm{d}\Omega_{k_f}} \\
&= N_{\mathrm{fi}} \frac{2\pi\eta_f}{1-\mathrm{e}^{-2\pi\eta_f}} \frac{2\pi\eta_i}{1-\mathrm{e}^{-2\pi\eta_i}} \frac{2\pi\eta_\kappa}{1-\mathrm{e}^{-2\pi\eta_\kappa}} \\
&\quad \cdot \Big[\Big|\int \mathrm{d}\mathbf{q}\,(\hat{C}^d_{\mathrm{fi}}(\mathbf{q})\,\hat{M}^d_{++++}(\mathbf{q}) - \hat{C}^{\mathrm{ex}}_{\mathrm{fi}}(\mathbf{q})\,\hat{M}^{\mathrm{ex}}_{++++}(\mathbf{q}))\Big|^2 \\
&\quad + \Big|\int \mathrm{d}\mathbf{q}\,\hat{C}^d_{\mathrm{fi}}(\mathbf{q})\,\hat{M}^d_{----}(\mathbf{q}) - \hat{C}^{\mathrm{ex}}_{\mathrm{fi}}(\mathbf{q})\,\hat{M}^{\mathrm{ex}}_{----}(\mathbf{q})\Big|^2 \\
&\quad + \Big|\int \mathrm{d}\mathbf{q}\,\hat{C}^d_{\mathrm{fi}}(\mathbf{q})\,\hat{M}^{\mathrm{d}}_{+-+-}(\mathbf{q})\Big|^2 \\
&\quad + \Big|\int \mathrm{d}\mathbf{q}\,\hat{C}^{\mathrm{d}}_{\mathrm{fi}}(\mathbf{q})\,\hat{M}^{\mathrm{d}}_{-+-+}(\mathbf{q})\Big|^2 \\
&\quad + \Big|\int \mathrm{d}\mathbf{q}\,\hat{C}^{\mathrm{ex}}_{\mathrm{fi}}(\mathbf{q})\,\hat{M}^{\mathrm{ex}}_{+-+-}(\mathbf{q})\Big|^2 \\
&\quad + \Big|\int \mathrm{d}\mathbf{q}\,\hat{C}^{\mathrm{ex}}_{\mathrm{fi}}(\mathbf{q})\,\hat{M}^{\mathrm{ex}}_{-+-+}(\mathbf{q})\Big|^2\Big]
\end{aligned} \tag{3.12}$$

where $\hat{M}^d_{s_f\sigma_f s_i\sigma_i}$ follows from $M^d_{s_f\sigma_f s_i\sigma_i}$ in (3.10) if the term $\exp(\pi\eta_\kappa/2)\,\Gamma(1-i\eta_\kappa)$ is omitted. The scattering matrix element $\hat{C}_{\mathrm{fi}}$ can be derived from Nordsieck's integral [20, 21]

$$\begin{aligned}
C^d_{\mathrm{fi}}(\mathbf{q}) &= \int \mathrm{d}\,\mathbf{r}\,\psi^*_{\mathbf{k}_f}(\mathbf{r})\,\mathrm{e}^{-i\mathbf{q}\mathbf{r}}\psi_{\mathbf{k}_i}(\mathbf{r}) \\
&= \mathrm{e}^{\pi\eta_i/2}\,\Gamma(1-i\eta_i)\,\mathrm{e}^{\pi\eta_f/2}\,\Gamma(1-i\eta_f)\,\hat{C}^d_{\mathrm{fi}} \\
\hat{C}^d_{\mathrm{fi}} &= -\frac{1}{(2\pi)^2}\,\mathrm{e}^{-\pi\eta_i}\,\alpha^{i\eta_i-1}\,\gamma^{i\eta_f-i\eta_i-1}(\gamma+\delta)^{-i\eta_f-1} \\
&\quad \cdot \Big\{{}_2F_1\left(1-i\eta_i, i\eta_f, 1; \frac{\alpha\delta-\beta\gamma}{\alpha(\gamma+\delta)}\right) \\
&\quad \cdot [\eta_f(k_f\gamma - k_i\delta) + \eta_i k_i(\gamma+\delta)] \\
&\quad + {}_2F_1\left(2-i\eta_i, 1+i\eta_f, 2; \frac{\alpha\delta-\beta\gamma}{\alpha(\gamma+\delta)}\right)\frac{(1-i\eta_i)\,\gamma\eta_f}{\alpha(\gamma+\delta)} \\
&\quad \cdot [k_i\delta(\alpha+\beta) - k_f\gamma(\alpha+\beta+\gamma+\delta)]\Big\}
\end{aligned} \tag{3.13}$$

where $\eta_i = Z_T/k_i$, $\eta_f = Z_T/k_f$ and ${}_2F_1$ is a hyergeometric function. For reasons of convergence, a coordinate transformation in the $\mathbf{q}$-integrals in (3.12) is necessary, $\mathbf{q}_1 = -\mathbf{q} - \mathbf{k}_f + \mathbf{k}_i$. Then, the variables take the following form

$$\begin{aligned}
&\mathbf{q} = \mathbf{k}_i - \mathbf{k}_f - \mathbf{q}_1 \\
&\alpha = q_1^2/2; \quad \beta = \mathbf{q}_1\mathbf{k}_f - i\varepsilon, \quad \varepsilon \to 0 \\
&\gamma = \mathbf{q}_1\,\mathbf{k}_i - q_1^2/2 + i\varepsilon; \\
&\delta = k_f\,k_i + \mathbf{k}_f(\mathbf{k}_i - \mathbf{q}_1) + i\varepsilon.
\end{aligned} \tag{3.14}$$

For plane waves, $C^d_{\mathrm{fi}}(\mathbf{q})$ is equal to a delta function $\delta(\mathbf{k}_i - \mathbf{k}_f - \mathbf{q}) = \delta(\mathbf{q}_1)$ and the result (3.9) is recovered. It should be noted, however, that $\hat{C}_{\mathrm{fi}}$ from (3.13) does *not* reduce to a δ-function in the limit $Z_T \to 0$, but vanishes instead. Rather, the δ-function emerges at $Z_T = 0$ from a second contribution to the derivative of Nordsieck's formula which is proportional to ε and omitted in (3.13). This is a similar behaviour as found for the Fourier transform of a Coulomb wave, and is peculiar to the Coulomb potential.

Even when $\hat{C}_{\mathrm{fi}}$ does not reduce to a delta function, the plane wave behaviour is found after carrying out the $\mathbf{q}_1$-integration: Although $\hat{C}_{\mathrm{fi}}$ becomes smaller for decreasing Z_T, it becomes more and more singular at $q_1 = 0$. The net result is a finite integral for $Z_T \to 0$.

4. Numerical results

We have performed calculations for 500 keV electrons on Ag and Ta for various polar angles of the two outgoing electrons in a coplanar geometry ($\varphi_{k_f} - \varphi_{\kappa_f} = 180°$, see Fig. 1). We have used experimental binding energies and hydrogenic wavefunctions with

the same Slater-screened nuclear charge for the bound and those free electronic states which are described by Coulomb functions. When Coulomb waves are used for the projectile, special care has to be taken as concerns the handling of the singularities in the $\mathbf{q}_1$-integral. Details of the numerical treatment are given in the appendix.

Figure 2 shows the differential cross section for Ta K-shell ionisation as a function of the kinetic electron energy $E_f = E_{k_f} - mc^2$ in comparison with experimental data [12]. Included are the calculations from Das and Konar [9] who use Dirac plane waves and the Ochkur approximation for the exchange contribution. This approximation not only strongly overestimates the experimental data, but in addition fails to reproduce the experimental slope and the symmetry around $E_f = 216.5$ keV for equal emission angles $\vartheta_{k_f} = \vartheta_{\kappa_f} = 30°$. Some improvement concerning the latter deficiency is obtained if the exchange contribution is treated according to (2.6). The replacement of the Darwin function by the product function (3.5) enhances the cross section only slightly. As far as the magnitude of the cross section is concerned, only the use of Coulomb waves brings about a noticable improvement; however, the theoretical values are still too large as compared to the data.

The strong angular and energy dependence of the electron spectra can be understood by recalling that in the plane wave case, the momentum dependence of the differential cross section is approximately given by

$$\frac{\mathrm{d}\sigma}{\mathrm{d}E_{\kappa_f}\,\mathrm{d}\Omega_{\kappa_f}\,\mathrm{d}\Omega_{k_f}} \sim \frac{1}{\mathbf{q}^4} |\langle \psi_{\kappa_f}(\mathbf{r}) | \, \mathrm{e}^{\mathrm{i}\mathbf{q}\mathbf{r}} | \psi_i(\mathbf{r}) \rangle|^2 \qquad (4.4)$$

since the prefactor of $A_{\mathrm{fi}}^{\pm}$ is small, $c/(E_i + mc^2) \ll 1$, and since the spinor part is not so strongly $\mathbf{q}$-dependent. From (4.4) it follows that the cross section is large if $q = |\mathbf{k}_i - \mathbf{k}_f|$ is small, but more importantly, if $\mathbf{q} \approx \boldsymbol{\kappa}_f$ for a spherical symmetric state ψ_i [14, 22]. Figure 1 shows for the specific example $\vartheta_{k_f} > \vartheta_{\kappa_f}$ that for small values of k_f, $\mathbf{q}$ is much more aligned with

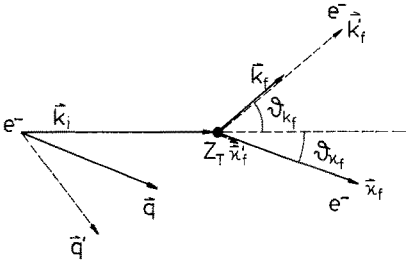

Fig. 1. Collision geometry, indicating the impinging electron (momentum $\mathbf{k}_i$), the scattered electron (momentum $\mathbf{k}_f$) and the ejected target electron (momentum $\boldsymbol{\kappa}_f$). Also given is the momentum transfer $\mathbf{q} = \mathbf{k}_i - \mathbf{k}_f$. Two cases are shown, small energy of the ejected electron (primed quantities) and large energy of the ejected electron (unprimed quantities)

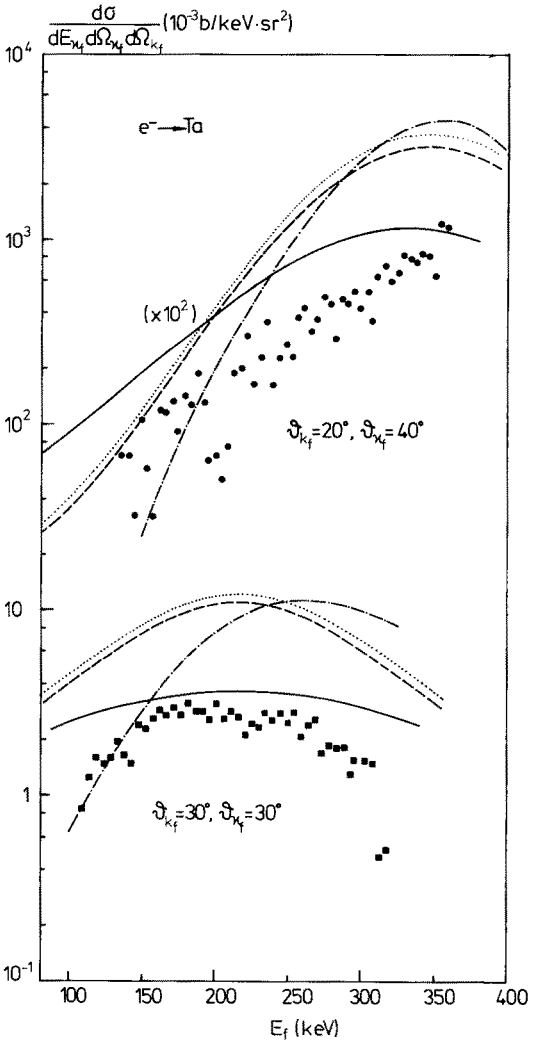

Fig. 2. Triply differential cross section for K-shell ionisation of Ta by 500 keV electrons in planar geometry ($\varphi_{k_f} - \varphi_{\kappa_f} = 180°$) as a function of the kinetic energy E_f of the scattered electron for emission angles $\vartheta_{k_f} = 20°$, $\vartheta_{\kappa_f} = 40°$ (top; all quantities are multiplied by a factor 100) and $\vartheta_{k_f} = \vartheta_{\kappa_f} = 30°$ (bottom). The experimental data (●, ■) from Ruoff and Nakel [12] are compared with calculations by Das and Konar [9] (dash-dotted curves, taken from [12]). The present calculations use Coulomb functions times Dirac spinors for all free electronic states (——), Dirac plance waves for the projectile and for the ejected target electron a Darwin function (——) or a Coulomb function times a Dirac spinor (.....)

$\boldsymbol{\kappa}_f$ than for large k_f. Correspondingly, the cross section increases with decreasing E_f (or increasing complementary energy $E_\kappa = E_{\kappa_f} - mc^2$, cf. Fig. 4). From exchange considerations it follows that for the other case, $\vartheta_{\kappa_f} > \vartheta_{k_f}$, the cross section increases with decreasing E_κ (or increasing E_f, see Fig. 2). For near-symmetric emission angles, a maximum shows up which eventually moves to the energy $E_\kappa = E_f = \frac{1}{2}(E_{k_i} + E_i) - mc^2$ for complete symmetry ($\vartheta_{\kappa_f} = \vartheta_{k_f}$).

If Coulomb waves are used instead of plane waves, the condition $\mathbf{k}_i - \mathbf{k}_f \approx \boldsymbol{\kappa}_f$ for large cross sections is

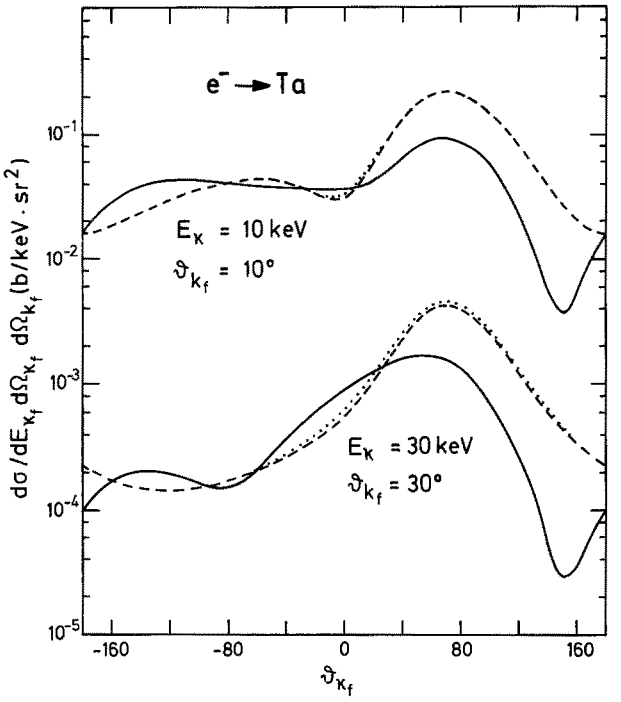

Fig. 3. Triply differential cross section for K-shell ionisation of Ta by 500 keV electrons in planar geometry ($\varphi_{k_f} - \varphi_{\kappa_f} = 180°$) as a function of the emission angle ϑ_{κ_f} for fixed kinetic energy $E_\kappa = 10$ keV and scattering angle $\vartheta_{k_f} = 10°$ (top) as well as for $E_\kappa = 30$ keV and $\vartheta_{k_f} = 30°$ (bottom). Calculations are shown for Dirac plane waves for the projectile together with a Darwin function for the ejected target electron, with exchange (----) and without exchange (.....), as well as for Coulomb functions times Dirac spinors for all free electrons without exchange (——)

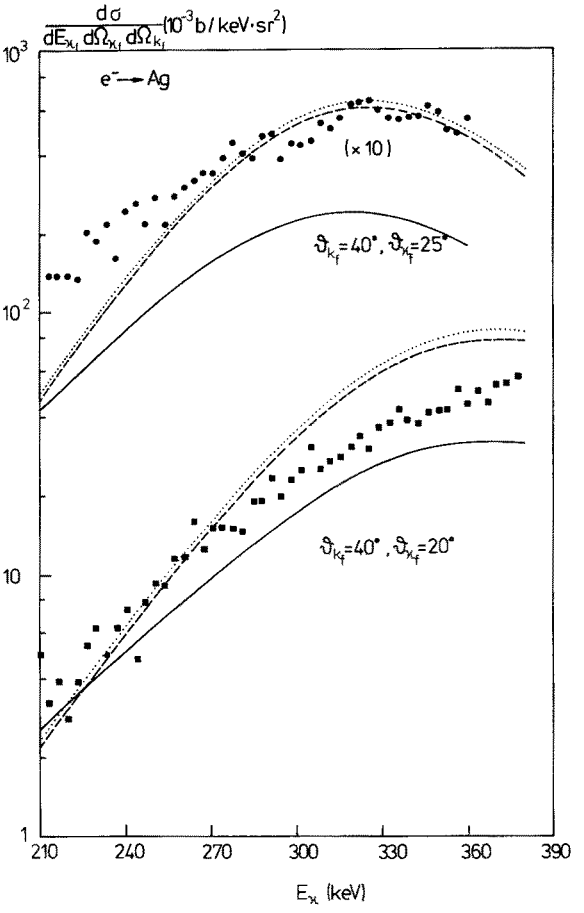

Fig. 4. Triply differential cross section for K-shell ionisation of Ag by 500 keV electrons in planar geometry ($\varphi_{k_f} - \varphi_{\kappa_f} = 180°$) as a function of the kinetic energy E_κ of the ejected electron for emission angles $\vartheta_{k_f} = 40°$, $\vartheta_{\kappa_f} = 25°$ (top; all quantities are multiplied by a factor of 10) and $\vartheta_{k_f} = 40°$, $\vartheta_{\kappa_f} = 20°$ (bottom). The experimental data (●, ■) from Schüle and Nakel [11] are compared with present calculations. For the definitions, see caption of Fig. 2

somewhat relaxed as $\mathbf{q}$ is smeared out around the value $\mathbf{k}_i - \mathbf{k}_f$, the more so, the heavier the target. Then, for $\mathbf{k}_i - \mathbf{k}_f \approx \boldsymbol{\kappa}_f$, the cross section is lowered in comparison with the plane wave case because there are nonaligned contributions to the $\mathbf{q}$-integral. Likewise, for the most mismatched case, the cross section will be higher. This results in a weaker energy dependence of the cross section than that obtained with plane waves.

For light targets such as He, apart from the "binary peak" at $\boldsymbol{\kappa}_f \approx \mathbf{q}$, another peak is observed in the opposite direction, $\boldsymbol{\kappa}_f \approx -\mathbf{q}$, if the momentum transfer to the target is small, and if in addition the energy E_κ of the ejected electron is low [23]. This double-lobe structure in an angular plot can be interpreted as the photoionisation limit [22] since the impact of a photon on spherically symmetric electronic states results in a p-wave pattern of the ejected electrons. The "recoil peak" should be observable when the collision energy is 5–10 times larger than the electronic binding energy [22]. Figure 3 shows that two peaks are present in the triply differential cross section as a function of the ejection angle ϑ_{κ_f} even for targets as heavy as Ta ($Z_T = 73$), although the relative intensity of the recoil peak diminishes rapidly with increasing scattering angle ϑ_{k_f} and electron energy E_κ. The current interpretation of the recoil peak as being due to a reflection of the electron on the target potential [23] is supported by the observation that this peak vanishes if the ejected electron is described by a plane wave [24]. Furthermore, the peak is more pronounced if scattering states are used for the impinging electron as well, instead of a free state (Fig. 3).

Figure 4 shows the energy dependence of the ionisation cross section in the case of an Ag target ($Z_T = 47$) at equal collision energy. As the binding energy is smaller, the cross section is in general higher than for Ta. The description with plane waves is much more successful for Ag than for Ta, in fact, this theory provides on the average the correct magnitude of the cross section as compared to experiment. The calcula-

tion with Coulomb waves improves on the slope of the cross section, but falls considerably below the experimental data, especially for the more symmetric case.

The reason for the discrepancies between the Coulomb wave theory and experiment for the present systems is not fully understood. The inclusion of screening effects in the continuum wavefunctions is supposed to alter the results only slightly, since the momentum transfer is so large that ionisation predominantly occurs at interelectronic distances which at most amount to the K-shell radius. Therefore, only the other K-shell electron and perhaps a few L-shell electrons will contribute to the screening. A calculation for Ag with a tentative effective charge of Z_T-4 in the Coulomb functions of the projectile electron changes the differential cross section by only ten percent or less. More seriously is probably the use of a Darwin function for the K-shell electron instead of an exact relativistic eigenfunction since the Darwin function does not possess the contraction factor r^{γ_K-1} with $\gamma_K=(1-Z_T^2/c^2)^{1/2}$ and hence will be inaccurate for very large momentum transfers. The comparison between Dirac and Darwin functions has been carried out for a uranium K-shell electron in the case of pair creation with subsequent K-shell capture, and has revealed differences of up to one order of magnitude, depending on the collision energy [25]. Generally, the influence of changes in the electronic wavefunctions on the differential ionisation cross section may be more significant if the target field is included in the projectile states than for the plane wave case, because the strong variation of the differential cross section with electron momentum produces a large sensitivity on the weight factor if the momentum transfer $\mathbf{q}$ is smeared out.

5. Conclusion

We have calculated triply differential cross sections for K-shell ionisation of heavy targets by using Dirac plane waves as well as an approximation to the Darwin functions for the projectile electron. A comparison between the two descriptions shows that with inclusion of the target Coulomb field, the cross section is in most cases lowered by a factor two or even more, and the energy dependence becomes weaker. Although the agreement with experiment is improved for the heavier target investigated, this is not the case for the lighter target, where the plane wave theory provides a rather good description of the data, in contrast to previous investigations [11] where exchange symmetry was not conserved [9]. For the heavy targets considered here and for an impact energy near or above 1 MeV, a first-order description in the electron-electron interaction should be sufficient, and also QED corrections should be small. An improvement of the theory may, however, be achieved by using more appropriate wavefunctions for the initial bound state as well as for the continuum states which should be mutually orthogonal. However, this will require a considerable increase of the numerical effort.

I should like to thank F. Bell and W. Nakel for stimulating this project, and P.A. Amundsen for helpful discussions. Support from GSI Darmstadt is gratefully acknowledged.

Appendix

In this appendix, numerical details for the evaluation of the continuum-continuum scattering integrals occuring in (3.12) are given. With the use of spherical coordinates and the coordinate transform $\mathbf{q}\to\mathbf{q}_1=-\mathbf{q}-\mathbf{k}_f+\mathbf{k}_i$, they are of the type

$$\int_0^\infty q_1^2\,\mathrm{d}q_1\int_{-1}^{1}\mathrm{d}(\cos\vartheta_{q_1})\int_0^\pi \mathrm{d}\bar{\varphi}_q\,\frac{1}{(\mathbf{q}_1+\mathbf{k}_f-\mathbf{k}_i)^2-q_0^2}\cdot\hat{C}_{fi}^{d}(\mathbf{q}_1)\,M(\mathbf{q}_1) \tag{A.1}$$

where $M(\mathbf{q}_1)$ is a well-behaved function, $\hat{C}_{\mathrm{fi}}$ is the scattering matrix element from (3.13) with (3.14), ϑ_{q_1} is the angle between $\mathbf{q}_1$ and $\mathbf{k}_i$ and $\bar{\varphi}_q\equiv\varphi_{q_1}-\varphi_{k_f}$. The quantisation direction is taken along $\mathbf{k}_i$.

There appear three singularities in the innermost $\bar{\varphi}_q$-integration: from $\hat{C}_{\mathrm{fi}}$ a branch cut at $\gamma+\delta=0$, as well as a strong singularity at $\alpha=-\beta$ (where the argument of the hypergeometric function becomes unity), and from the retarded Coulomb field a first-order pole at $q^2=(\mathbf{q}_1+\mathbf{k}_f-\mathbf{k}_i)^2=q_0^2$. Fast convergence requires an analytical treatment of the $\alpha=-\beta$ singularity at

$$\varphi^*=\arccos\left[-\left(\frac{q_1}{2k_f}+\cos\vartheta_{k_f}\cos\vartheta_{q_1}\right)\Big/(\sin\vartheta_{k_f}\sin\vartheta_{q_1})\right],$$

if φ^* lies inside the integration interval $(0,\pi)$:

$$\begin{aligned}&\int_0^\pi \mathrm{d}\bar{\varphi}_q(\alpha+\beta)^{i\eta_i-i\eta_f-1}F(\bar{\varphi}_q)\\&=\int_0^\pi \mathrm{d}\bar{\varphi}_q(q_1^2/2+\mathbf{q}_1\,\mathbf{k}_f-i\varepsilon)^{i\eta_i-i\eta_f-1}[F(\bar{\varphi}_q)-F(\varphi^*)]\\&\quad+F(\varphi^*)\,\pi(A+B)^{i\eta_i-i\eta_f-1}\\&\quad\cdot{}_2F_1\left(1-i\eta_i+i\eta_f,\tfrac{1}{2},1;\frac{2B}{A+B}\right)\\&A=q_1^2/2+q_1\,k_f\cos\vartheta_{q_1}\cos\vartheta_{k_f}-i\varepsilon\\&B=q_1\,k_f\sin\vartheta_{q_1}\sin\vartheta_{k_f}\end{aligned} \tag{A.2}$$

where F denotes the remaining integrand which is well-behaved at φ^*. In addition, the $\bar{\varphi}_q$ integral should be split at $\bar{\varphi}_q=\varphi^*$ and a logarithmic variable substitution should be made. Also the $\mathbf{q}^2=q_0^2$ singularity requires the change to a logrithmic variable. Fortunately, these

two singularities never coincide and in general do not simultaneously fall into the integration interval.

The singularity at φ^* propagates into the second integral over $\cos\vartheta_{q_1}$ when $|\cos\varphi^*|=1$ at

$$x\equiv\cos\vartheta_{q_1}=-q_1\cos\vartheta_{k_f}/2k_f\mp\sin\vartheta_{k_f}(4-q_1^2/k_f^2)^{1/2}/2,$$

yielding two square-root singularities. Likewise, the pole at $(\mathbf{q}_1+\mathbf{k}_f-\mathbf{k}_i)^2=q_0^2$ produces another pair of square-root singularities. In addition, the integrand diverges strongly at $\gamma=0$ (i.e. at $\cos\vartheta_{q_1}=x^*=q_1/2k_i$) which requires an analytical treatment in the surrounding of that point if $|x^*|<1$

$$\begin{aligned}
&\int_{x_1}^{x_2}\mathrm{d}(\cos\vartheta_{q_1})\,\gamma^{i\eta_f-i\eta_i-1}\,G(\cos\vartheta_{q_1})=q_1^{i\eta_f-i\eta_i-1}\\
&\quad\cdot\left\{\int_{x_1}^{x_2}\mathrm{d}(\cos\vartheta_{q_1})\left(k_i\cos\vartheta_{q_1}-\frac{q_1}{2}+i\varepsilon\right)^{i\eta_f-i\eta_i-1}\right.\\
&\quad\cdot(G(\cos\vartheta_{q_1})-G(x^*))\\
&\quad+G(x^*)\frac{1}{k_i(i\eta_f-i\eta_i)}\left[\left(k_i x_2-\frac{q_1}{2}+i\varepsilon\right)^{i\eta_f-i\eta_i}\right.\\
&\quad\left.\left.-\left(k_i x_1-\frac{q_1}{2}+i\varepsilon\right)^{i\eta_f-i\eta_i}\right]\right\}
\end{aligned}\tag{A.3}$$

where G comprises the in x^* well-behaved remainder.

The integration limits $x_1\geqq-1$ and $x_2\leqq1$ are chosen such that none of the other singularities falls into this region. Altogether, the second integral contains (at most) five singularities, and in each surrounding a logarithmic variable substitution is necessary for fast convergence.

The third integral (over q_1) contains a branch cut at $q_1=2k_i$ from the $\gamma=0$ pole, another branch cut at $q_1=2k_f$ where the two square-root singularities from $\alpha=-\beta$ coincide, and a strong singularity at $q_1=0$ which again calls for an analytical treatment (plus a logarithmic variable substitution, $q_2=\ln q_1$)

$$\begin{aligned}
&\int_{\delta_0}^{q_{\max}}\mathrm{d}q_1\,q_1^{-1+i\eta_f+i\eta_i}H(q_1)\\
&=\int_{\ln\delta_0}^{\ln q_{\max}}\mathrm{d}q_2\,q_1^{i\eta_f+i\eta_i}(H(q_1)-H(0))\\
&\quad+H(0)\frac{1}{i\eta_f+i\eta_i}(q_{\max})^{i\eta_i+i\eta_f},\\
&q_{\max}\to\infty,\ \delta_0\to0
\end{aligned}\tag{A.4}$$

H denoting the remaining integrand. Generally, a rather small step number (~20) in each of the subsections of the three-dimensional integral is sufficient. There is, however, a pathological region near $\vartheta_{k_f}=0°$ or 180° where the poles do not appear in the $\bar{\varphi}_q$ integral, which results in an enhancement of the singularities in the second integral. Not only coincide the two singularities from $\alpha=-\beta$ at $x=-q_1/(2k_f\cos\vartheta_{k_f})$ (with $|\cos\vartheta_{k_f}|=1$), but also the two singularities from the retarded Coulomb field at $x=[q_0^2-(q_1^2+k_f^2+k_i^2)+2k_ik_f\cos\vartheta_{k_f}]/(2q_1(k_f\cos\vartheta_{k_f}-k_i))$ and produce a further (logarithmic) singularity in the q_1-integral at $q_1=k_i-k_f\cos\vartheta_{k_f}\pm q_0$. The slow convergence in this ϑ_{k_f}-region affects predominantly the exchange contribution.

References

1. Møller, C.: Ann. Phys. (Leipzig) **14**, 531 (1932)
2. Bethe, H.A.: Z. Phys. **76**, 293 (1932)
3. Rester, D.H., Dance, W.E.: Phys. Rev. **152**, 1 (1966)
4. Middleman, L.M., Ford, R.L., Hofstadter, R.: Phys. Rev. A**2**, 1429 (1970)
5. Li-Scholz, A., Collé, R., Preiss, I.L., Scholz, W.: Phys. Rev. A**7**, 1957 (1973)
6. Moiseiwitsch, B.L.: Adv. At. Mol. Phys. **16**, 281 (1980)
7. Davidović, D.M., Moiseiwitsch, B.L., Norrington, P.H.: J. Phys. B**11**, 847 (1978)
8. Das, J.N.: Nuovo Cimento **12**B, 197 (1972)
9. Das, J.N., Konar, A.N.: J. Phys. B**7**, 2417 (1974)
10. Darwin, C.G.: Proc. R. Soc. A**118**, 654 (1928)
11. Schüle, E., Nakel, W.: J. Phys. B**15**, L639 (1982)
12. Ruoff, H., Nakel, W.: J. Phys. B**20**, 2299 (1987)
13. Ochkur, V.I.: Sov. Phys. JETP **18**, 503 (1964)
14. Byron Jr, F.W., Joachain, C.J., Piraux, B.: J. Phys. B**18**, 3203 (1985)
15. Pindzola, M.S., Buie, M.J.: Phys. Rev. A**37**, 3232 (1988)
16. Eissner, W., Seaton, M.J.: J. Phys. B**5**, 2187 (1972)
17. Jakubowicz, H., Moores, D.L.: J. Phys. B**14**, 3733 (1981)
18. Geltman, S.: J. Phys. B**7**, 1994 (1974)
19. Bjorken, D., Drell, S.D.: Relativistische Quantenmechanik. pp. 120, 149. Mannheim: Bibliographisches Institut 1964
20. Nordsieck, A.: Phys. Rev. **93**, 785 (1954)
21. Jakubaßa-Amundsen, D.H.: J. Phys. B**16**, 1767 (1983)
22. Ehrhardt, H.: Comments At. Mol. Phys. **13**, 115 (1983)
23. Ehrhardt, H., Hesselbacher, K.H., Jung, K., Willmann, K.: J. Phys. B**5**, 1559 (1972)
24. Bell, F.: Private communication
25. Becker, U.: J. Phys. B**20**, 6563 (1987)