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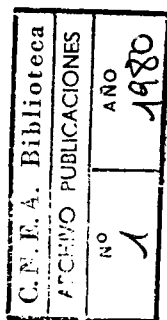
The emission of energetic electrons from atoms by fast ions considered as a charge-transfer process

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Received 10 July 1978, in final form 16 October 1979



Abstract. The ejection of energetic electrons from atoms by fast ions is described using as final electron states the continuum orbitals in the field of the projectile. The electronic distribution in the first-order Born approximation is equal to the distribution for direct ionisation where the final electron state is described by a plane wave times the Coulomb factor centred on the projectile. In the second-order Born approximation the distribution of ejected electrons is significantly decreased, and it is shown that it is equivalent to the correct distribution for direct ionisation in first order times the Coulomb factor around the projectile. For the case of ejected electrons with negligible momentum in the frame of the projectile, it is shown that the electron distribution centred on the projectile is isotropic to order v^{-12} , while the double scattering term in v^{-11} depends on the direction of motion of the electron.

1. Introduction

The first-order Born approximation has been widely used for the description of doubly differential cross sections for electron emission from atoms by fast charged particles; this process can be viewed as a direct electronic excitation to a continuum state of the target, assuming that the distortion of the final state by the projectile is negligible (Massey and Mohr 1933, Manson *et al* 1975). The results agree well with experiment except for electrons ejected with velocities close to that of the projectile; for them more appropriate final states are continuum orbitals on the field of the travelling charge, and the process can be classified as charge exchange to a continuum state.

Several theoretical approaches have been proposed that give a reasonable description of the angular and energy distributions of the ejected electrons. Salin (1969) considers a distorted-wave Born approximation where the distortion of the final electron state by both projectile and the residual target ion is taken into account. Macek (1970) uses Faddeev's equations for the final-state wavefunction, treating equally the influence of the projectile and target on the free electron. Dettmann (1972) and Dettmann *et al* (1974) view the process as a charge exchange to the continuum and calculate it in the second-order Born approximation; here the effect of the projectile on the final electron state is fully incorporated into the formalism, and the action of the residual target is partially considered through the successive orders of the Born series.

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The approaches of Salin and Macek are suitable to describe the electron distribution for a wide range of ejection velocities, but their formalisms are not as simple as the one used by Dettmann *et al.* On the other hand, the charge exchange to the continuum mechanism describes only slow electrons in the frame of the projectile, but it can easily incorporate the second-order Born correction to the cross section.

In this work we try to keep the simplicity of Dettmann's formulation, and to extend its validity to fast electrons emitted at larger angles in the frame of the target. For those electrons that are also fast in the frame of the projectile our results will tend to those resulting from the treatment of direct ionisation from the target, while for slow electrons in this frame our results will reproduce the peak of the distribution around the projectile, including the substantial correction introduced by the second-order Born approximation to charge-exchange processes; the reason for such a large contribution from the second-order Born term will be established, it being connected with the long-range behaviour of the Coulomb target potential, whose action on a captured electron cannot be neglected, even in the limit of high projectile velocities. We shall consider the case of a target with a single active electron in a general s state, and the results obtained can be extended with minor changes to states of any given orbital angular momentum. In this way we propose a simple approach applicable to all energetic electrons emitted by the target, and that also gives the best description of those ejected with small velocities in the frame of the projectile.

2. Theory

Let us assume a three-particle system, where a bare projectile of charge Z_1 interacts with an atom composed of core 2 and electron e , which will be the only one active in the collision. For the pairs of particles 1- e , 2- e , (2+ e)-1, 2-(1+ e) the relative coordinates between centres of mass will be \mathbf{r}_1 , \mathbf{r}_2 , \mathbf{R}_2 , \mathbf{R}_1 respectively, while the reduced masses of those pairs of particles are

$$\mu_j = M_j/(M_j + 1) \quad \nu_j = M_i(M_j + 1)/(M_i + M_j + 1) \quad (1)$$

where $j \neq i = 1, 2$ and M_1, M_2 are the masses of projectile 1 and core 2 respectively. The interaction between 1 and e is $V_1(\mathbf{r}_1) = -Z_1/r_1$, and for 2- e is a potential $V_2(\mathbf{r}_2)$ that depends on the core 2 considered. Atomic units are used throughout this paper.

We shall consider an initial state where the pair 2- e is in the bound s state 'i' and projectile 1 moves with relative momentum \mathbf{K}_i

$$\psi_i = e^{i\mathbf{K}_i \cdot \mathbf{R}_2} \phi_i(\mathbf{r}_2). \quad (2)$$

3. Direct ionisation

We are interested in final states

$$\psi_f = e^{i\mathbf{K}_2 \cdot \mathbf{R}_2} \phi_{\kappa_2}(\mathbf{r}_2) \quad (3)$$

where the projectile moves with momentum \mathbf{K}_2 with respect to the centre of mass 2- e , and the electron is in a continuum orbital centred on the target, with ingoing wave boundary conditions and asymptotic momentum κ_2 . The distortion of the electron state by the projectile has been neglected in (3).

The first-order Born approximation to the transition amplitude is (McDowell and Coleman 1970)

$$T_1 = -\frac{4\pi Z_1}{P^2} \int d\mathbf{r}_2 \phi_{\kappa_2}(\mathbf{r}_2) e^{i\mu_2 \mathbf{P} \cdot \mathbf{r}_2} \phi_i(\mathbf{r}_2) \quad (4)$$

where $\mathbf{P} = \mathbf{K}_i - \mathbf{K}_2$ is the transferred momentum. If it were possible to assume that the final electron state is not distorted either by the target or the projectile, we could replace $\phi_{\kappa_2}(\mathbf{r}_2)$ by a plane wave and (4) is simplified to

$$T_{\text{PW}} = (2\pi)^{-3/2} \tilde{V}_1(\mathbf{P}) \tilde{\phi}_i(\mathbf{K}) \quad (5)$$

here

$$\mathbf{K} = \kappa_2 - \mu_2 \mathbf{P}$$

and the Fourier transforms are defined by

$$\tilde{f}(\mathbf{k}) = \int d\mathbf{r} f(\mathbf{r}) e^{-i\mathbf{k} \cdot \mathbf{r}} \quad (6)$$

so that

$$\tilde{V}_1(\mathbf{P}) = -4\pi Z_1 / P^2. \quad (7)$$

We shall see later on that the use of a plane wave as a final electron state, equivalent to the binary encounter approximation, gives poor results for the ejected-electron distribution.

The triple differential cross section (TDCS), defined per unit solid angle Ω_2 of the projectile final scattering direction and unit volume of the ejected electron momentum κ_2 , is

$$\Sigma_\alpha^3 = (\nu_2 / 2\pi)^2 (K_2 / K_i) |T_\alpha|^2 \quad (8)$$

where T_α stands for T_{PW} or T_1 . The doubly differential cross section (DDCS) is defined as

$$\Sigma_\alpha^2 = \int d\Omega_2 \Sigma_\alpha^3. \quad (9)$$

4. Charge exchange to the continuum

4.1. First-order Born approximation

When we are interested in taking account of the distortion set up by the projectile on the electron distribution, this can be accomplished by considering the ionisation as a charge-transfer process to a continuum state centred on the projectile. The two equivalent forms for the first order Born approximation are

$$T'_1 = \langle \psi'_f | V_1 | \psi_i \rangle = \langle \psi'_f | V_2 | \psi_i \rangle \quad (10)$$

where

$$\psi'_f = e^{i\mathbf{K}_1 \cdot \mathbf{R}_1} \phi_{\kappa_1}^{(-)}(\mathbf{r}_1) \quad (11)$$

represents the final state with the centre of mass of $(1+e)$ moving with momentum \mathbf{K}_1 with respect to 2, and $\phi_{\kappa_1}^{(-)}$ is the Coulomb wavefunction describing an electron moving

with asymptotic momentum κ_1 in the frame of the projectile (Dettmann *et al* 1974)

$$\phi_{\kappa}^{(-)}(\mathbf{r}) = f_c(n)(2\pi)^{-3/2} e^{i\kappa\mathbf{r}} {}_1F_1(-in, 1; -i\kappa\mathbf{r} - i\kappa\mathbf{r}) \quad (12)$$

where

$$n = \mu Z/\kappa \quad \text{and} \quad f_c(n) = e^{n\pi/2} \Gamma(1+in) \quad (13)$$

is the so-called Coulomb factor. We do not consider the internuclear potential in (10) because its contribution is cancelled with that coming from the second-order Born terms, at least in the high-velocity limit (Drisko 1955).

The transition amplitude for the electron ejection viewed as a charge-exchange process is obtained by replacing (2) and (11) in (10)

$$\begin{aligned} T'_1 = & -(2\pi)^{-3/2} f_c^*(n_1) Z_1 \iint d\mathbf{R}_2 d\mathbf{r}_2 \exp(-i\mathbf{K}_1\mathbf{R}_1 - i\kappa_1\mathbf{r}_1) \\ & \times {}_1F_1(in_1, 1; i\kappa_1\mathbf{r}_1 + i\kappa_1\mathbf{r}_1) r_1^{-1} \exp(i\mathbf{K}_i\mathbf{R}_2) \phi_i(\mathbf{r}_2). \end{aligned} \quad (14)$$

Using the relation $\mathbf{K}_1\mathbf{R}_1 + \kappa_1\mathbf{r}_1 = \mathbf{K}_2\mathbf{R}_2 + \kappa_2\mathbf{r}_2$, and the Fourier representation of ${}_1F_1$ (see McDowell and Coleman 1970, p 364), (14) results:

$$\begin{aligned} T'_1 = & -(2\pi)^{-9/2} f_c^*(n_1) \int d\mathbf{k} G_1(\mathbf{k}, \kappa_1) \tilde{V}_1(k) \int d\mathbf{R}_2 \exp[i(\mathbf{P} - \mathbf{k})\mathbf{R}_2] \\ & \times \int d\mathbf{r}_2 \exp(-i\kappa_2\mathbf{r}_2 + i\mu_2\mathbf{k}\mathbf{r}_2) \phi_i(\mathbf{r}_2) \end{aligned} \quad (15)$$

where

$$G_1(\mathbf{k}, \kappa_1) = (1 - 2k\kappa_1/k^2)^{-in_1}. \quad (16)$$

The delta function resulting from the \mathbf{R}_2 integration reduces (15) to a simple analytic expression; using (5):

$$T'_1 = f_c^*(n_1) G_1(\mathbf{P}, \kappa_1) T_{\text{PW}}. \quad (17)$$

The TDCS for electron ejection taken as a charge-transfer process is defined by

$$\Sigma_1^{3'} = (\nu_1\nu_2/4\pi^2)(K_1/K_i) |T'_1|^2 \quad (18)$$

since it can be shown that $2\mathbf{P}\kappa_1/P^2 < 1$ the phase factor $G_1(\mathbf{P}, \kappa_1)$ present in (17) satisfies $|G_1| = 1$, and the influence of the hypergeometric function appearing in the transition amplitude T'_1 in (14) is completely removed from the differential cross section (18). The doubly differential cross section is defined now by

$$\Sigma_1^{2'} = \int d\Omega_2 \Sigma_1^{3'} \quad (19)$$

recalling the results (5) and (9) for the DDCS taken as a direct excitation process, we obtain from (17) and (19)

$$\Sigma_1^{2'} = |f_c^*(n_1)|^2 \Sigma_{\text{PW}}^2. \quad (20)$$

We conclude that, within the first-order Born approximation, the probability of electron transfer to a continuum state centred on the projectile is equal to the probability of direct excitation if the corresponding continuum state centred on the target is approximated by a plane wave times the Coulomb factor relative to the projectile. Here, by corresponding state we mean a state with

$\kappa_2 = \kappa_1 + \mathbf{K}_1/v_1$. The presence of the Coulomb factor in (20) accounts for the well known peak of capture to the continuum in the electron distribution (Dettmann *et al* 1974).

4.2. Second-order Born approximation

We shall try to incorporate into our results the main contribution of the second-order Born approximation to the transition amplitude, because it is well known that this term plays a dominant role in charge-exchange processes. The second-order Born term for the transition operator expanded in powers of the free-particle Green's operator G_0^+ is

$$T_2' = \langle \psi_f' | V_2 G_0^+ V_1 | \psi_i \rangle. \quad (21)$$

It is difficult to obtain the explicit form of T_2' , even through a numerical calculation (Kramer 1972); we shall then restrict our attention to the high-energy region, where an expansion of T_2' in inverse powers of the collision velocity is dominated by the lowest-order term. This has been treated for capture to a discrete state (Dettmann 1971), or to a continuum state of negligible energy (Dettmann *et al* 1974). We shall consider the case of a general continuum state of momentum κ_1 in the frame of the projectile: going to the Fourier space of the electron coordinates, equation (21) is expressed as

$$T_2' = (2\pi)^{-6} \iint d\mathbf{k}_1 d\mathbf{k}_2 \widehat{\phi_{\kappa_1}^{(-)*}}(\mathbf{k}_1) \tilde{V}_1(\mathbf{K}' - \mathbf{k}_1) G_0^+(\mathbf{k}_1, \mathbf{k}_2) \tilde{V}_2(\mathbf{K} - \mathbf{k}_2) \tilde{\phi}_i(\mathbf{k}_2) \quad (22)$$

where, neglecting terms of order v_i/M

$$G_0^+(\mathbf{k}_1, \mathbf{k}_2) = D - \mathbf{K}\mathbf{k}_1 - \mathbf{K}'\mathbf{k}_2 - k_1^2/2v_1 - (k_1 - k_2)^2/2\mu_1 \quad (23a)$$

$$\mathbf{K}' = \mathbf{P} - \kappa_1 \quad (23b)$$

$$\mathbf{K} = \kappa_2 - \mathbf{P} \quad (23c)$$

$$D = \epsilon_i + v_i^2/2 - K^2/2 + i\eta \quad (23d)$$

ϵ_i being the electron binding energy in state i , and η the usual small positive quantity that is taken to zero after integrations are performed; \mathbf{K} and \mathbf{K}' are equivalent to the parameters \mathbf{K}^ω and $\mathbf{K}^{\omega'}$ of Dettmann (1971).

The Fourier transform $\tilde{\phi}_i(\mathbf{k})$ is concentrated around $k \sim 0$ and its width, the momentum spread of the state i , is much smaller than the collision velocity v_i ; the continuum state $\widehat{\phi_{\kappa_1}^{(-)*}}(\mathbf{k})$ is centred on $\mathbf{k} = -\kappa_1$ and its width is also small compared with v_i ; both functions behave asymptotically as k^{-4} . The Fourier transform of the Coulomb potential V_1 is proportional to k^{-2} ; the target potential V_2 is Coulombic for small r , therefore it also behaves asymptotically as k^{-2} (see Dettmann 1971, p 156).

We shall consider the case where κ_1 and κ_2 can be large, while at the same time \mathbf{K} and \mathbf{K}' do not cancel and remain of the order of v_i . Therefore, the overlap between the Fourier transforms in (22) is produced when either the electronic states or the potentials reach their asymptotic forms, and the contribution of lowest order in v_i^{-1} comes from the region where the functions $\tilde{\phi}$ are centred, and the potentials are slowly varying functions of $\mathbf{k}_1, \mathbf{k}_2$ that can be taken as constants outside the integral (peaking approximation). The Green's function G_0^+ can also be taken outside the integral after

evaluating it at $\mathbf{k}_1 = -\boldsymbol{\kappa}_1$, $\mathbf{k}_2 = 0$. The lowest order in v_i^{-1} (22) is then equal to

$$T'_2 = \tau_2/D_0 \quad (24a)$$

where

$$\tau_2 = \phi_{\boldsymbol{\kappa}_1}^{(-)*}(0)\phi_i(0)\tilde{V}_1(\mathbf{P})\tilde{V}_2(\mathbf{K}) \quad (24b)$$

$$D_0 = G_0^+(-\boldsymbol{\kappa}_1, 0) = \epsilon_1 + \mathbf{v}_i\mathbf{P} - P^2/2 + i\eta. \quad (24c)$$

The peaking approximation cannot be applied to G_0^+ in the neighbourhood of a zero of D_0 ; those values of \mathbf{P} correspond to the so-called critical angle of scattering, and it is necessary to approximate $G_0^+(\mathbf{k}_1, \mathbf{k}_2)$ by additional terms of its expansion around $(-\boldsymbol{\kappa}_1, 0)$ (linearisation of G_0^+):

$$T'_2 \approx (2\pi)^6 \tilde{V}_1(\mathbf{P})\tilde{V}_2(\mathbf{K}) \int d\mathbf{k}_1 d\mathbf{k}_2 \widetilde{\phi_{\boldsymbol{\kappa}_1}^{(-)*}}(\mathbf{k}_1)\tilde{\phi}_i(\mathbf{k}_2)/|D_0 - (\mathbf{v}_i - \mathbf{P})(\mathbf{k}_1 - \boldsymbol{\kappa}_1) - \mathbf{P}\mathbf{k}_2|. \quad (25)$$

Using an integral representation for the denominator of (25):

$$T'_2 \approx -i(2\pi)^6 \tau_2 \int_0^\infty dS \exp[-i(D_0 + iZ_2P)S] {}_1F_1(in, 1, i|v_i - \mathbf{P}|\boldsymbol{\kappa}_1 S - i(\mathbf{v}_i - \mathbf{P})\boldsymbol{\kappa}_1 S) \quad (26)$$

which can be solved without further approximations (Magnus *et al* 1966):

$$T'_2 = -i(2\pi)^6 \tau_2 G_2(\mathbf{P}, \boldsymbol{\kappa}_1)/(D_0 + iZ_2P) \quad (27a)$$

with

$$G_2(\mathbf{P}, \boldsymbol{\kappa}_1) = |1 + (|v_i - \mathbf{P}|\boldsymbol{\kappa}_1 - (\mathbf{v}_i - \mathbf{P})\boldsymbol{\kappa}_1)/(D_0 + iZ_2P)|^{-in_1}. \quad (27b)$$

Due to the peaking approximation in the potentials, the result (27) constitutes the asymptotic approximation to the transition amplitude T'_2 . Using (7) and (24c) we see that the leading term is of order v_i^{-6} everywhere except for $\mathbf{v}_i\mathbf{P} = P^2/2$, where it changes to v_i^{-5} (critical angle region).

Equation (27) is valid for a general $\boldsymbol{\kappa}_1$, but the same result can be obtained if we replace ${}_1F_1$ by one in (26), since $G_2(\mathbf{P}, \boldsymbol{\kappa}_1) \sim v_i^{-1}$ except for $\boldsymbol{\kappa}_1 \rightarrow 0$. Our results will then coincide for $\boldsymbol{\kappa}_1 \neq 0$ with those of Dettmann *et al* (1974) who made ${}_1F_1 = 1$ for their calculation of the leading term in v_i ; furthermore, (27) is equivalent in the limit $\boldsymbol{\kappa}_1 \rightarrow 0$ to the result of Shakeshaft and Spruch (1978a, b) who approximated ${}_1F_1$ by its Bessel function limit when $\boldsymbol{\kappa}_1 \rightarrow 0$. It is then natural to expect that our results and those of Shakeshaft and Spruch will differ from the ones of Dettmann *et al* at the limit $\boldsymbol{\kappa}_1 \rightarrow 0$, where these are not valid since G_2 is then of order v_i^0 .

The first- and second-order Born transition amplitudes (17) and (27) can be related by using Schrödinger's equation for the initial state in Fourier space

$$(K^2/2\mu_2 - \epsilon_i)\tilde{\phi}_i(\mathbf{K}) + (2\pi)^{-3} \int d\mathbf{k} \tilde{V}_2(\mathbf{K} - \mathbf{k})\tilde{\phi}_i(\mathbf{k}) = 0.$$

Applying the peaking approximation, to principal order in v_i we get, for the case of an initial s state where $\phi_i(0) \neq 0$:

$$-K^2\tilde{\phi}_i(\mathbf{K})/2\mu_2 = \tilde{V}_2(\mathbf{K})\phi_i(0)$$

that replaced in (27) produces

$$T'_2 = F(\mathbf{P}, \boldsymbol{\kappa}_2) T'_1 \quad (28)$$

where

$$F(\mathbf{P}, \boldsymbol{\kappa}_2) = -G_1^*(\mathbf{P}, \boldsymbol{\kappa}_1) G_2(\mathbf{P}, \boldsymbol{\kappa}_1) (\mathbf{P} - \boldsymbol{\kappa}_2)^2 / (2v_i \mathbf{P} - P^2 + i2Z_2). \quad (29)$$

The TDCS in the second-order Born approximation is related to the first-order result (18); from (28):

$$\Sigma_2^{3'} = (\nu_1 \nu_2 / 4\pi^2) (K_1 / K_i) |T'_1 + T'_2|^2 = \Sigma_1^{3'} |1 + F(\mathbf{P}, \boldsymbol{\kappa}_2)|^2. \quad (30)$$

The DDCS is obtained by integration of (30) over the orientations of \mathbf{K}_2 , which amounts to summing over the allowed momentum transfers \mathbf{P} . Since the scattering angles θ of interest are very small, the momentum transferred in the forward direction can be taken as constant and equal to $K_i - K_2 = \kappa_2^2 / 2v_i$ when terms of order v_i^{-1} are neglected, while the variable transverse component is $-K_2 \sin \theta$. Let us analyse the dependence of the resulting DDCS on the orientation of $\boldsymbol{\kappa}_2$: electrons emitted from the target with a given energy are represented by a constant value of κ_2 ; for them $\mathbf{K} = \boldsymbol{\kappa}_2 - \mathbf{P}$ cancels when the electron ejection angle α satisfies

$$\cos \alpha = \kappa_2 / 2v_i. \quad (31)$$

The vector $\boldsymbol{\kappa}_2$ obeying (31) defines a sphere of radius v_i centred on the projectile (see figure 1). We observe from (17) that integration of $\Sigma_1^{3'}$ over \mathbf{P} will produce a distribution $\Sigma_1^{2'}$ of ejected electrons concentrated on the surface of this sphere, and its width is that of $|\tilde{\phi}_i(\mathbf{k})|^2$. This is the so-called binary region of the electron distribution, similar to the one described by Drepper and Briggs (1976) for electron loss.

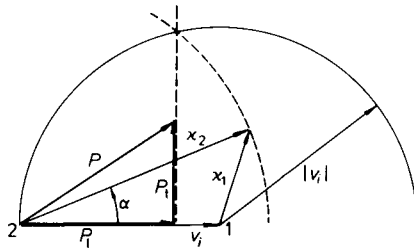


Figure 1. Kinematical relations among the relevant velocities and momenta for the ionisation process: the binary region for ejected electron velocities is the sphere of radius v_i centred on the projectile 1; the allowed momentum transfers \mathbf{P} define a plane normal to v_i at a distance $P_1 = \kappa_2^2 / 2v_i$ from the target 2; the variable transverse component is $P_1 = -K_2 \sin \theta$.

The TDCS in second order (30) cannot be used in the binary region because the peaking approximation fails for $K \approx 0$; since the real part of the denominator in (29) cancels for the same value of \mathbf{P} , this is also the region of the critical angle of double scattering. We have calculated T'_2 for the special case where $K = 0$ by making a peaking approximation only in the variable \mathbf{k}_1 of (22), and since we are in the critical angle region the denominator is conserved into the integral. We arrive at $T'_2 = T'_1 / v_i$, where $T'_1 \sim v_i^{-2}$; so in the binary region the second-order Born contribution can be neglected.

5. Results

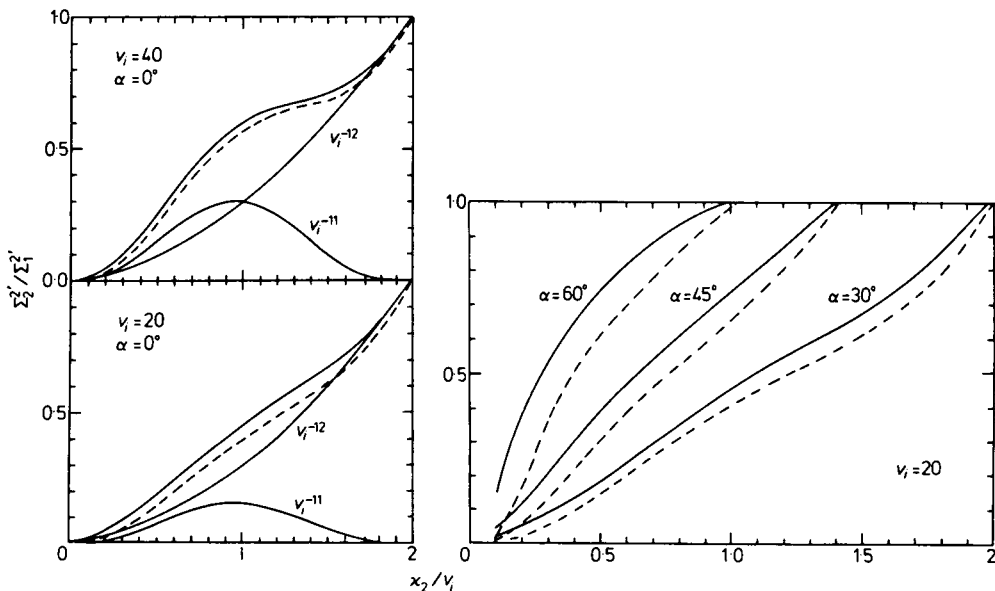
5.1. Electrons ejected with finite velocity in the frame of the projectile

We consider the ionisation process from the point of view of charge exchange to a continuum state of momentum κ_1 in the frame of the projectile: the DDCS in the second-order Born approximation $\Sigma_2^{2'}$ can be obtained in closed form for an initial 1s hydrogenic state. The results are presented in figure 2 for several angles of ejection and collision velocities; the partial contributions of order v_i^{-11} and v_i^{-12} are also shown, being the analytic expression for the coefficient of the first:

$$\lim_{v_i \rightarrow \infty} \Sigma_2^{2'} v_i^{11} = 16 |f_c(n_1)|^2 Z_2^4 Z_1^2 X^{-9} (2 - X \cos \alpha) / (2 \cos \alpha - X)^3 \quad (32)$$

with $X = \kappa_2/v_i$, while the analytic form of the term in v_i^{-12} is too complicated to be useful.

Due to the use of the peaking approximation, the only terms of significance in (30) are those that give contributions of order v_i^{-11} and v_i^{-12} to the DDCS; the phases G_1 and G_2 produce contributions of higher order, except for G_2 when $\kappa_1 \rightarrow 0$ where it modifies the term in v_i^{-11} . In the limit of $v_i \rightarrow \infty$ where our asymptotic expansion is strictly valid, the action of the phase G_2 on the v_i^{-11} term appears only at $\kappa_1 = 0$. Figure 2 also shows that, even though the TDCS (30) is not valid in the binary region because the width of this region is negligible when $v_i \rightarrow \infty$ the DDCS obtained from (30) goes to the correct limit for $\kappa_1 = v_i$: $\Sigma_2^{2'} = \Sigma_1^{2'}$. From the comparison between the first- and second-order Born results given in figure 2 it can be seen that the distribution of ejected electrons is decreased significantly by the second-order term, not only for slow electrons in the



Figures 2. Relation between second- and first-order Born DDCS for charge transfer $\Sigma_2^{2'}/\Sigma_1^{2'}$ for several collision velocities v_i and angles α of electron ejection in the frame of the target. Partial contributions of order v_i^{-11} and v_i^{-12} are presented. Broken lines correspond to the case where $\Sigma_2^{2'}$ is replaced by the projectile Coulomb factor $|f_c(Z_1/\kappa_1)|^2$ times the first-order Born DDCS for direct ionisation $\Sigma_1^{2'}$.

frame of the projectile, as was shown by Dettmann *et al* (1974), but also for electrons ejected in regions far away from the target and projectile.

Figure 3 presents the DDCS when the electron ejection and projectile velocities have the same magnitude; we note that the second-order result $\Sigma_2^{2'}$ compares favourably with the experimental measurements of Toburen and Wilson (1972) while $\Sigma_1^{2'}$ is too high.

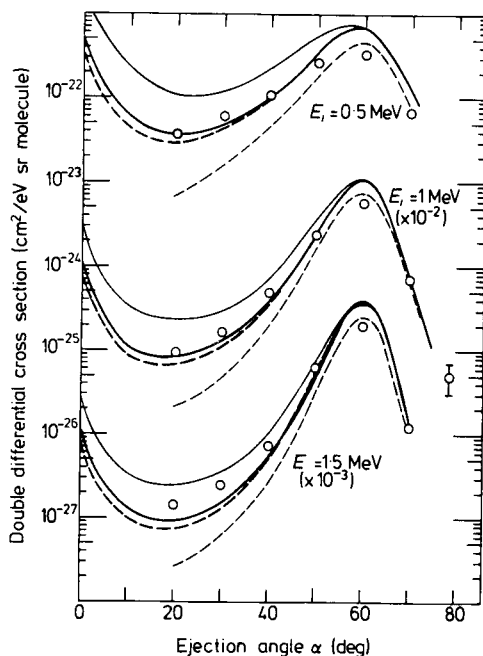


Figure 3. Angular dependence of the DDCS for electrons ejected with the same velocity of the projectile. The light full curve represents the first-order Born DDCS for charge exchange $\Sigma_1^{2'}$, the heavy full curve the corresponding second-order Born result $\Sigma_2^{2'}$, the light broken curve is the first-order Born DDCS for direct ionisation $\Sigma_1^{2'}$, and the heavy broken curve is $|f_c(Z_1/\kappa_1)|^2 \Sigma_1^2$. Experimental points are taken from Toburen and Wilson (1972) who use molecular hydrogen as the target. We assumed that H_2 is roughly equivalent to two H atoms for the calculation of the theoretical curves.

We have seen in § 4.1 that the description of the ionisation as a charge-exchange process to a continuum state of the projectile is equivalent, within the first-order Born approximation, to the direct excitation of that electron to a continuum state of the target approximated by a plane wave times the Coulomb factor (13). One may think that the replacement of the continuum state by a plane wave is appropriate for energetic electrons; this is not the case, as the TDCS for ionisation from a 1s hydrogenic orbital shows (Landau and Lifshitz 1965):

$$\Sigma_1^3 = \Sigma_{PW}^3 |f_c(n_2)|^2 4P^2 \exp[-2Z_2 \tan^{-1}(2Z_2\kappa_2/\Gamma)/\kappa_2] \times |(P - \kappa_2\gamma)^2 + (Z_2\gamma)^2| / |\Gamma^2 + (2Z_2\kappa_2)^2| \quad (33)$$

where

$$\gamma = \hat{P}\hat{\kappa}_2 \quad \text{and} \quad \Gamma = P^2 - \kappa_2^2 + Z_2^2.$$

The factor accompanying Σ_{PW}^3 is a non-trivial function of κ_2 which does not approach

unity for large κ_2 and v_i . Thus, the failure of $\Sigma_1^{2'}$ to reproduce the electron distribution far away from the target may be connected with the unsuitability of replacing the continuum state around the target by a plane wave. The second-order contribution will compensate, at least partially, for such a replacement: the transition amplitude to second order is, from (10) and (21),

$$T'_1 + T'_2 = \langle \Psi'_f | (1 + V_2 G_0^+) V_1 | \Psi_i \rangle = \langle (1 + G_0^- V_2) \Psi'_f | V_1 | \Psi_i \rangle. \quad (34)$$

For the first-order Born contribution we have seen that, apart from the Coulomb factor and a phase of higher order in v_i^{-1} , only the plane wave of the continuum state plays a role in the transition amplitude, and the main contribution of the second-order term is obtained through the peaking approximation, which is equivalent to replacing the continuum state by a plane wave times its Coulomb factor; therefore, in our procedure the dependence of Ψ'_f on the electronic coordinate is given by a plane wave. The factor $1 + G_0^- V_2$ in (34) represents the first two terms of an expansion of $1 + G_2^- V_2$ in powers of V_2 , where $1 + G_2^- V_2$ operating on a plane wave generates the exact continuum state around the target; we then conclude that the second-order Born transition amplitude $T'_1 + T'_2$ is equivalent, up to terms of order V_2 , to the first-order direct transition T_1 times the Coulomb factor around the projectile; for DDCS this reads

$$\Sigma_2^{2'} \approx |f_c(n_1)|^2 \Sigma_1^2. \quad (35)$$

To account for the distortion of the final electron state by the projectile it is then only necessary to multiply the DDCS for direct ionisation by the Coulomb factor of the projectile. We see that (35) is verified by the results presented in figures 2 and 3.

5.2. Electrons ejected with negligible velocity in the frame of the projectile

Shakeshaft and Spruch (1978b) have considered the process of charge exchange to the continuum in the limit $\kappa_1 \rightarrow 0$; their interest was centred in the possible angular dependence of the peak of electron density around the projectile. Since they use the peaking approximation for the second-order Born term their results, like ours, are only valid to lowest order in an expansion in powers of v_i^{-1} . The transition amplitudes (17) and (27) when $\kappa_1 \rightarrow 0$ reduce to

$$T'_1 = 2^5 \pi^2 Z_1 Z_2 P^{-2} K^{-4} \phi_{\kappa_1}^{(-)*}(0) \phi_i(0) \exp(2iZ_1 \hat{P} \hat{\kappa}_1 / P) \quad (36)$$

$$T'_2 = T'_1 K^2 (K^2 - v_i^2 + 2iZ_2 P)^{-1} \exp[-2iZ_1 |\hat{P} \hat{\kappa}_1 / P + (K - \mathbf{K} \hat{\kappa}_1) / (v_i^2 - K^2 + 2iZ_2 P)|] \quad (37)$$

where $\mathbf{K} = \kappa_2 - \mathbf{P} = \mathbf{v}_i - \mathbf{P}$.

The leading terms in v_i to the DDCS $\Sigma_2^{2'}$ come from two regions of the domain of integration in momentum transfers \mathbf{P} : outside the critical angle, given by $P = v_i$, $|T'_1 + T'_2|^2$ is of order v_i^{-12} ; furthermore, the only difference with charge transfer to a discrete state is the presence of the Coulomb factor—the rest of the term is exactly the Brinkmann–Kramers result multiplied by 0.3 due to the use of the second-order Born approximation. The orientation $\hat{\kappa}_1$ present in (17) and (27b) does not appear in $\Sigma_2^{2'}$ to order v_i^{-12} , since the relative phase between T'_1 and T'_2 in (36) and (37) is of order v_i^{-1} outside the critical angle region. When we perform the part of the P integral in a neighbourhood of width v_i^{-1} around $P^2 = 2\mathbf{v}_i \cdot \mathbf{P}$ (i.e. $P \approx v_i$, $\mathbf{K} = |\mathbf{v}_i - \mathbf{P}| \approx v_i$), we see from (27) that $T'_2 \sim T'_1 v_i$ and $|T'_1 + T'_2| \sim v_i^{-10}$ so $\Sigma_2^{2'}$ gets a term of order v_i^{-11} . This is the contribution of the critical angle of double scattering, first considered by Thomas (1927): the final electron state is produced by a first scattering with the projectile, where

it receives its final momentum intensity $\kappa_2 = v_i$, since in the second interaction, now with the target, the electron can only change its momentum orientation.

We shall now obtain the partial contribution of order v_i^{-11} to the DDCS in the limit $\kappa_1 \rightarrow 0$, complementing the result (32); using as an independent variable the transverse component \mathbf{P}_t of the transferred momentum \mathbf{P} (see figure 1):

$$\mathbf{P} = \mathbf{v}_i/2 + \mathbf{P}_t \quad \mathbf{K} = \mathbf{v}_i/2 - \mathbf{P}_t \quad (38)$$

$$|T_2'|^2 = 2^{19}3^{-6}Z_1^2Z_2^5|f_c(n_1)|^2v_i^{-12}(x + \frac{1}{3})^{-4}\beta^{-2}\chi(x, \beta)e^{-\delta\chi(x, \beta)} \quad (39)$$

where

$$\chi(x, \beta) = \beta^2[(x-1)^2 + \beta^2]^{-1} \quad x = (2P_t/v_i)^2/3$$

and, for $k \approx v_i$:

$$\begin{aligned} \beta &= 8Z_2P/3v_i^2 \approx 8Z_2/3v_i \\ \delta &= 2Z_1(1 - \hat{\mathbf{K}}\hat{\kappa}_1)/Z_2 \approx Z_1(2 + \hat{\kappa}_1\hat{v}_i - \sqrt{3}|\hat{\kappa}_1 + \hat{v}_i|\cos\psi)/Z_2 \end{aligned} \quad (40)$$

ψ being the azimuthal angle of $\hat{\mathbf{K}}$ measured from the plane of $\hat{\kappa}_1$ and \mathbf{v}_i . The integral over the final orientations of the projectile can be replaced by an integration over the two dimensions of \mathbf{P}_t :

$$\Sigma_2^{2'} = 2^{14}3^{-5}Z_1^2Z_2^5|f_c(n_1)|^2\pi^{-2}v_i^{-12}\int_0^{2\pi}d\psi\int_0^\infty dx(x + \frac{1}{3})^{-4}\beta^{-2}\chi(x, \beta)e^{-\delta\chi(x, \beta)}. \quad (41)$$

The result (32) gives the isotropic contribution of order v_i^{-11} produced by (41); to this order, the $\hat{\kappa}_1$ -dependent part is given by

$$\lim_{v_i \rightarrow \infty} (2^6Z_1^2Z_2^5|f_c(n_1)|^2/3v_i\pi^2)\int^\pi d\psi\int_0^\infty dx\chi(x, \beta)\beta^{-2}(e^{-\delta\chi(x, \beta)} - 1). \quad (42)$$

Only the x -integral can be done analytically in the limit $\beta \ll 1$; when the electron is scattered in the forward or backward directions the parameter δ is independent of ψ , and from (42) we obtain

$$\lim_{\substack{v_i \rightarrow \infty \\ \kappa_1 \rightarrow 0}} \Sigma_2^{2'}v_i^{11} = 2^4Z_1^2Z_2^4|f_c(n_1)|^2e^{-\delta/2}J_0(i\delta/2) \quad (43)$$

with $\delta = 2 + \hat{\kappa}_1\hat{v}_i$ restricted to the cases $\hat{\kappa}_1\hat{v}_i = \pm 1$, and J_0 is the Bessel function of the first kind. Equation (43) replaces (31) in the limit $\kappa_1 \rightarrow 0$, and coincides with the result given by Shakeshaft and Spruch (1978a), who made the calculation by replacing the confluent hypergeometric function of the continuum state by

$$J_0\{2[Z_1r(1 - \hat{\mathbf{K}}\hat{r})]^{1/2}\} \quad \text{valid for } \kappa_1 \rightarrow 0.$$

Since the contribution of order v_i^{-11} is very small compared with the term in v_i^{-12} in the range of non-relativistic collision velocities we conclude that, up to order v_i^{-12} , there is no angular dependence of the peak of capture to the continuum in the limit $\kappa_1 \rightarrow 0$; to obtain the whole contribution to the DDCS of order v_i^{-13} , or higher, and see its angular dependence it is necessary to relax the peaking approximation, which will be done in a forthcoming paper (Miraglia and Ponce 1979).

6. Conclusions

We have studied the process of ejection of energetic electrons from a target with one active *s* electron by a fast heavy charge, taking the point of view of a charge-transfer process to a continuum state of the projectile. A hydrogenic target has been assumed in order to obtain specific numerical results, but the conclusions brought by this work are equally valid for a general state of an independent electron model of the target. Using a Born expansion in electron-target and electron-projectile potentials we obtained the first-order Born approximation (20) to the DDCS without approximations; the only effect of describing the process as a charge transfer is the presence of the Coulomb factor (13) centred on the projectile, which multiplies a term identified as the DDCS for direct ionisation where the electronic continuum state is replaced by a plane wave.

The second-order Born contribution cannot be obtained exactly, so we calculated the dominant terms of its asymptotic expansion in v_i ((27)–(29)). The resulting distribution of ejected electrons is appreciably decreased from the first-order result, and the relation between DDCS $\Sigma_2^{2'}/\Sigma_1^{2'}$ (figure 2) increases monotonically with the ejection velocity κ_2 , regaining the value 0.3 for $\kappa_2 = v_1$, which also applies to charge transfer to a discrete state. When $\kappa_1 \rightarrow v_1$ that relation approaches unity, and in this binary region the first-order Born approximation is dominant.

From the calculations of the transition amplitudes in first and second order (34) it can be seen that the final electronic state acts like a plane wave multiplied by the Coulomb factor (equations (17) and (22)–(23)), so that the second-order Born contribution merely provides the linear perturbation of that free-particle state by the target; within the approximation determined by the first two terms of the Born expansion we concluded that the second-order Born approximation to the DDCS for charge exchange $\Sigma_2^{2'}$ (35) is equivalent to the first-order direct ionisation result Σ_1^2 times the Coulomb factor around the projectile.

For the case of electrons ejected with negligible momentum κ_1 in the frame of the projectile, we showed that the term of order v_i^{-11} presents a dependence on the orientation $\hat{\kappa}_1$ (equation (43)), while the contribution in v_i^{-12} is isotropic. The anisotropy found for the electronic distribution around the projectile (Shakeshaft and Spruch 1978b) should come from terms of order v_i^{-13} or higher, but to take full account of the contributions to $\Sigma_2^{2'}$ in those orders it is necessary to go beyond the peaking approximation used in this work.

We have then obtained a simple way to account for the distortion produced by the projectile on the final electron distribution. We may visualise it by assuming that as a first step the projectile interacts with the target electron and produces a distribution of ejected electrons Σ_1^2 governed only by the residual target potential; in the second step the projectile distorts this distribution and is surrounded by a cloud of electronic density that diverges on the location of the projectile. This distortion is accounted for by the Coulomb factor $|f_c(Z_1/\kappa_1)|^2$ that multiplies the original distribution Σ_1^2 ; since f_c goes to unity for large values of κ_1 the electronic distribution will tend to the original of the direct ionisation process far away from the projectile.

Acknowledgments

The authors wish to thank Professor W Meckbach for many helpful discussions. This work was partially supported by the Organization of American States through the Multinational Program in Physics.

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