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Selection rules for electron transfer to the continuum in ion-atom collision

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Résumé. — Nous considérons le processus de transfert d'un électron à un état du continuum au premier ordre de l'approximation de Born. Nous étudions le développement de la section efficace doublement différentielle en puissances de la vitesse et de l'angle d'éjection de l'électron. Les coefficients de ce développement obéissent à des règles de sélection. Nous comparons ces règles de sélection, qui prédisent une forme asymétrique pour le pic de transfert électronique vers le continuum, aux résultats expérimentaux récents.

Abstract. — We consider the process of electron transfer to the continuum in first order Born approximation. We analyse the expansion of the double-differential cross section in series of electron velocity and ejection angle. We found that the coefficients obey precise selection rules. We discuss the relation of these rules, which predict an asymmetric shape for the electron loss to the continuum cusp, with the interpretation of recent experimental results.

The distribution of electrons emitted in an ion-atom collision exhibits a cusp-shaped peak centred at $\mathbf{v}_e = \mathbf{v}_p$, where $\mathbf{v}_e$ and $\mathbf{v}_p$ are the electron and incident projectile velocities respectively [1]. This effect is attributed to the final state interaction between the electron and the projectile of charge Z_p, and has been called electron transfer to continuum (ETC). Actually, in a first perturbative order treatment, the electron is dragged along in a Coulomb wave centred at the projectile [2]. The normalization of this state introduces in the electronic double-differential cross section (DDCS) $\mathrm{d}\sigma/\mathrm{d}\mathbf{v}_e$ a factor (we shall use atomic units)

$$| f_c(v) |^2 = \frac{2\,\pi Z_p/v}{1 - \exp\left(-\dfrac{2\,\pi Z_p}{v}\right)} \qquad (1)$$

with $\mathbf{v} = \mathbf{v}_e - \mathbf{v}_p$, the electron-projectile relative velocity. This factor leads to a spherically symmetric peak around $\mathbf{v}_e = \mathbf{v}_p$ [3]. However, a more complicated structure in the DDCS has been experimentally found in ion-gas target collisions [4]. In fact, recent experiments on ETC clearly show the presence of an anisotropic structure which has been investigated with considerable interest during the past few years. This activity has been triggered by recent detailed measurements of the three-dimensional distributions [5].

The nonisotropic structure of the cusp shape can be conveniently described by the parametric double expansion of the DDCS [4, 6] :

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\mathbf{v}_e} = | f_c(v) |^2 \sum_{J,n=0}^{\infty} B_J^{(n)}(v_p)\, v^n\, P_J(\cos\theta) \qquad (2)$$

with $\cos\theta = \mathbf{v}_p \cdot \mathbf{v}/v_p \cdot v$. This expansion in powers of the velocity includes physically significant terms that are eliminated when the electron energy $E = v^2/2$ is introduced as a variable [7]. Naturally the contribution of each of the expansion coefficients in equation (2) depends on the features of the ETC process which is under analysis. For ion-gas target collisions, under single collision conditions, there are two ETC processes for the production of the so called « convoy electrons » : electron capture (ECC) and electron loss (ELC) to the continuum. If the impinging projectile is a stripped ion, ECC is the only possible transfer process. In this case a violent collision with a large momentum transfer determined by the ion velocity $\mathbf{v}_p$ is required in order to eject a target electron into a low lying continuum state of the projectile. On the other hand, if the initial charge of the projectile is lesser than its atomic number, a weak momentum transfer of the order ε_i/v_p is enough to produce the loss

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into the continuum of a projectile electron. Here ε_i is the binding energy. In fact both ECC and ELC processes contribute. However, a neutral projectile has not a pure Coulomb interaction with a target electron and the ELC process dominates.

Theoretical and experimental evaluation of the coefficients $B_J^{(n)}$ enable a precise description of the nonisotropic structure of the DDCS due to both ETC mechanisms, and a clear comparison between theory and experiment [8]. In view of the divergence of the DDCS, such a comparison strongly depends on the detector resolution, and equation (2) must be integrated over the resolution volume [4] in the velocity space. This volume is defined by the velocity resolution (R) and the angular acceptance (θ_0) of the spectrometer. The electronic distribution results :

$$Q(\mathbf{v}_e) = \int_{R,\theta_0} \frac{d\sigma}{d\mathbf{v}_1} d\mathbf{v}_1 = = \sum_{J,n=0}^{\infty} B_J^{(n)}(v_p)\, U_J^{(n)}(\mathbf{v}_e) \quad (3)$$

with

$$U_J^{(n)}(\mathbf{v}_e) = \int_{R,\theta_0} |f_c(v)|^2\, v^n\, P_J(\cos\theta)\, d\mathbf{v}_1 . \quad (4)$$

Near the peak top the main contribution to $Q(\mathbf{v}_e)$ arises from terms with $n = 0$. In particular the term $B_0^{(0)}\, U_0^{(0)}$ gives the usual divergence of the Coulomb factor f_c in $\mathbf{v}_e = \mathbf{v}_p$. Terms with $n \neq 0$ correspond to non-singular contributions to the cross section and dominate at the tails of the peak.

The theoretical contribution of each term in equation (2) depends on the features of the active ETC mechanism, and also on the perturbative approach under consideration. In the present paper we will show that certain selection rules are obtained in the first Born approximation, which reduces the number of contributing coefficients $B_J^{(n)}$. These selection rules are very important since they may be confronted with the experimental electronic distribution, thus probing the first Born approximation in the convoy electron production mechanism.

The ELC process results from a weak collision which suffices to excite a projectile electron into a low lying continuum state. Consequently, the first Born approximation should be valid for large projectile velocities [9]. Let us consider a hydrogenic ion of nuclear charge Z_p which collides with a neutral atom of nuclear charge Z_T. In first Born approximation the DDCS for electron loss is given by

$$\frac{d\sigma}{d\mathbf{v}_e} = \sum_\alpha \frac{4}{v_p} \int \frac{d\mathbf{Q}}{Q^4} |\langle \psi_{\mathbf{v}}^- | e^{i\mathbf{Q}.\mathbf{r}} | \psi_{1s} \rangle|^2 \cdot \left| \left\langle \alpha \left| \sum_J^N e^{-i\mathbf{Q}.\mathbf{r}_J} - Z_T \right| 0 \right\rangle \right|^2 \delta\!\left(\frac{Q^2}{2\mu} - \mathbf{Q}\cdot\mathbf{v}_p + \frac{1}{2}(Z_p^2 + v^2) + \Delta\varepsilon_\alpha \right) \quad (5)$$

where $\left| \left\langle \alpha \left| \sum_J^N e^{-i\mathbf{Q}.\mathbf{r}_J} - Z_T \right| 0 \right\rangle \right|^2$ is the target atomic form factor for the transition from its ground state $| 0 \rangle$ to an arbitrary excited state $| \alpha \rangle$, with a change $\Delta\varepsilon_\alpha$ in electronic energy. On the other hand the ionic form factor is known analytically

$$|\langle \psi_{\mathbf{v}}^- | e^{i\mathbf{Q}.\mathbf{r}} | \psi_{1s} \rangle|^2 = \frac{2^6 Z_p^5}{\pi^2} |f_c(v)|^2 \frac{[(Q^2 - \mathbf{Q}\cdot\mathbf{v})^2 + (Z_p/v)^2 (\mathbf{Q}\cdot\mathbf{v})^2]}{[(\mathbf{Q}-\mathbf{v})^2 + Z_p^2]^4} \times \times \frac{\exp[-(2 Z_p/v) \arctan(2 Z_p v/(Q^2 + Z_p^2 - v^2))]}{(Q^2 + Z_p^2 - v^2)^2 + 4 Z_p^2 v^2} . \quad (6)$$

This expression may be expanded in powers of v and $\mathbf{Q}\cdot\mathbf{v}$

$$|\langle \psi_{\mathbf{v}}^- | e^{i\mathbf{Q}.\mathbf{r}} | \psi_{1s} \rangle|^2 = = |f_c(v)|^2 \sum_{l,m=0}^{\infty} a_{lm}(Q, Z_p)\, v^{2(m-1)} (\mathbf{Q}\cdot\mathbf{v})^l \quad (7)$$

with adequate coefficients $a_{lm}(Q, Z_p)$.

We express the momentum transfer $\mathbf{Q}$ in spherical polar coordinates Q, δ and ϕ, with $\hat{\mathbf{z}} = \hat{\mathbf{v}}_p$, and execute the integration with respect to the polar angle :

$$\int_0^{2\pi} (\hat{\mathbf{Q}}\cdot\hat{\mathbf{v}})^l\, d\phi = \sum_{i=0}^{[l/2]} b_{li}\, P_{l-2i}(\cos\delta)\, P_{l-2i}(\cos\theta) . \quad (8)$$

We replace equations (7) and (8) in the DDCS (Eq. (5)) and note that the energy-conserving Dirac δ only contributes with even powers of the electron projectile velocity v. Finally we obtain the parametric expansion (2), with the following selection rules :

$$B_J^{(n)} = 0 \quad \text{if} \quad n + J = \text{odd} \quad (9)$$

$$B_J^{(n)} = 0 \quad \text{if} \quad J > n + 2 . \quad (10)$$

Restricting ourselves to the zero-velocity limit, these selection rules lead to the following expression for the ELC distribution

$$Q(\mathbf{v}_e) = B_0^{(0)} U_0^{(0)} + B_2^{(0)} U_2^{(0)} . \tag{11}$$

This equation is generally believed to be valid close to the peak top [9] and has been employed for the interpretation of experimental data [10]. However its validity seems to be doubtful farther from of the ECC peak. The next terms of the parametric expansion tend to predominate when the electron-projectile velocity is not so small. Thus a four term generalization of the previous expression, compatible with the selection rules, is more adequate.

$$Q(\mathbf{v}_e) = B_0^{(0)} U_0^{(0)} + B_2^{(0)} U_2^{(0)} + B_1^{(1)} U_1^{(1)} + B_3^{(1)} U_3^{(1)} . \tag{12}$$

The relative importance of the anisotropic terms $B_1^{(1)}$ and $B_3^{(1)}$ by comparing with the singular terms $B_0^{(0)}$ and $B_2^{(0)}$, calculated in the closure approximation [9], is shown in figure 1 for the collision H^0 + He. As a matter of fact these additional terms do not appear when the ELC mechanism is interpreted as the ionization limit of Rydberg states excitation [11].

In figure 1 we see that $B_1^{(1)}$ is positive, and consequently it produces a weak skewness towards high electron velocities as it is shown in figure 2. On the other hand the anisotropic terms $B_2^{(0)}$ and $B_3^{(1)}$ become negative for $v_p \gtrsim Z_p$. This change of sign is related to the zeros of the Legendre function $P_J(\hat{\mathbf{Q}} \cdot \hat{\mathbf{v}}_p)$ which is included in $B_J^{(n)}$.

Finally it is possible that the first Born approximation oversimplifies the anisotropic structure of the electron loss DDCS, particularly at intermediate projectile velocities. Very recent experimental data for H^0 + He collisions seem to confirm this conjecture [5, 10]. However a similar highly complicated structure is observed in ECC experiments, but not in beam foil convoy electron distributions [10]. This feature may indicate the presence of a systematic error in the experimental device [5, 12]. Actually much care must be taken with respect to a possible variation of the experimental effective beam-gas interaction volume with the ejection angle. Anyhow a more careful comparison between the experimental evidence and the previous selection rules would provide a conclusive proof for the validity of the first order Born approximation in the electron loss to the continuum process.

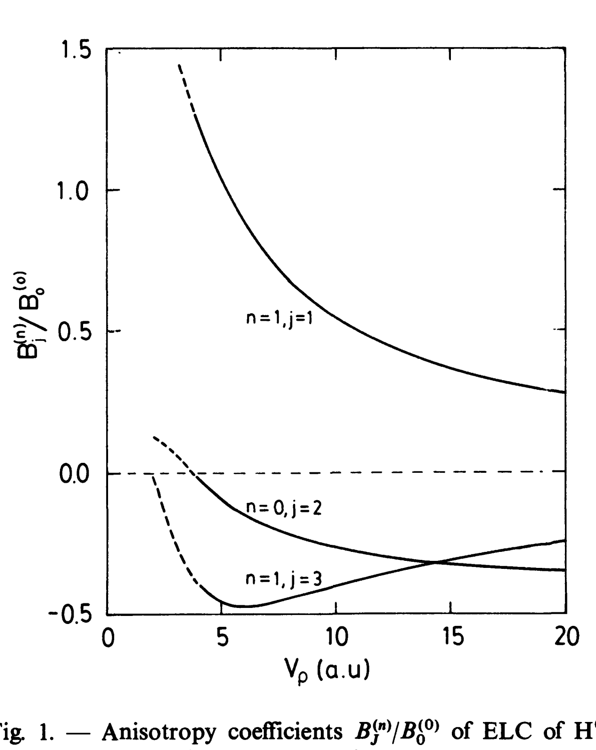

Fig. 1. — Anisotropy coefficients $B_J^{(n)}/B_0^{(0)}$ of ELC of H^0 on He as function of projectile velocity v_p.

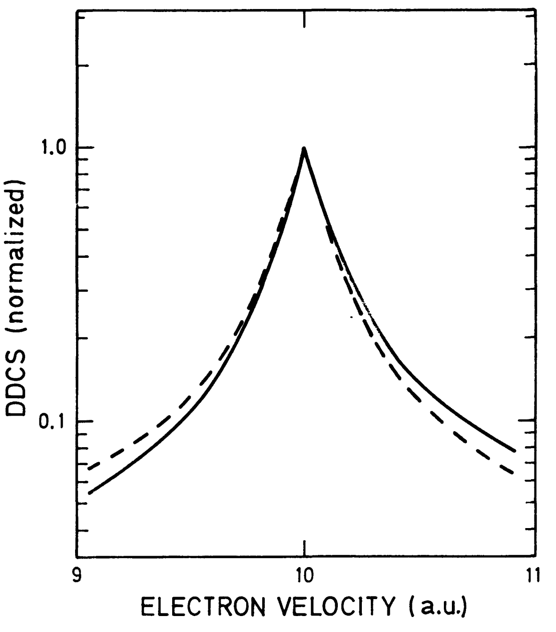

Fig. 2. — Electron loss to the continuum cusp at 0° for the collision H^0 + He, v_p = 10 a.u. It is assumed that the detector has an acceptance angle θ_0 = 1° and an energy resolution R = 0.002. (---), theory of Briggs and Day, equation (11). (——), present result, equation (12).

In ECC processes a noticeable skewness of the peak towards low electron velocities is experimentally found in stripped ion-gas target collisions [4]. This feature clearly suggests the presence of an asymmetric singular term with $B_1^{(0)} \neq 0$ in the parametric expansion of the DDCS. Recently this term $B_1^{(0)} U_1^{(0)}$ has been fitted to experimental data [4, 8] and its relevance to the peak position as a function of the electron ejection angle has been considered [13]. However the first order Born approximation for charge exchange to the continuum from a 1s hydrogenic target state gives the following selection rules for the coefficients of the parametric expansion :

$$B_J^{(n)} = 0 \quad \text{if} \quad n + J = \text{odd} \tag{13}$$

$$B_J^{(n)} = 0 \quad \text{if} \quad J > n . \tag{14}$$

These selection rules clearly exclude the asymmetric singular term $U_1^{(0)}$.

In order to prove equations (13) and (14) let us consider the collision of a stripped ion of charge Z_p with a hydrogenic atom of effective charge Z_T. The first order approximation for charge exchange to a continuum state centred at the projectile gives the following expression for the DDCS :

$$\frac{d\sigma}{d\mathbf{v}_e} = | f_c(v) |^2 \frac{2^5}{\pi} \frac{Z_p^2 Z_T^5}{v_p} \times$$
$$\times \int \frac{d\mathbf{Q}}{|\mathbf{Q}+\mathbf{v}|^4} \frac{1}{(Z_T^2+Q^2)^4} \delta\left(\frac{Q^2}{2\mu} - \mathbf{Q}\cdot\mathbf{v}_p + \frac{1}{2}(v^2+Z_T^2)\right) \tag{15}$$

with μ the reduced mass of the ion-atom system.

Expanding in powers of v and $\mathbf{Q}\cdot\mathbf{v}$ we obtain

$$\frac{1}{|\mathbf{Q}+\mathbf{v}|^4} = \sum_{l,m=0}^{\infty} \binom{l+m}{l} \frac{2^l(-)^{l+m}(l+m+1)}{Q^{4+2(l+m)}} \times$$
$$\times\ v^{2m}(\mathbf{Q}\cdot\mathbf{v})^l \,. \tag{16}$$

Once more the transfer moment $\mathbf{Q}$ is expressed in spherical polar coordinates, with $\hat{\mathbf{z}} = \hat{\mathbf{v}}_p$, and the integration with respect to the polar angle is executed. We replace equations (8) and (16) in the DDCS, and equations (13) and (14) follow.

As the first Born approximation does not explain the observed asymmetry, higher orders of perturbation are required. In this context, the second Born approximation [14], the continuum distorted wave approximation [15] and a multiple scattering theory [6] have to be mentioned. In the latter approach the first four coefficients $B_0^{(0)}$, $B_1^{(0)}$, $B_0^{(1)}$ and $B_1^{(1)}$ were calculated, giving reasonable agreement with a fit to experimental H^+ + He data [8].

The singular terms $U_0^{(0)}$ and $U_1^{(0)}$ give the main contribution to the ECC peak. However the remaining two terms $U_0^{(1)}$ and $U_1^{(1)}$, which account for the non-singular part of the scattering amplitude, tend to predominate at the tails of the peak, and cannot be excluded in an analysis of the electron capture to the continuum process.

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