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Forward Electron Ejection in Ion Collisions

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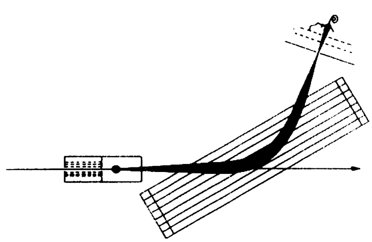

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THEORETICAL DESCRIPTION OF THE CUSP ELECTRONS EJECTED IN ASYMMETRIC HEAVY-ION COLLISIONS

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Abstract

Starting from the Faddeev equations a series expansion for the transition amplitude for electron emission is given, which serves as a basis for the discussion of approximations used in the literature and their range of validity for a given collision system and momentum of the ejected electron. Both target and projectile electron emission will be considered. Emphasis is laid on the asymmetry of the forward peak and its variation with system parameters, such as collision velocity and charge ratio Z_P/Z_T. The theoretical results will be confirmed by a comparison with experimental data.

1.Introduction

Electron spectroscopy has received a great deal of attention lately, since the production of electrons by fast ion impact is of principal interest in many branches of physics. In particular, the so-called cusp electrons which are emitted with nearly zero velocity relative to the projectile, i.e. appear in the target frame in forward direction with a momentum that equals the collision velocity v have been focused in a variety of experimental and theoretical investigations (see i.e. Meckbach and Burgdörfer, proceedings of this conference). The spectral distribution of the cusp electrons provides a sensitive test for the applicability of first-order theories, and I will show in the following that these theories are invalid not only for electrons initially bound to the target, but also for electron loss from the projectile in asymmetric collision systems, even at very high impact velocity.

2.Faddeev Theory

The basic formalism for electron emission is most easily described in the three-particle picture, where the effect of all electrons of the projectile-target system except the active one is incorporated into the potentials. Let Ψ_i^A be the initial electronic bound state (with A denoting either target T or projectile P), V_A the interaction field between the electron and A, and V_B the electronic perturbation in the initial channel. In the semiclassical theory the transition amplitude is given by (in atomic units)

$$a_{fi} = -i \int_{-\infty}^{\infty} dt \langle \Psi_f^- | V_B | \Psi_i^A \rangle \tag{2.1}$$

where Ψ_f^- is the exact solution to the electronic two-center problem with the boundary condition of a free electron in the final state. For fast collisions, which I shall concentrate on, the internuclear motion can be described by a classical straight-line path, thus neglecting the internuclear potential.

According to Faddeev[1], Ψ_f^- can be written as a sum of wavefunctions which are determined by a set of two coupled equations

$$|\Psi_f^-\rangle = |\Psi_{o,f}\rangle + |\Psi_1\rangle + |\Psi_2\rangle \tag{2.2}$$

$$|\Psi_1\rangle = G_B V_B |\Psi_{o,f}\rangle + G_B V_B |\Psi_2\rangle$$

$$|\Psi_2\rangle = G_A V_A |\Psi_{o,f}\rangle + G_A V_A |\Psi_1\rangle$$

where $\Psi_{o,f}$ is an electronic plane wave, and $G_{A,B}$ is a Green's function defined by $G_{A,B} = (i\partial/\partial t + \Delta/2 - V_{A,B} - i\varepsilon)^{-1}$ with $\varepsilon \rightarrow 0$. In order to avoid convergence problems from the long-range Coulomb fields it is assumed here and in the following that V_A, V_B are screened Coulomb potentials, with the well-defined limit of screening $\rightarrow$ 0 taken in the final T matrices. From (2.2), series expansions for Ψ_f^- can be derived. Using the definition of an eigenstate to nucleus A, $\Psi_f^A = (1 + G_A V_A)\,\Psi_{o,f}$ the series can be written in three different ways

$$|\Psi_f^-\rangle = (1 + G_B V_B + G_A V_A + G_B V_B G_A V_A + G_A V_A G_B V_B + \dots)\,|\Psi_{o,f}\rangle \tag{2.3a}$$

$$= (1 + G_A V_A + G_B V_B G_A V_A + \dots)\,|\Psi_f^B\rangle \tag{2.3b}$$

$$= (1 + G_B V_B + G_A V_A G_B V_B + \dots)\,|\Psi_f^A\rangle \tag{2.3c}$$

where the form (2.3a) is a symmetric expansion allowing for both a projectile or target electronic final state.

For practical purposes, these series have to be truncated, such that it is no longer irrelevant, which of them is used. It is thus crucial to determine from the momentum k and the direction ϑ of the ejected electron relative to the parent nucleus, as well as from the charge ratio Z_A/Z_B, whether V_A or V_B will be the dominating potential, in order to truncate the appropriate series. An estimate for the potential acting on the electron a time τ after the collision can be found by using the Coulomb formula

$$V_A \approx \frac{Z_A}{k\tau} \quad , \quad V_B \approx \frac{Z_B}{\tau\left[(v - k\cos\vartheta)^2 + k^2\sin^2\vartheta\right]^{1/2}} \tag{2.4}$$

Restricting the discussion to the cusp electrons, one has to use (2.3c) for $k \to 0$ if $Z_A \gg Z_B$ (because V_A is dominant), and (2.3b) for $k \to v$ and $\vartheta \to 0$ if $Z_B \gg Z_A$ (as V_B is dominant), but in the cases $k \to 0$, $Z_A \ll Z_B$ as well as $k \to v, \vartheta \to 0$, $Z_B \ll Z_A$, the symmetric series (2.3a) should be preferred.

3.Approximations for the Calculation of the Forward Peak: Target Ionisation

Let me first consider the case where bare projectiles are impinging on the target atom, such that only target electrons are contributing to the forward peak. Solid state effects, as for example capture into high-lying bound projectile states which are eventually participating in the convoy electron production[2], will not be discussed here. In this case, A is identified with the target T, B with the projectile P.

a) First-order Born Approximation

The first Born approximation for target ionisation is obtained by retaining the first term in the series (2.3c), such that the transition matrix element reads

$$M_{fi}^{1.B.} = \langle \Psi_f^T \mid V_P \mid \Psi_i^T \rangle \tag{3.1}$$

Pioneer experiments on the forward peak in collisions of H^+ on He by Rudd and coworkers[3] have clearly demonstrated that (3.1) strongly underestimates the number of electrons ejected with beam velocity near 0^o.

b) First-order Faddeev Approximation

From the estimate (2.4) it is obvious that in this case the projectile field must not be neglected in the expansion of Ψ_f^-. Using the symmetric series (2.3a) and retaining the first three terms $1 + G_P V_P + G_T V_T$, i.e.

$$M_{fi}^{1.FA} = \langle \Psi_f^P \mid V_P \mid \Psi_i^T \rangle + \langle \Psi_f^T \mid V_P \mid \Psi_i^T \rangle - \langle \Psi_{o,f} \mid V_P \mid \Psi_i^T \rangle \tag{3.2}$$

Macek[4] could explain the enhanced intensity of the cusp electrons. It originates from the normalisation of the projectile eigenstate Ψ_f^P, and diverges like $F_o = 2\pi Z_P/|\vec{k}_f - \vec{v}|$ as the momentum $\vec{k}_f$ of the electron approaches $\vec{v}$, unless the finite detector resolution is taken into account. However, a careful analysis of the peak shape[5] reveals an enhanced intensity of electrons with $k_f < v$ as compared to those with $k_f > v$, a feature which can not be reproduced by the symmetric factor F_o contained in (3.2).

c) Second-order Born Approximation

Incidentally, the insufficiency of a first-order theory for the description of charge transfer to the continuum (CTC) which is the basic process leading to the cusp electrons, is not surprising. It is known from bound-state charge transfer that the Brinkman-Kramers theory provides the wrong high-velocity limit which has only recently been verified experimentally[6], and also gives a wrong relative occupation probability of the final subshells. Therefore, Dettmann[7], Shakeshaft[8] and coworkers have applied the second Born approximation, which consists in retaining the fields up to first order in the series (2.3b):

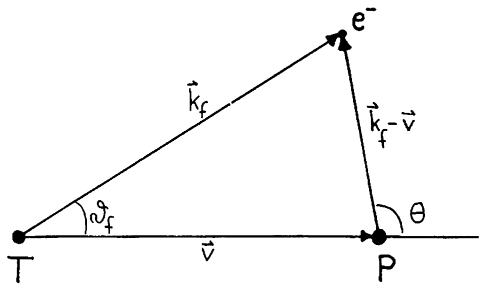

Fig.1 Momenta of the ejected electron in the projectile or target frame

$$M_{fi}^{2.B.} = \langle \Psi_f^P \mid V_P + V_T G_0 V_P \mid \Psi_i^T \rangle \qquad (3.3)$$

where G_0 is the free propagator. The asymmetry property of the cusp electrons is readily displayed by writing the doubly differential cross section in terms of a partial wave expansion

$$\frac{d^2\sigma}{dE_f d\Omega_f} \sim \frac{1}{|\vec{k}_f - \vec{v}|} \sum_l a_l P_l(\cos\theta) \qquad (3.4)$$

where $E_f = k_f^2/2$, P_l a Legendre polynomial and θ the electron emission angle in the projectile frame with respect to $\vec{v}$. It has been shown[9] that the assumption of continuity of the capture amplitude across the ionisation threshold leads to finite a_l (including odd values of l) in the limit $\vec{k}_f \to \vec{v}$. This is satisfied for the second Born theory[8,10], whereas a_l $(l > 0)$ vanishes in the first-order theory. For zero emission angle ϑ_f in the target frame, electrons with $k_f > v$ are emitted at $\theta = 0$, such that $P_l = 1$, while electrons with $k_f < v$ appear in the backward direction $\theta = \pi$, where $P_l = (-1)^l$, resulting in a discontinuity of the cross section at $k_f = v$. The increased intensity at $\theta = 0$ may be explained by the fact that these electrons are ejected in the same direction as the target motion (when viewed from the projectile frame).

Another distinction between the Brinkman-Kramers and the second Born approximation is found for the position E_{peak} of the forward peak as a function of emission angle ϑ_f. From (3.4) it can be verified[10] that the first-order theory shows a quadratic dependence on ϑ_f for small angles, while the second Born theory displays a linear decrease of E_{peak} with ϑ_f. The latter dependence is clearly verified by experiment in He^{++} on Ar (refs. 10,11) and H^+ on He collisions[12].

d) Impulse Approximation (IA)

If the projectile is much heavier than the target, a first-order treatment of the potential V_P in the T matrix is not sufficient. Instead, a consistent first-order expansion of ψ_f^- in the weak target field V_T leads with the help of (2.3b) to

$$|\psi_f^-\rangle = (1 + G_0V_T + G_PV_PG_0V_T)\,|\psi_f^P\rangle$$

$$M_{fi}^{IA} = \langle\psi_f^P\,|\,V_T(1 + G_PV_P)\,|\psi_i^T\rangle \qquad (3.5)$$

where use has been made of the relations $G_P = G_0 + G_PV_PG_0$ and $\langle\psi_f^P|\,V_P|\psi_i^T\rangle = \langle\psi_f^P|\,V_T|\psi_i^T\rangle$. An insertion of a complete set of plane waves $\psi_{0,\vec{q}}$ behind the operator $(1 + G_PV_P)$ in (3.5) allows for the description of the CTC process in terms of ejection of a target electron into an intermediate projectile state with momentum $\vec{q} + \vec{v}$, with a subsequent scattering by the target field into the final state ψ_f^P.

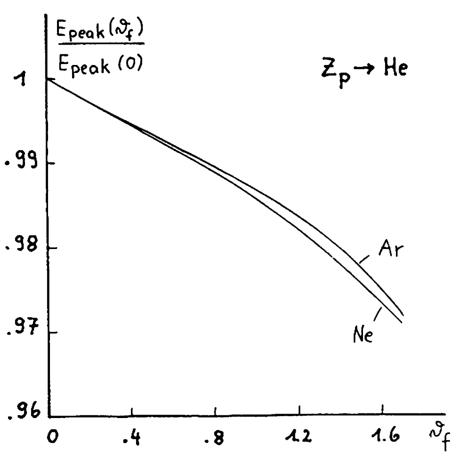

Fig.2 Ratio of peak energy to $v^2/2$ as a function of ϑ_f for collisions of Ar^{18+}(v=18.1 a.u.) and Ne^{10+} (v=17.62 a.u.) with He

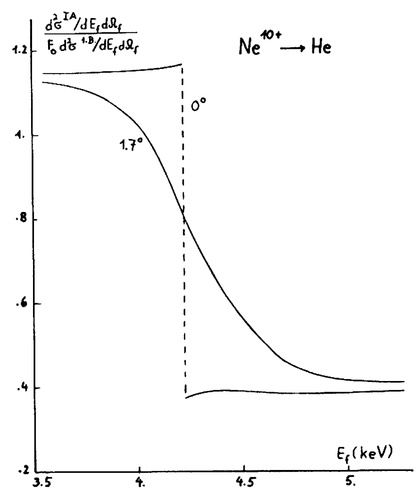

Fig.3 Cross section ratio between impulse approximation and first Born theory times $F_0=2\pi Z_P/|\vec{k}_f-\vec{v}|$ at $\vartheta_f=0^0$ and 1.7^0 for 155 MeV Ne^{10+} on He

Off-shell effects for CTC are expected to be small[13] and neglected in the following.

As the impulse approximation reduces to the second Born theory for asymptotic collision velocities, it is expected to show similar features characteristic for a higher-order theory. Fig.2 displays the linear dependence of E_{peak} on ϑ_f for small angles in collisions of Ar^{18+} and Ne^{10+} with He at nearly equal impact velocities. In order to make the discontinuity of the differential cross section at $\vec{k}_f = \vec{v}$ visible, Fig.3 shows the ratio $d^2\sigma^{IA}/(F_0 d^2\sigma^{1.B.})$ which is finite at $E_f = v^2/2$. At nonzero angles the discontinuity is replaced by a rather steep fall-off of the ratio when E_f is increased.

In order to study the dependence of the discontinuity on the projectile charge and collision velocity, let me define the ratio

$$S = \frac{d^2\sigma/dE_f d\Omega_f(k_f^{<}, \vartheta_f=0)}{d^2\sigma/dE_f d\Omega_f(k_f^{>}, \vartheta_f=0)} \tag{3.6}$$

where the electron momenta $k_f^{<}$ and $k_f^{>}$ are chosen such that $\eta = Z_p/|k_f - v|$ is equal (and $\gg 1$, but finite for numerical reasons) for both, with $k_f^{<} < v$ and $k_f^{>} > v$. As the electron is in a final projectile state, the field strength Z_p is taken as

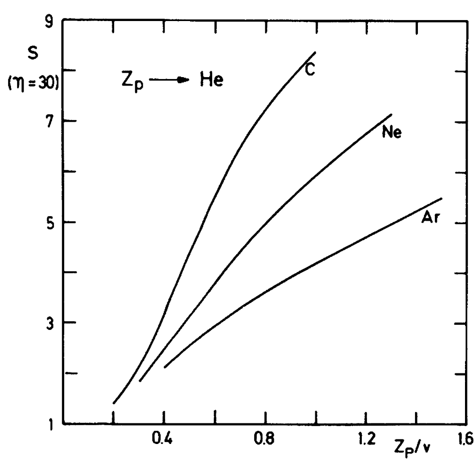

Fig.4 Discontinuity S at $\vartheta_f=0$ and $\eta=30$ as a function of inverse velocity for collisions of C^{6+}, Ne^{10+} and Ar^{18+} with He

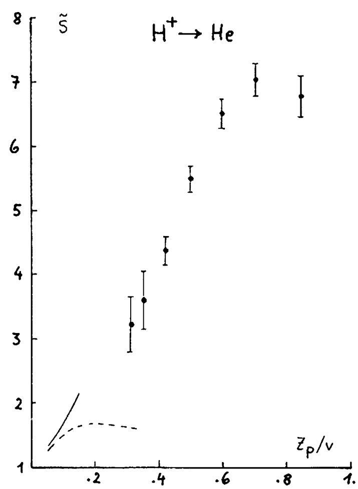

Fig.5 Discontinuity $\tilde{S}$ at $\vartheta_f \approx 0$ as a function of Z_p/v in $H^+ \rightarrow He$ collisions. Shown are results for the IA (——) and the asymptotic second Born theory (---). Data are from Dahl[12]

reference parameter also with respect to the velocity v. Fig.4 shows S in the IA for C^{6+}, Ne^{10+} and Ar^{18+} impinging on a He target. For large collision velocities, $v \gg Z_P$, a peaking approximation reveals[13] that in the limit of $k_f \longrightarrow v$, $\vartheta_f \longrightarrow 0$ the matrix element in (3.5) becomes proportional to a confluent hypergeometric function, the argument of which is $x \approx 16iZ_P/3v$ for $k_f \gtrsim v$ and $x \approx 0$ for $k_f \lesssim v$. Thus the discontinuity vanishes ($S \longrightarrow 1$) for $Z_P/v \longrightarrow 0$. At fixed Z_P/v which may also be considered as parameter of the initial perturbing field, S increases when Z_P/Z_T becomes smaller, i.e. when the relative influence of the target becomes stronger.

In the case of $H^+ \longrightarrow$ He collisions, the systematics of the discontinuity has recently been investigated experimentally[12]. In Fig.5 the related quantity $\tilde{S} = \vec{k}_f^{>} F_0(\vec{k}_f^{>})\, d^2\sigma(\vec{k}_f^{<},0)/[\vec{k}_f^{<} F_0(\vec{k}_f^{<})\, d^2\sigma(\vec{k}_f^{>},0)]$ is shown, where $(\vec{k}_f^{<} - v)^2 = (\vec{k}_f^{>} - v)^2 = 2 \times 10^{-3}$ eV. However, the data are taken at relatively low v where the IA is no longer valid. Nevertheless, the trend shown in Fig.4 is in good agreement with the experiment. That the theory extrapolated to H^+ projectiles lies above the data results from the average over the angular acceptance in the experiment, which reduces the discontinuity (cf. Fig.3). For comparison, the second Born results are also shown for $H^+ \longrightarrow$ He at $\vartheta_f = 0$, applying the high-velocity formula from ref.8. It is seen that even at rather high velocity, this formula breaks down, whereas at the highest velocity investigated, agreement is found with the IA within the numerical accuracy of the latter.

The discontinuity S reveals itself as a decisive parameter for the shape of the forward peak. Considering only partial waves with $l \leq 1$ in the expansion (3.4), the differential cross section may be approximated by

$$\frac{d^2\sigma}{dE_f d\Omega_f} = \frac{2\kappa Z_P}{|\vec{k}_f - \vec{v}|} \; a \left[(S+1) - (S-1)\cos\theta \right] \qquad (3.7)$$

$$\cos\theta = \frac{k_f \cos\vartheta_f - v}{|\vec{k}_f - \vec{v}|}$$

which has the property that at $\vartheta_f = 0$, $d^2\sigma(k_f^{<},0)/d^2\sigma(k_f^{>},0) = S$, while $d^2\sigma$ is continuous for $\vartheta_f \neq 0$. In order to compare with experimental peak shapes, (3.7) has to be integrated over the angular acceptance ϑ_0, giving a simple analytic formula, and over the energy resolution ΔE_f. The constant a in (3.7) accounts for the absolute value which hitherto has not been determined experimentally. In the case of 155 MeV Ne^{10+} colliding with He ($\vartheta_0 = 1.4^0$, $\Delta E_f = 2.2\%$) the peak shape is compared with experimental data[14] in Fig.6. The dashed line is the formula (3.7) with S from Fig.4, and gives a reasonable fit to the peak shape. The agreement between the IA and (3.7) in the tails might be improved by introducing the energy dependence of the first Born theory into the constant a, as suggested from Fig.3. For the collision system $O^{8+} \longrightarrow$

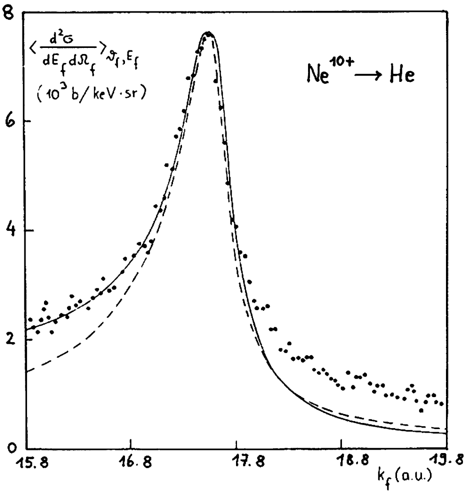

Fig.6 Differential cross section for cusp electron emission in $Ne^{10+} \rightarrow He$ collisions at v=17.62 a.u. Full line, IA, dashed line, (3.7) normalised at the peak. Data are from Berry et al[14]

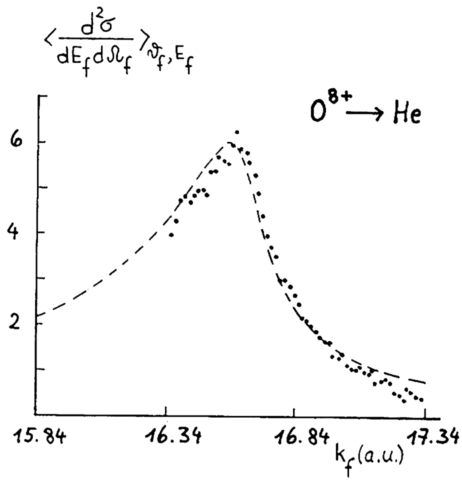

Fig.7 Differential cross section for cusp electron emission in $O^{8+} \rightarrow He$ collisions at v=16.64 a.u. The dashed line is the formula (3.7), the data are from Berry et al[14] (arbitrary units)

He (ϑ_0 = 1.4^0, ΔE_f = 1.4%) the formula (3.7) with S = 3.49 also compares well with the experimental data[14]. Note that apart from the normalisation of the peak height there are no free parameters in this theory.

4. Projectile Ionisation

When the projectile is not fully stripped, electron loss will in general provide the dominant contribution to the forward peak at high collision velocities. Then in the formulas (2.1) - (2.3), A has to be identified with the projectile P, B with the target T.

a) First-order Born Approximation

The first Born approximation for projectile ionisation, which is obtained from the first term in the series (2.3c), yielding

$$M_{fi}^{1.B.} = \langle \psi_f^P \,|\, V_T \,|\, \psi_i^P \rangle \qquad (4.1)$$

has been frequently applied[15,16] for the description of the forward peak in systems with $Z_P \gtrsim Z_T$ and large v. In a similar way as for target ionisation, the differential cross section near $\vec{k}_f = \vec{v}$ can be decomposed into partial waves

$$\frac{d^2\sigma}{dE_f d\Omega_f} \sim \frac{1}{|\vec{k}_f - \vec{v}|} \sum_{l=0}^{2n} a_l P_l(-\cos\theta) \tag{4.2}$$

where in the first Born theory, l can only take even values[17,18] such that the cross section does not exhibit a discontinuity when θ is switched from 0^o to 180^o. Experiments show[19] that the electron loss peak is much more symmetric than the corresponding CTC peak which would support the applicability of the first Born theory; however, the dependence of the peak width on velocity in collisions of e.g. Si with Ne and O with Ar show deviations[19] from first Born predictions, and a detailed study[20] of the angular distribution for H $\rightarrow$ He collisions in the cusp region indicates that more partial waves than present in (4.2) should contribute.

b) Second-order Faddeev Approximation

For asymmetric systems with $Z_P \ll Z_T$ a treatment of the target field V_T in first order is not sufficient, as long as the collision velocity is not very much greater than Z_T. As in the cusp region both potentials will be important, the symmetric series (2.3a) for ψ_f^- should be used. The second-order Faddeev approximation includes all terms explicitly written in (2.3a), such that the transition matrix element becomes

$$\begin{aligned} M_{fi}^{2.FA} = & \langle \psi_f^T | (1 + V_P G_P) V_T | \psi_i^P \rangle \\ & + \langle \psi_f^P | (1 + V_T G_T) V_T | \psi_i^P \rangle \\ & - \langle \psi_f^T | V_T | \psi_i^P \rangle - \langle \psi_f^P | V_T | \psi_i^P \rangle \\ & + \langle \psi_{0,f} | V_T | \psi_i^P \rangle \end{aligned} \tag{4.3}$$

where the last three terms correct for double counting and are nothing but the first-order Faddeev approximation. The first term, M_1, describes the charge transfer to the target continuum and influences the tails of the forward

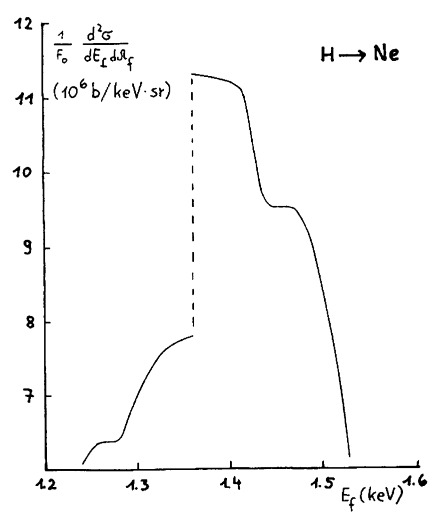

Fig.8 Cross section divided by F_0 for electron emission in 2.5 MeV H $\rightarrow$ Ne collisions at ϑ_f=0. Only the second term in (4.3) is included

peak[21], whereas the second term, M_2, accounts for the projectile ionisation via an intermediate target continuum state and is dominant for $\vec{k}_f \approx \vec{v}$. At $\vartheta_f = 0$, the matrix element corresponding to this second term[21] exhibits a phase proportional to $Z_P \cos\Theta$ which gives rise to a discontinuity as k_f traverses v. Unfortunately, this phase depends also on integration variables which cannot be fixed by a simple peaking approximation. In Fig.8 the discontinuity of the cross section calculated only from M_2 is clearly visible. In contrast to the target ionisation, the high-energy side is enhanced, because the electrons which are ejected with $\Theta = 0$ move in the same direction as the projectile from which they originate. Note that the wings of the peak will be influenced by M_1 which is not included in the calculation.

Again, one may define the ratio S according to (3.6) as a measure for the discontinuity. Fig.9 shows S as a function of Z_P/v for H on C, Ne and Ar targets. While the first Born theory always gives a ratio close to 1, the deviation from unity in the Faddeev approximation is the larger, the heavier the target atom and the lower the collision velocity, indicating the importance of the target field. In Fig.10 the absolute values of the differential cross section at $k_f \gtrless v$ and $\vartheta_f = 0$ are compared to the first Born results. Considerable deviations are found even for a C target, and the Born theory becomes only valid at $v \gg Z_T$.

In conclusion, it has been shown for asymmetric collision systems, using the impulse approximation for target ionisation and the second Faddeev approximation for electron loss that the forward peak displays a discontinuity for zero emission angle

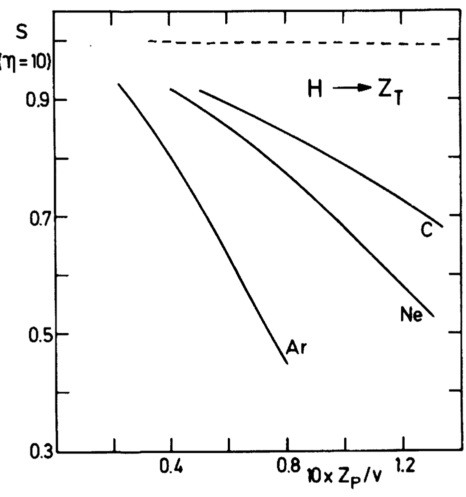

Fig.9 Discontinuity S at ϑ_f=0 and η =10 as function of inverse velocity for H colliding with C, Ne and Ar

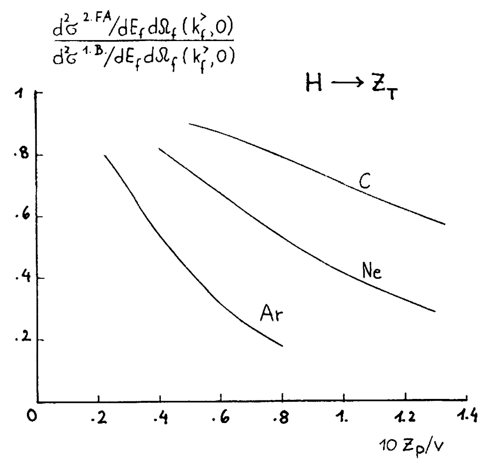

Fig.10 Cross section ratio between the Faddeev and the Born approximation for H colliding with C, Ne and Ar at ϑ_f=0 and η =10

at $k_f = v$ irrespective whether the electrons originate from the target or the projectile. The magnitude of this discontinuity can be closely related to the experimental peak shapes which provide strong evidence for the necessity of a higher-order theory.

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