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Inverted cusps in electron spectra near zero electron velocity in inelastic ion-atom collisions

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Expressions for inverted cusps in electron spectra near zero velocity from inelastic ion-atom collisions are derived by the plane-wave Born approximation. In addition, it is shown that for $2p_0$ ionization not only the cusp-shaped electron-loss peak is inverted but the binary-encounter peak too.

Recently, Burgdörfer[1] showed that the usual cusp-shaped electron spectrum from inelastic ion-atom collisions is inverted for $2p_0$ ionization of the projectile. Here it is assumed that the cusp is dominated by electron loss to the continuum (ELC).[2] Thus the cusp shows a dip at an electron velocity $v_e = v_p$ which gets more pronounced with increasing projectile velocity v_p. Burgdörfer[1] obtained his results by an algebraic $O(4,2)$ approach and showed a few graphical examples of electron spectra. In this Rapid Communication we will give a formula for the inverted cusp which shows a general scaling for arbitrary projectile-target combinations at any projectile velocity. This scaling is correct for hydrogenic wave functions of the initial and final electron state and for an unscreened Coulomb interaction. In the first-order Born approximation the double-differential cross section for the ejection of a projectile electron from an arbitrary state $|nlm\rangle$ is easily obtained by means of partial derivatives of the ionization matrix element of the $1s$ state. In the limit of vanishing electron velocity u (in the projectile frame), this matrix element acquires a simple form, such that the cross section reduces to a series of Legendre polynomials:

$$\lim_{u\to 0}\left(u\frac{d\sigma}{d\vec{u}}\right) = \sigma_0\left(1+\sum_{\lambda=1}^{n} a_{2\lambda}P_{2\lambda}(\cos\theta)\right) \quad . \tag{1}$$

The target is thereby left in its ground state. θ is the electron ejection angle relative to $-\hat{v}_p$ and the beam direction is taken as quantization axis of the magnetic substates. σ_0 and $a_{2\lambda}$ are independent of θ. The coefficients $a_{2\lambda}$ scale with v_p/v_{or}, where $v_{or} = Z_p/n$ is the orbital velocity of the electronic initial state and Z_p the projectile charge, but their structure depends on n, l, and m. An equivalent expression for the double-differential cross section for the special case of $1s$ ionization has been given by Day[3,4] and Briggs and Day.[5] For the $2p_0$ ionization the angular distribution is determined by the coefficients a_2 and a_4. Figure 1 shows a_2 and a_4 as a function of v_p/v_{or}. Transforming Eq. (1) to the laboratory frame and integrating over the angular acceptance θ_0 of the electron spectrometer (neglecting finite energy resolution) gives the scaled cusp yield I_{cusp} as a function of the laboratory frame electron velocity v_e,

$$I_{cusp}(\eta) = \text{const}\left[(A+B-C)|\eta| - (1+\eta^2)^{1/2}\left(\frac{A\eta^4}{(1+\eta^2)^2}+\frac{B\eta^2}{1+\eta^2}-C\right)\right] \ , \tag{2}$$

with

$$A = 35a_4/24;\quad B = 3a_2/2 - 15a_4/4 \ ,$$
$$C = 1 - a_2/2 + 3a_4/8;\quad \eta = (v_e - v_p)/(v_e v_p)^{1/2}\theta_0 \ . \tag{3}$$

For $v_p \to 0$ one obtains $a_2 = a_4 = 0$ and for $v_p \to \infty$ the coefficients are $a_2 = \frac{5}{7}$, $a_4 = -\frac{12}{7}$. The latter values hold for an

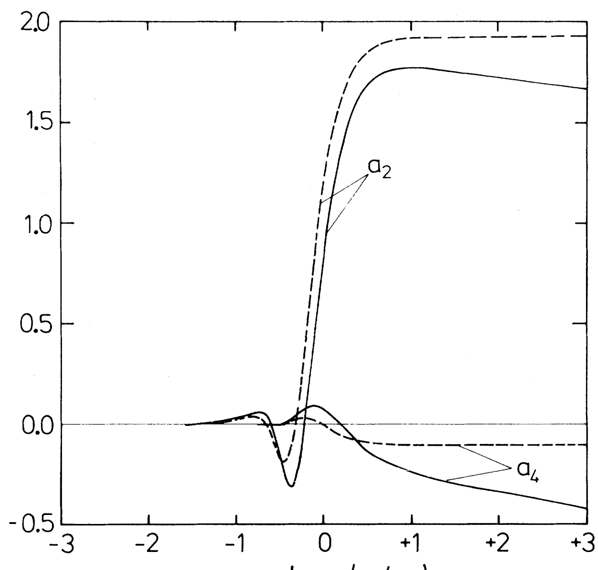

FIG. 1. Angular distribution parameters a_2 and a_4 as a function of v_p/v_{or}. Solid lines: unscreened Coulomb interaction; dashed lines: exponentially screened Coulomb interaction. The Thomas-Fermi screening parameter $\lambda = 1.13Z_T^{1/3}$ (Z_T is the target atomic number) was chosen to be that of an argon target (Ref. 6).

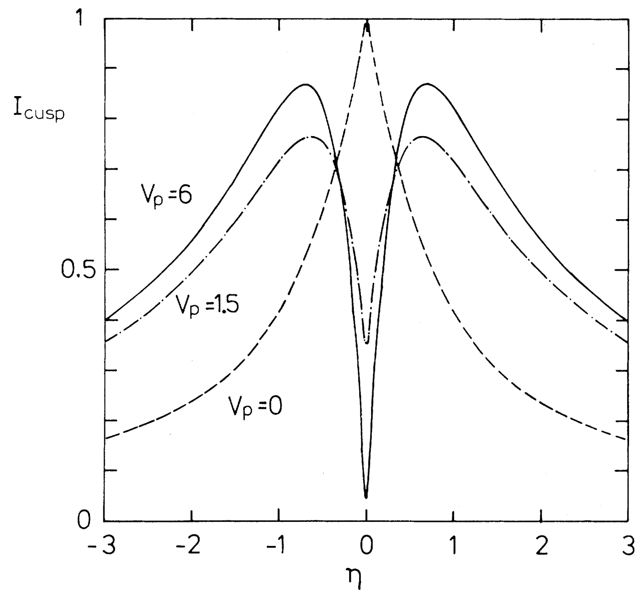

FIG. 2. The cusp yield I_{cusp} as a function of the scaled electron velocity (see text). The curves belong to different projectile velocities v_p ($v_{\text{or}}=1$).

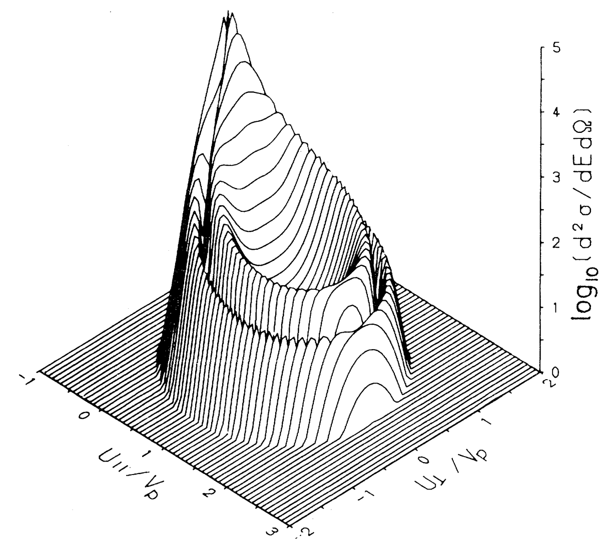

FIG. 3. An isometric plot of the double-differential cross section for $2p_0$ ionization (in units of b/keV sr) of a Ne target by protons with $v_p = 20$ a.u.

unscreened Coulomb interaction. Inspection of Fig. 1 reveals that a_2 and a_4 approach these limiting values logarithmically only. It follows that for small projectile velocities v_p one gets the usual cusp-shaped electron peak ($A = B = 0$, $C = 1$), but for $v_p \rightarrow \infty$ the dip within the cusp reaches even zero electron yield ($C = 0$). Figure 2 shows the cusp yield as a function of the scaled electron velocity η for different projectile velocities. The curve for $v_p = 0$ might be somewhat unrealistic since the plane-wave Born approximation ceases to be valid in this limit. Clearly, the development of the cusp inversion with increasing projectile velocity can be seen.

In general, an inversion occurs for $2a_2 - 8a_4/3 - 1 \geq 0$. This condition holds not only for $2p_0$—but also for $1s$ ionization, where $a_4 = 0$.[3,4] Thus even the cusp from $1s$ ionization could be inverted for $a_2 \geq \frac{1}{2}$,[4] at least in principle. It is interesting to note that, within the first Born approximation, a_2 always stays below 0.5.[3] In addition, we have investigated $2s$ ionization where both a_2 and a_4 do not vanish identical but again the condition for cusp inversion cannot be fulfilled within the whole v_p range. In our treatment of cusp inversion we have neglected the simultaneous excitation of the target atom. For a He^+/Ar interaction Burgdörfer[1] has found that this excitation did not seriously affect the dip structure since the doubly inelastic contribution was a small fraction of the total cusp cross section only.

Whereas Eqs. (1) and (2) hold only for zero electron velocity u in the projectile reference frame, Fig. 3 displays an isometric plot of $d^2\sigma/dE\,d\Omega$ as a function of the scaled electron velocities $u_\perp$ and $u_\parallel$, perpendicular and parallel to the beam direction. $E = 0.5u^2$ is the electron energy and the cross section is plotted logarithmically. The ring-shaped pattern is the binary-encounter peak located at $u = 2v_p \cos\theta$. It is clearly seen that the peak is inverted to a dip. Thus not only the cusp at $u = 0$ is inverted but the binary-encounter peak too. Physically this is easy to understand. Since the cross section at the location of the binary-encounter peak is proportional to the electron momentum density projected on the beam direction,[7] the usual peak gets a dip: The $2p_0$ momentum distribution is vanishing everywhere perpendicular to the beam direction; thus the projection is zero. In contrast, the $2p_1$ distribution peaks perpendicular to the beam direction. This yields an ordinary peak of the cross section at $u = 2v_p \cos\theta$. It follows that the Fano-Macek alignment parameter A_0^{col} (Ref. 8) reaches its maximum possible positive value $A_0^{\text{col}} = +0.5$ at the position of the binary-encounter peak. This holds for projectile velocities where the peak is really inverted, i.e., for $v_p/v_{\text{or}} > 1$. From the discussion above it is evident that every magnetic substate shows peak inversion if the momentum distribution has a nodal plane perpendicular to the beam direction. Thus any substate $|nlm\rangle$ shows inversion if the sum $(l+m)$ is odd. In conclusion, we note that peak inversion is a general property of certain magnetic substates and occurs in any first-order theory both for ionization and bound-state charge transfer.[9]

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