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ANGULAR MOMENTUM OF CAPTURED ELECTRONS: THE CLASSICAL OVER-BARRIER MODEL AND ITS LIMITATIONS

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An existing model which incorporates angular momentum conservation for the captured electron relative to the capturing ion throughout the capture event into the classical overbarrier model is improved and extended by introducing an angular momentum uncertainty. The extended model is shown to reproduce experimental average angular momenta of captured electrons satisfactorily.

Electron capture by slow highly charged ions can in a first approximation be described by the classical over-barrier model [1]. In this model capture is assumed to take place at a crossing of the diabatic potential curves if at the same time the electron – in a classical description – can overcome the potential barrier between the ionic charges of target and projectile. This model has been proven to be fairly successful in predicting the total cross section σ for charge exchange and the distribution of principal quantum numbers n of the transferred electron. Recently we have suggested an extension of the model [2] in order to describe the angular momentum distribution of this electron. Our extension is based on the observation that, in a frame attached to the projectile ion, the electron "traveling" with the target atom has an angular momentum of the order of bv with b the impact parameter and v the relative velocity of the collision partners. The total charge exchange cross section σ can therefore be decomposed into rings within which the angular momentum L, carried into the collision by the target electron, can be accommodated in the corresponding subshell. In this approximation one obtains subshell cross section σ_L given by

$$\sigma_L = A 2\pi \int_0^{R_c} W_L(b) b \, \mathrm{d}b, \tag{1}$$

with a proportionality factor A and $W_L(b)$ a probability function given by

$$W_L(b) = \theta(L + 1 - bv)\ \theta(bv - L) \tag{2}$$

in which the step functions θ represent the main assumption of conservation of the classical angular momentum during the electron transfer process. In [2] we have made a comparison of the average angular momentum $\langle L \rangle$ as calculated from eq. (1) by means of

$$\langle L \rangle = \left(\sum_{L=0}^{n_f - 1} (L + \tfrac{1}{2}) \sigma_L \right) \left(\sum_{L=0}^{n_f - 1} \sigma_L \right)^{-1}, \tag{3}$$

with experimental values of $\langle L \rangle$ as obtained from the measurements of Dijkkamp et al. [3]. In this comparison we assumed an L-independent proportionality factor A and a maximum internuclear distance R_c for electron transfer, which in the simplest approximation was also independent as given by the classical overbarrier model [1] and which in a better approximation was calculated by taking the centrifugal potential of the electron with angular momentum L into account, leading to

$$R_c(n(L)) = \frac{2(q-1)}{-2|I_t| + q^2/n(L)^2}, \tag{4}$$

with q the initial charge of the projectile, I_t the ionization potential of the target atom and $n(L)$ the principal quantum number of the captured electron, given by

$$n(L) = q \left(\frac{2q^{1/2} + 1}{2|I_t|(q + 2q^{1/2})} \right)^{1/2} \times \left(1 + \frac{(q-1)(1+q^{1/2})^2 |I_t| L^2}{2q(2q^{1.2}+1)^3} \right)^{-1/2}. \tag{5}$$

Another improvement of the description can be obtained by introducing an L-dependence of the proportionality factor A by means of

$$A_L = (2L + 1)/(2L + 1 + n_t^2), \tag{6}$$

which represents the statistical weight of L-states in the projectile ion related to the weight of all states available

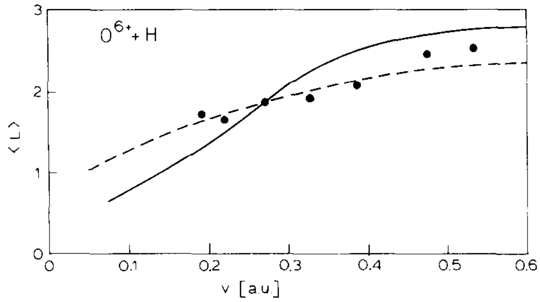

Fig. 1. Average angular momentum $\langle L \rangle$ as function of the projectile velocity for electron capture in the process $O^{6+} + H \to O^{5+}(n = 4) + H^{+}$. Solid line: calculations with eqs. (1)–(6). Dashed line: calculations with eq. (14). Points: experimental results obtained from the data of Dijkkamp et al. [3].

to the electron in either the projectile or target. Fig. 1 shows a comparison of theoretical and experimental values of $\langle L \rangle$ for the case of O^{6+} + H collisions, leading to O^{5+} ($n = 4$). The agreement between experimental and theoretical values is better than in [2].

Although, as said in [2], the partial cross sections σ_L themselves should not be taken too serious, we show a set of σ_L – again for the case of O^{6+} + H collisions – in fig. 2, since this allows a better discussion of the short-

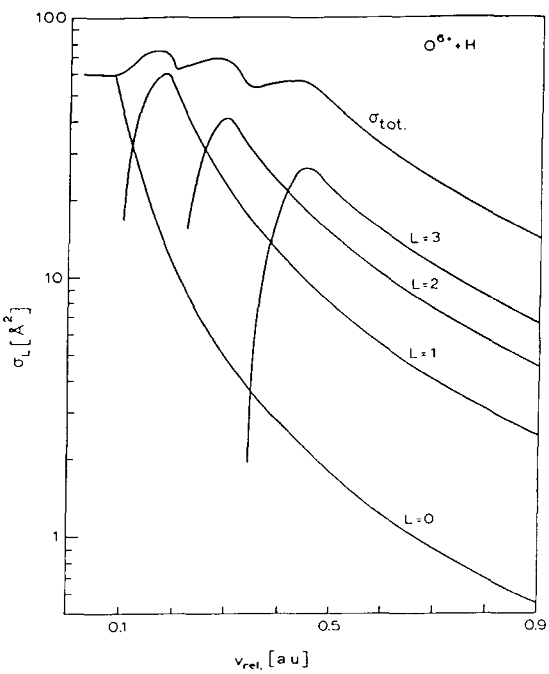

Fig. 2. Partial cross sections σ_L as function of the projectile velocity v as calculated from eqs. (1), (2), (4)–(6).

comings in the description. The cross sections σ_L as calculated from eqs. (1), (2), (4)–(6), are sharply peaked and at low velocities there are no contributions from higher L-values at all. As opposed to this the experiments [3] show that even at very low velocities there are significant contributions of charge exchange into 4d and 4f substates.

To improve the theoretical description of the classical model one could take into account that even for well defined impact parameter b and collision velocity v a distribution of angular momenta will occur due to (1) the finite size of the electron cloud in the target atom and (2) due to the uncertainty of the barrier-height in the limited time available for the transfer process. Especially the latter effect can be shown to have an important influence and will be discussed in more detail below.

Following Niehaus [4] we assume an uncertainty in the energy of the barrier height given by

$$\Delta E = \sqrt{V_{\text{rad}} \cdot \mathrm{d}V_b/\mathrm{d}R} \tag{7}$$

which represents the minimum of δE given by the uncertainty relation on one hand and by the classical variation of the barrier height on the other hand, when the time interval Δt of observation is varied.

As a consequence the electrons have – on the average – some extra energy when they pass the barrier. For this extra energy E we assume a distribution given by

$$W(E) = 2\pi^{-1/2}\Delta E^{-1} \exp\left[-(E/\Delta E)^2\right]. \tag{8}$$

This leads to a momentum distribution $W(p) = pW(E)$. From this distribution we calculate the absolute value of the projection of the average momentum in some arbitrary direction, $\bar{p}_x$, by the relations

$$\langle p_x^2 \rangle = \frac{\int_{\text{solid angle}} \mathrm{d}\Omega \, \sin^2\vartheta \, \cos^2\varphi}{4\pi} \int_0^\infty \mathrm{d}E \, W(E) p^2$$

$$= \frac{2}{3\sqrt{\pi}} \Delta E, \tag{9}$$

$$\bar{p}_x = \sqrt{\frac{2}{3\sqrt{\pi}} \Delta E}. \tag{10}$$

In the coordinate frame of the projectile, this momentum corresponds to an extra angular momentum of the captured electron. For a collision with impact parameter b, and capture of the electron at distance R_c, the angular momentum values of the captured electron will therefore be distributed around the value $L_0^* = vb$, with a width of the distribution given by

$$|\Delta L| = R_c \bar{p}_x. \tag{11}$$

To relate the angular momentum L^* to its quantum number we use $L^* = L + \frac{1}{2}$. The distribution around $L_0^* = vb$ we assume to be a Gaussian of width $|\Delta L|$.

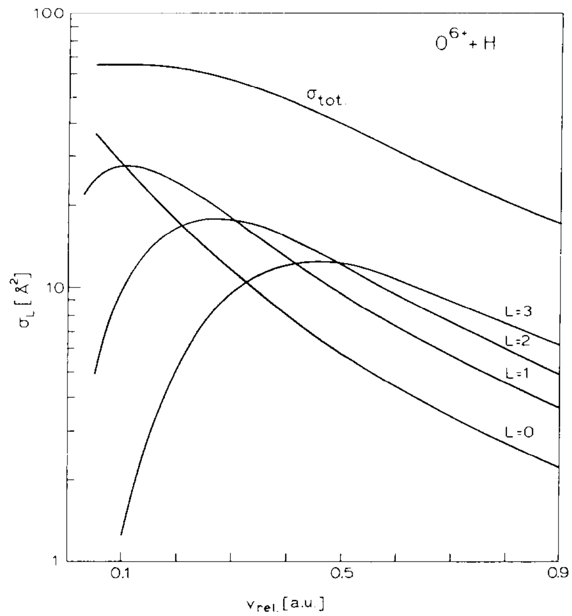

Fig. 3. Partial cross sections σ_L as function of the projectile velocity v, calculated from eq. (14), which takes the distribution of L around bv into account.

This gaussian replaces in our model the unit step function $W_L(b)$ given by eq. (2). The step function was normalized as

$$\int_0^\infty W_L(b)\,\mathrm{d}(vb) = 1, \tag{12}$$

independently of L. We require the same normalization for the Gaussian. This leads to the following expression:

$$W_L(b) = \frac{1}{\sqrt{\pi}\Delta L}\left\{\exp-\left(\frac{L^* - vb}{\Delta L}\right)^2 + \exp-\left(\frac{L^* + vb}{\Delta L}\right)^2\right\}. \tag{13}$$

with the relations (1), (6) and (13) we thus obtain for the subshell cross section σ_L:

$$\sigma_L = \frac{2L+1}{2L+1+n_t^2}\,\frac{2\sqrt{\pi}}{\Delta L}\int_0^{R_c(L)} b\,\mathrm{d}b\left\{\exp-\left(\frac{L^* - vb}{\Delta L}\right)^2 + \exp-\left(\frac{L^* + vb}{\Delta L}\right)^2\right\}. \tag{14}$$

In fig. 3 we show the cross sections as function of the relative velocity v of the collision partners. The cross sections are less sharply peaked than in fig. 2 and contributions to higher L values can now be seen at much lower velocities. The calculated average values $\langle L \rangle$ are even in very good agreement with the experimental values [4]. The description by eq. (14) thus represents a significant improvement and clearly demonstrates that the distribution of L values due to the energy uncertainty should not be neglected. On the other hand one should keep in mind that this simple description can only serve as a rather rough first approximation. More detailed quantum mechanical calculations as e.g. those from Fritsch and Lin [5] are necessary to obtain dependable results on partial cross sections σ_L.

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