Orientation and alignment in H^+-H collisions

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We have calculated probabilities, orientation parameters, and alignment angles for $2p$ excitation and capture in proton-hydrogen collisions at 50- and 100-keV projectile energy. The results, obtained from solving the Schrödinger equation in a multistate atomic-orbital expansion, are compared to those of a similar, recently published investigation. In both studies, similar results for excitation are found, and also for capture at large impact parameters. The origin of different predictions for capture at intermediate impact parameters is discussed.

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Total cross sections for excitation and capture in proton-hydrogen collisions are well established from experiments [1] and various theoretical treatments [2–4]. Only a few studies address more detailed aspects of the final states, such as calculations or measurements of parameters that give information about the collision amplitudes for excited states. Experimental results exist for the integral alignment [5] but differential measurements have not yet been performed.

The orientation parameter and the alignment angle for the excited (captured) $2p$ state as a function of impact parameter have been calculated in an extensive general study of orientation and alignment of collisionally excited atomic states by Lin *et al.* [6], in the following referred to as LSJF. An interesting point is their conclusion for capture: that the orientation parameter is negative at large and very small impact parameters, and positive at intermediate impact parameters ($b \approx 1.0$ a.u.) and that no systematic behavior exists for the alignment angle. They suggest that future experiments and/or theoretical calculations should test these predictions and address their possible simple interpretations.

In this paper, we present new calculations and compare our results to the results of LSJF, and also to previously established propensity rules for orientation [7–9]. Our independent calculations of coherence parameters not only address the physics of the processes, but also serve as a sensitive test of computer codes: Total cross sections, formed by squaring the collision amplitudes and integrating over impact parameter, represent much less sensitive tests.

Our discussion will be referring to the natural frame of reference, $\mathbf{v}=(v,0,0)$ and to collisions with positive impact parameter $\mathbf{b}=(0,b,0)$ [10]. Atomic units will be used unless otherwise stated. The orientation parameter and the alignment angle are defined by

$$L_\perp(b,v)=\frac{|a_+|^2-|a_-|^2}{|a_+|^2+|a_-|^2}\ , \tag{1}$$

$$\gamma(b,v)=\tfrac{1}{2}[\pi+\arg\,(a_-a_+^*)]\ . \tag{2}$$

Here a_+ and a_- are the $2p_{+1}$ and $2p_{-1}$ amplitudes for excitation or capture. We note that the orientation parameter $L_\perp(b,v)$ gives the expectation value of the angular momentum projection for the excited (captured) state and that the alignment angle γ defines the major axis of the excited (captured) $2p$ charge cloud. We expect that the orientation parameter will be negative for direct transitions at intermediate to large b in a velocity region where the phase criterion

$$\frac{\Delta\varepsilon a}{v}+\Delta m\,\pi\approx 0 \tag{3}$$

can be fulfilled [7–9]. In this equation a denotes an effective interaction range typically of the order 10–30 depending on system and processes, v is the collision velocity, and $\Delta\varepsilon$ is the energy change from the initial to the final state. For $2p$ excitation in H^+-H collisions $\Delta\varepsilon=0.375$, so for a typical $a\approx 10$ it is clear that a propensity rule for negative orientation is expected at quite large velocities ($v\sim 1$–2). However, the fact that the $n=2$ states are degenerate gives rise to couplings which may blur the relative clear picture of negative orientation observed for other systems [11,12].

For capture it has been shown [8] that the modulus of the coupling matrix element between an s state and a p_{-1} state generally is larger in magnitude than the one between an s and a p_{+1} state. We may therefore expect negative orientation in capture even for very high velocities, also in accordance with intuitive classical considerations [10].

We have expanded the wave function in terms of the electron translational factor modified eigenstates of the $n=1$, 2, and 3 shells on each center and solved the time-dependent Schrödinger equation in the constant velocity, impact-parameter approach [14–16]. This basis of 28 traveling hydrogen states reduces to 20 effective states since coupling to states of negative reflection symmetry vanishes. This expansion corresponds to the expansion of LSJF, however, their calculation includes additional excited states and pseudostates. We have also performed the calculations including the $4s$ and $4p$ states on each center without observing any significant effects on the $2p$ capture and $2p$ excitation predictions.

In Fig. 1 we show the $2p$ probabilities, orientation parameters, and alignment angles at 50-and 100-keV projectile energy, $v=1.4$ and 2.0, respectively. We also present the degree of linear polarization $P_l=\sqrt{1-L_\perp^2}$ since this parameter is easier to access experimentally than $L_\perp$. These results should be compared to Figs. 6,7, and 10 of LSJF, and we find that our results for excitation are in fair agreement.

For capture we compare in Fig. 2 directly our results with those of LSFJ. We first note that the probabilities, orientations, linear polarizations, and alignment angles agree at larger impact parameters. Also the cross sections are in fair agreement with previous results, cf. Table I. At intermediate impact parameters, however, the probabilities and the orientation and shape parameters differ significantly.

At 50 keV [Fig. 2(a)] the orientation parameter in our calculation is negative except for a narrow b window at $b \approx 1.5$, and at 100 keV [Fig. 2(b)] the orientation is negative for all impact parameters. The propensity rule is thus observed for capture in our calculation. Studies of the time development of the charge cloud show that the b window of positive $L_\perp$ at 50 keV and $b \approx 1.5$ originates from strong mixing between the states of the $n=2$ shell, which tends to invalidate the first-order prediction leading to Eq. (3), and hence the propensity rule. This mixing will generally lead to oscillatory behavior of $L_\perp$ at lower energies.

The alignment angle γ for excitation approaches $\pi/2$ at large b as expected from the first Born approximation. The alignment angle for capture in our calculation generally appears to be more stable and close to 0. This is connected with the reluctance of the captured charge cloud to rotate with the internuclear axis through the collision. Studies of the collision dynamics at selected impact parameters confirm a previously discussed slippage phenomenon [13].

(i) The $2p$ excitation charge cloud receives probability

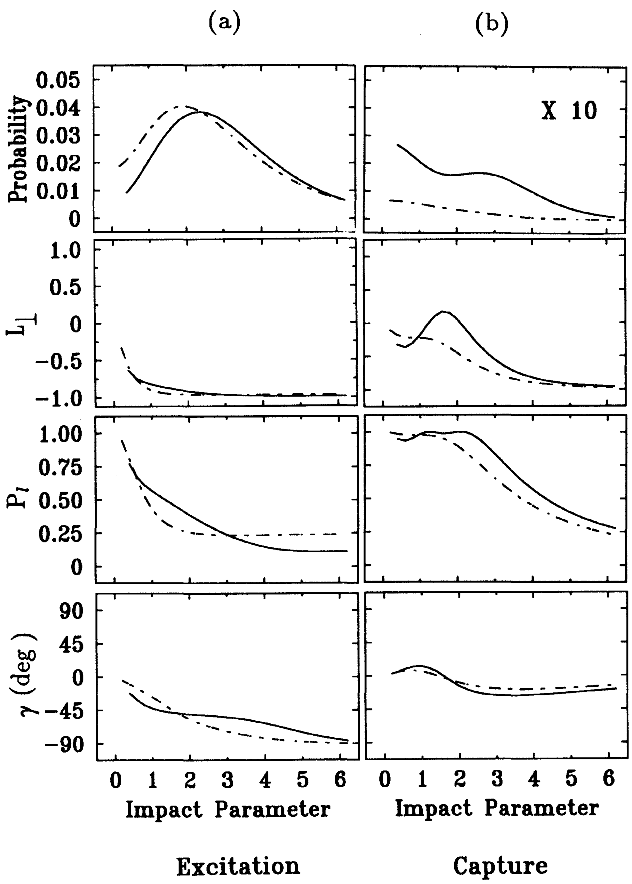

FIG. 1. Probability, orientation parameter $L_\perp$, linear polarization P_l, and alignment angle γ as functions of impact parameter for (a) $2p$ excitation and (b) $2p$ capture. Solid line, 50-keV projectile energy; chain line, 100-keV projectile energy.

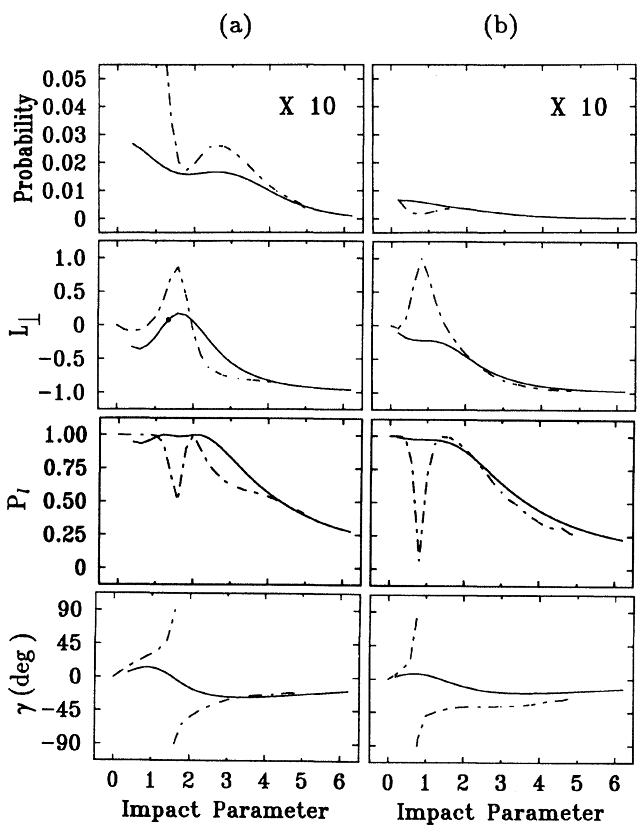

FIG. 2. Comparison between present results and the results of LSFJ (Ref. [6] and databank at JILA) for $2p$ capture at (a) 50- and (b) 100-keV projectile energy. Solid line, present results; chain line, LSFJ.

TABLE I. Total cross sections in 10^{-17} cm^2 for $2s$, $2p$ excitation and $2s,2p$ capture: (a) present results, (b) from Ref. 2 and from databank at JILA (note the data presented at 100 keV have been evaluated by extrapolation from graphs); (c) from Ref. 3 (interpolated at 100 keV).

	50 keV		100 keV	
	$2s$	$2p$	$2s$	$2p$
		Excitation		
(a)	1.4	7.9	1.1	8.0
(b)	1.8	7.4	1.5	5.7
(c)	1.8	6.9	1.1	8.1
		Capture		
(a)	1.5	0.3	0.2	0.04
(b)	1.3	0.5	0.2	0.03
(c)	1.4	0.4	0.2	0.02

flow from the initial state. This buildup allows the $2p$ states to couple rotationally, and gives rise to the slippage effect.

(ii) The $2p$ capture state is much less populated by the coupling from the target $1s$ state. Initially a state aligned with the internuclear vector, nearly parallel with the x axis, is populated. During collision the flow of probability into the $2p$ states is too small to change the initial alignment significantly. As a result, the $2p$ aligned state only wiggles slightly around the initial p_x shape and the alignment angle stays close to 0.

An interesting discussion concerns the differences between the present work and LSFJ for $2p$ capture at intermediate impact parameters. The inclusion of pseudostates suggests the possibility of two-step processes of strong potential Born type [17], i.e., excitation to the continuum followed by capture to the projectile $2p$ state. If the pseudostates used in the calculation of LSFJ allow for such mechanisms, it may well give an oscillatory behavior of $L_\perp$ for capture. If this speculation is correct the $L_\perp$ parameter for capture can be a sensitive parameter describing the capture dynamics at higher velocities.

We have tested this hypothesis by introducing four pseudostates in the form (s states)$e^{-\lambda r}$, with $\lambda=2.5$, 1.5, 0.75, 0.2. These states were orthonormalized to the discrete states of the target and the target Hamiltonian was diagonalized. This gave four pseudostates with energies $\varepsilon=-0.0028$, 0.07, 1.2, 7.5.

A recalculation at 100 keV showed little effect on the excitation parameters. For capture the alignment angle was influenced by this only to about $\pm 10°$, however, a narrow b window of positive $L_\perp$ indeed appeared around $b=1.0$ ($L_\perp \simeq 0.05$). This indicates that capture via continuum states may play an important role in this b range and points to an explanation of the strong positive $L_\perp$ prediction seen by LSJF and the accompanying sudden change in γ in the b range where $L_\perp \approx 1$ (Fig. 2). The effect seems to be very sensitive to the precise representation of the continuum, albeit the choice and the number of pseudostates included in the wave-function expansion. From the point of view of the simple phase criterion [cf. Eq. (3)], one may speculate that the transition sequence $1s^A \to ks^A \to 2p_m^B$ indeed will predict a preferred $2p_{+1}$ capture state, since the transition from the s continuum is exoergic ($\Delta\varepsilon < 0$).

In summary we have calculated $2p$ excitation and $2p$ capture probabilities, orientation parameters, linear polarizations, and alignment angles at 50 and 100-keV projectile energy. The results confirm earlier predictions for the orientation parameters and suggest a simple explanation of the positive orientation seen by LSJF for capture at intermediate impact parameters. We strongly encourage experiments to be carried out, since measurements of these parameters seem to probe the capture dynamics very sensitively.

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