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Spin effects in slow $(H\text{-}He)^+$ collisions

R. Hippler, H. Madeheim, and H. O. Lutz
Fakultät für Physik, Universität Bielefeld, Postfach 8640, Universitätsstrasse 25, D-4800 Bielefeld 1, Federal Republic of Germany

M. Kimura and N. F. Lane
Argonne National Laboratory, Argonne, Illinois 60439
and Department of Physics, Rice University, Houston, Texas 77251

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The integral alignment A_{20} was investigated for $H(2p)$ excitation in slow $(H\text{-}He)^+$ collisions. Pronounced differences are observed between H^+-He and He^+-H collisions; they are attributed to the different (singlet and triplet) spin channels which dominate the respective excitation process.

The investigation of electronic processes in simply structured atomic collision systems is not only fundamentally important for our understanding of collision dynamics; it is also of practical importance for a variety of fields such as fusion technology and astrophysics. Besides the most simply structured (one-electron) system H^+-H, two-electron systems like H-H or $(H\text{-}He)^+$ are of considerable interest as electron-electron interaction during the collision may provide a significant part of the total interaction. Usually, electron-electron interaction during the collision is considered not to be dominant to govern the collision dynamics; it could show up, however, in slow atomic collisions where the collision partners transiently form a quasimolecule,[1] and also in fast atomic collisions in which all perturbations are weak.[2] Here "slow" refers to the projectile velocity v_p being small compared to the (classical) velocity v_e of the bound electrons under consideration. This quasimolecular model of atomic collisions has been widely used for an understanding of electronic processes involving inner and outer atomic shells (e.g., Ref. 3 and references therein). Figure 1 displays a schematic *diabatic* correlation diagram for the $(H\text{-}He)^+$ singlet system, i.e., the binding energy of an electron in a given molecular orbital (MO) as a function of the internuclear distance R. For this and similar collision systems, $H(2p)$ excitation provides a conspicuous and well studied reaction channel (e.g., Ref. 4). As can be seen from Fig. 1, excitation to the $H(2p)$ state in singlet He^+-H collisions occurs dominantly at small internuclear separations via couplings of the $2p\sigma$ MO with other near-degenerate MO's (for example, $2p\pi$ or $2s\sigma$; σ and π refer to the projection of the angular momentum on the internuclear axis). In H^+-He collisions, on the other hand, $H(2p)$ excitation is thought to arise from a two-step mechanism. In a first step an important radial coupling between $1s\sigma$-$2p\sigma$ at $R\approx 2.5$ a.u. populates the charge exchange channel He^+-H; then the second step, as before, involves couplings of the $2p\sigma$ MO with other high-lying MO's leading to $H(2p)$ excitation. This difference in the two incident channels of the singlet $(H\text{-}He)^+$ collision complex will give rise to a large difference in the differential[5] and total cross sections leading to $H(2p)$ excitation.[6] We note that within the singlet manifold al-

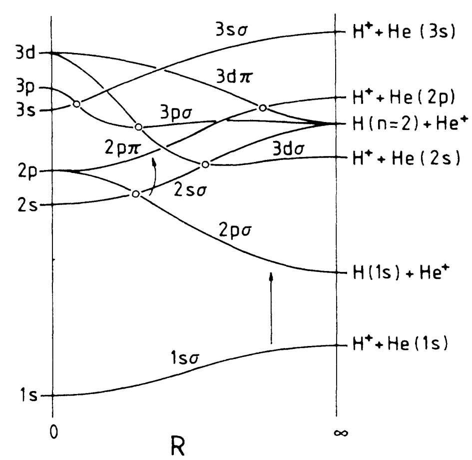

FIG. 1. Schematic (*diabatic*) energy-level diagram for (singlet) H^+-He collisions. The binding energy of an electron moving in the field of two approaching nuclei is shown as a function of internuclear separation R.

though the two incident channels and, hence, the flux-exit mechanism are different, they both proceed to arrive at the H(2p) state via the same intermediate states and the same couplings that are thus identical for H^+-He and He^+-H (singlet) collisions at low velocities. The similarity of the H^+-He and He^+-H collisions should then be reflected in certain characteristic signatures of the collision. For example, the alignment[7] [i.e., the relative population of the different H(2p) substates] depends sensitively on the contribution of σ and π states to the excitation process. However, in H^+-He collisions there exists only one (singlet) spin manifold, whereas in He^+-H collisions a second (triplet) manifold can contribute, and because of the smaller energy defect for the triplet state, it is expected to contribute significantly. Therefore, it is natural to expect a different behavior of the two different incident channels of (H-He)$^+$ collision complex, and in turn a different alignment in the two collision systems H^+-He and He^+-H.

In this Rapid Communication, we discuss experimental and theoretical results for

$$\left.\begin{matrix} He^+ + H \\ H^+ + He \end{matrix}\right\} \rightarrow H(2p) + He^+ \qquad (1)$$

collisions in the energy range of 1–25 keV. The quantity of interest, i.e., the integral alignment A_{20}, provides detailed information about the collision dynamics as a function of the collision energy and is defined as (e.g., Ref. 4)

$$A_{20} = \frac{\sigma_1 - \sigma_0}{\sigma(2p)}, \qquad (2)$$

where σ_0 and σ_1 are the total cross sections for excitation into the H(2p_0) and H(2p_1) magnetic substates, respectively, and $\sigma(2p) = \sigma_0 + 2\sigma_1$. A_{20} is thus a measure of the relative population of the H(2p_m) magnetic substates; it is obtained from a measurement of the linear polarization P of Ly-α radiation emitted during the radiative decay of H(2p) to the H(1s) ground state. The degree of linear polarization P is defined as

$$P = \frac{I_\parallel - I_\perp}{I_\parallel + I_\perp}, \qquad (3)$$

where $I_\parallel$ and $I_\perp$ are the light intensities with the electric vector parallel and perpendicular to the proton beam direction. The emitted light was measured perpendicularly to the direction of the incident ion beam with a polarization-sensitive device.[8,9] This consisted of a LiF plate arranged at Brewster's angle (about 60°) followed by a solar-blind photomultipler (EMR 542 J). The integral alignment A_{20} is related to the degree of linear polarization through

$$A_{20} = \frac{6P}{P-3}, \qquad (4)$$

which accounts for the depolarization due to the fine-structure interaction in H(2p). Hyperfine-structure interaction is weak in atomic hydrogen and was neglected. The experimental setup[8,9] further consists of an ion gun producing beams of fast hydrogen or helium ions with kinetic energies up to 25 keV. The ions are crossfired onto a thermal atomic hydrogen or helium target; the atomic hydrogen target was produced with the help of a Wood's discharge tube. Typically, the degree of dissociation was ≈85%; it was measured *in situ* by means of time-of-flight spectroscopy.[9] The measured linear polarizations have been corrected for the incomplete dissociation. It was, therefore, necessary to measure the degree of linear polarization in He^+-H_2 collisions as well; these results will be published in a forthcoming communication.[10]

Our experimental and theoretical results (dashed line) for the He^+-H collision system are displayed in Fig. 2, together with recent calculations of Errera, Mendez, and Riera[11] (dash-dotted line). Also shown on an equal-velocity scale are previous experimental and theoretical results (solid line) for the reverse system H^+-He.[12–14] As expected, a marked difference between the alignment for the two different incident channels of the (H-He)$^+$ collision complex is observed. In the following we will discuss the origin of this difference in more detail. This is facilitated by the fact that the (H-He)$^+$ collision complex has been studied quite thoroughly. In particular, recent differential measurements[8] have demonstrated that for incident H^+-He collisions the 2$p\sigma$-2$p\pi$ rotational coupling dominates at impact parameters $b \approx 1$ a.u.; this excitation mechanism populates the H(2$p_{\pm1}$) magnetic substates. At smaller b a double-rotational coupling 2$p\sigma$-2$p\pi$-2$s\sigma$ leads to H(2p_0) excitation.[15] This 2$s\sigma$ state population is also produced by the radial coupling among the 2$s\sigma$ and 2$p\sigma$ states around $R \approx 0.4$ a.u. At low incident energies of a few keV the integral populations caused by these two couplings are roughly equal; as a consequence, the integral alignment A_{20} is approximately zero. This does not hold for the reverse system He^+-H, where we observe a significantly larger (positive) alignment. It indicates that the above double-rotational coupling mechanism now ap-

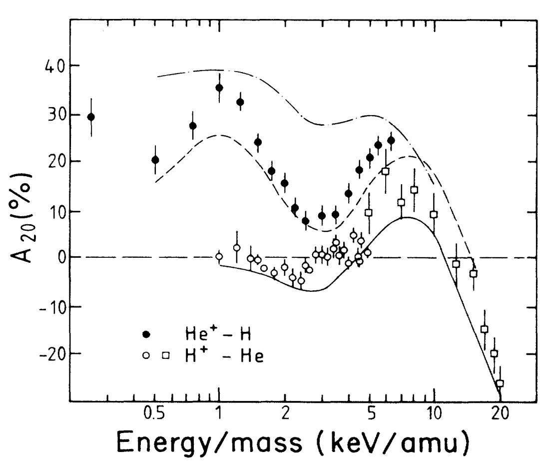

FIG. 2. Integral alignment A_{20} for H(2p) production in H^+-He and He^+-H collisions vs incident energy. Present experimental results for He^+-H collisions (●) and previous results for H^+-He collisions (○, Ref. 8; □, Ref. 13) are compared with the present calculations (dashed and solid lines, respectively) and with recent calculations by Errera, Mendez, and Riera (Ref. 11) (dash-dotted line) for He^+-H.

pears to be of a lesser importance. This experimental result is confirmed by our theoretical calculations, in which the molecular states for both singlet and triplet manifolds were obtained by the full configuration interaction method; the present molecular states are equivalent in precision to those of Green *et al.*[16] A molecular-orbital expansion method with inclusion of molecular electron translation factors was used in the semiclassical approximation.[17] It is clear from *adiabatic* potential-energy diagrams for the spin-singlet and -triplet manifolds that these two classes of potentials show quite different features. As is illustrated in Fig. 3, the most notable feature is that, for the triplet manifold, the separated-atom energy of $H^+ + He(2^3P)$ lies lower than the $H(n=2) + He^+$ levels, while the situation is just the opposite for the singlet manifold. This difference is of fundamental importance for our understanding of the underlying collision dynamics of excitation and electron-capture processes. A series of radial and rotational couplings mix a number of states that are in a sensitive energy dependence involved in these inelastic collisions. However, it is still possible to identify the effects of the most significant couplings. For example, in the *singlet* case, 1Σ-1Π and 1Σ-2Σ-1Π ($2p\sigma$-$2s\sigma$-$2p\pi$ in diabatic notation) are important couplings which produce $H(2p_{\pm 1})$ population at lower energies, whereas $H(2p_0)$ excitation is produced by the 1Σ-1Π-3Σ ($2p\sigma$-$2p\pi$-$3p\sigma$) couplings. At low energies, these contributions produce Σ and Π states with comparable probability, and the integral alignment in H^+-He collisions (pure singlet case) is small. In singlet He^+-H collisions, the integral alignment is also small similar to the H^+-He collision and is sensitive to the collision energy below 2 keV/amu.

The above couplings also operate in the *triplet* manifold; however, the important difference is that here they do *not* lead to excitation of the $H(2p)$ states. This is because for the triplet channel neither of the 1Π nor 3Σ states correlates with the $He^+ + H(n=2)$ outgoing channel; instead, they correlate with $He(2^3P) + H^+$. For the triplet manifold, 1Σ-2Σ-1Π-2Π and 1Σ-1Π-2Π coupling mechanisms in addition to the 1Σ-2Π coupling are dominant at lower energies. This leads to the results that $H(2p)$ excitation in He^+-H collisions at low incident energies is dominated by rotational couplings leading to outgoing Π states. This has the consequence that predominantly the $H(2p_{\pm 1})$ magnetic substates become populated; it is reflected in the much larger positive alignment than compared to that for the singlet manifold. The electron flux, as a function of impact parameter and of collision energy, is in a rather complicated and sensitive manner exchanged among the involved states, and this behavior is responsible for the dip in A_{20} around 3 keV/amu in the He^+-H data.

As the incident energy increases, direct (impulsive) excitation to $H(2p)$ through 1Σ-3Σ or 4Σ couplings within the singlet manifold and via 1Σ-4Σ or 5Σ couplings in the triplet manifold becomes important, resulting in preferred $H(2p_0)$ population in both collision systems. This causes the sign change of A_{20} at ≈ 15 keV/amu. The contribution to A_{20} from the singlet and triplet manifolds becomes very similar compared to each other above ~ 5 keV/amu, giving the statistical weights, i.e., $\frac{1}{4}$ and $\frac{3}{4}$ for the singlet and triplet manifolds, respectively, in the total A_{20}. Above several 10 keV/amu the theoretical curves for H^+-He and He^+-H collisions appear to approach one

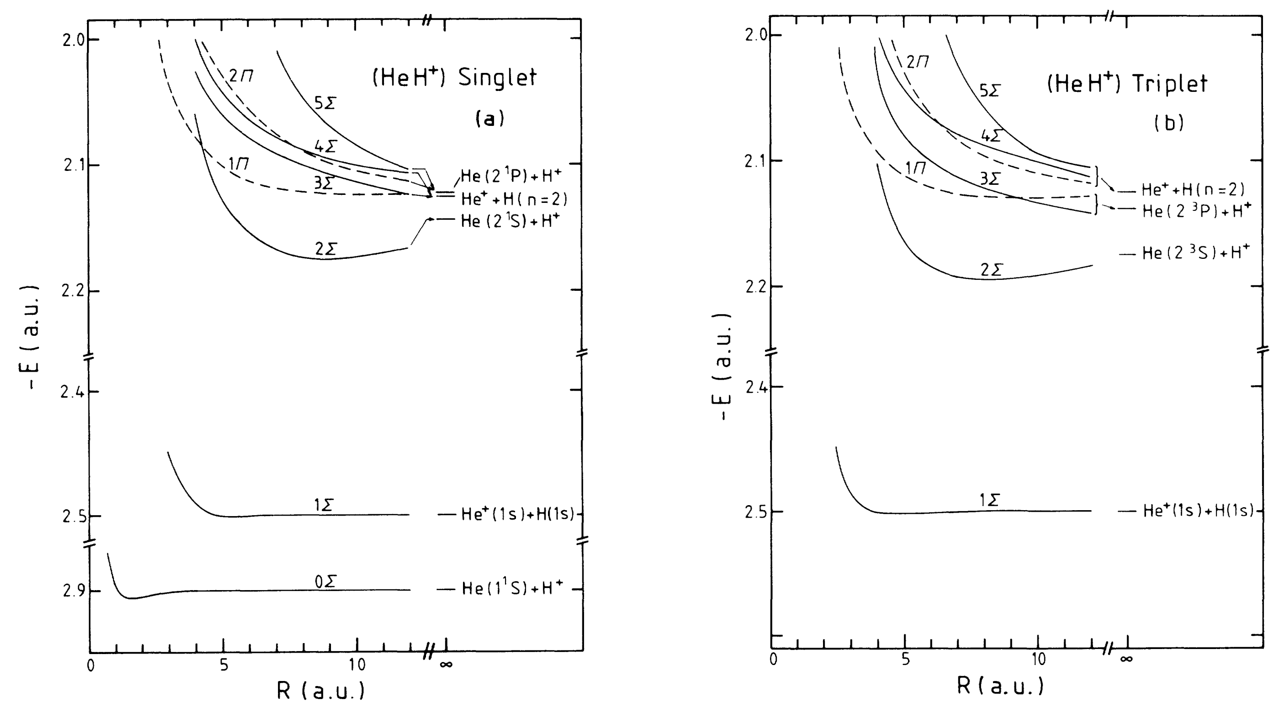

FIG. 3. *Adiabatic* potential energy diagram for He^+-H collisions for (a) singlet- and (b) triplet-spin channels as a function of internuclear separation R.

another; as expected since the spin effects discussed here should be of minor importance at large collision energies.

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