

Coplanar and non-coplanar differential cross sections for ionization of aligned H_2 molecules by electron impact

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Synopsis The single ionization of fixed-in-space hydrogen molecules by electron impact is studied theoretically for transitions from the ground (*gerade*) state to final ground (*gerade*) and first excited (*ungerade*) states of H_2^+ . We consider coplanar and non-coplanar geometries, and asymmetric kinematical conditions for intermediate and high incident energies. The computed cross sections are presented and discussed in the framework of recent experimental findings.

In this work, the single ionization of hydrogen molecules is investigated theoretically as a function of the molecular alignment. The interest is focused here on coplanar (the target electron is ejected into the scattering plane, defined by both the incident and scattered electron momenta) and non-coplanar geometries. Also, asymmetric kinematical conditions are analyzed in which one slow and one fast electron are detected in the final channel. Attention is paid to the role played by interference effects arising from the two-center nature of the molecular target.

In a previous work [1], molecular transition amplitudes obtained within the MBBK approximation [2] were described as an *effective* one-center contribution modulated by an interference factor similar to the one appearing in experiments with light. The ionization process was considered in those works, as a pure *vertical* electronic transition from the ground electronic (*gerade*) state of the H_2 target to the non-dissociative ground electronic state of the residual H_2^+ ion [1], which is the one that gives the dominant contribution for the electron ionization reaction. The MBBK model was successfully used to explain experimental cross sections integrated over all molecular orientations [2] in asymmetric coplanar arrangements as well as many evidences of interference patterns (see for instance [3] and references quoted therein). Furthermore, it was predicted recently for the case of *oriented* molecules that destructive interferences coming from the coherent

emission from both molecular centers may provoke the suppression of the binary peak in the differential cross sections [4].

Also recently, experimental studies of electron impact ionization of hydrogen molecules for different molecular orientations have been performed [5,6]. In the experiments, the alignment of the molecule is determined from fragmentation of the residual H_2^+ molecular ion following an ionizing collision.

In the present study, multiple differential cross sections (MDCS) at a fixed internuclear orientation are computed for both the ground non-dissociative (*gerade*) and first excited (*ungerade*) final H_2^+ states. Coplanar and non-coplanar geometries are considered at intermediate and high impact energies. The MBBK model is employed to obtain the MDCS for fixed orientations of the molecule with respect to the momentum transfer direction [4]. It is shown that the interference pattern changes strongly with both the final state of the residual molecular ion and the molecular orientation.

References

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