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Fully differential cross sections for ionization of H_2 molecules by proton impact: single- and two-centre effects

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Synopsis Fully differential cross sections for ionization of H_2 by 75 keV proton impact are compared with recent experimental data. Calculations were obtained by using a two-effective centre approximation within the CDW-EIS approach.

In this work, single ionization of hydrogen molecules by 75 keV proton impact is studied. Our goal is focused on the analysis of theoretical fully differential cross sections (FDCS), depending on the emitted electron momentum and on the transverse momentum transfer. To this end, different emission geometries and projectile kinematical conditions are considered. The present theory is compared with recent measurements made by Hasan *et al.* [1] .

Regarding the theory, a two-effective centre approximation (TEC) within the continuum distorted wave-eikonal initial state (CDW-EIS) approach, is employed to obtain FDCS. In this case, all the interactions present in the exit channel are considered on an equal footing. It should be mentioned that, as it happens for atomic targets, since the present differential cross sections depend on the momentum transfer, the interaction between the projectile and each molecular nuclei must be included in the formulation. Thus, it may play a relevant role in the corresponding calculations, depending on the energies of the emitted electron and momentum transfer values [2]. It is worth noting that the present theoretical method allows us then to compute two kind of FDCS, each one of them associated to different effects arising from the different interactions between the heavy particles during the reaction. In the so-called *two-centre FDCS*, interferences due to the presence of the two molecular nuclei is taken into account, whereas the *single-centre FDCS* are defined in such a way that only the effect related to the interaction between the projectile and each target nucleus is considered. This allows us to asses the contribution of each one of the mentioned interactions in the FDCS.

A reasonable good agreement between our theory and the measurements is achieved, in particular when a coplanar geometry where the electron emission plane coincides with the projectile dispersion one (the *scattering* plane) is analysed. Moreover, in some cases the agreement between experiment and the CDW-EIS–FDCS is better than for the case of more sophisticated schemes. However, substantial differences appear, for non-coplanar emission geometries and for large values of the momentum transfer. Also our approach appears to be perfectly suitable to tackle other *unconventional* electron emission geometries, for instance, those recently presented in [1], where the interference effects are clearly enhanced [3].

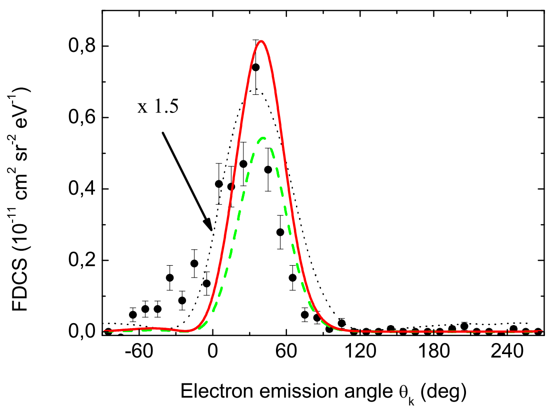

Figure 1. FDCS for electrons emitted with an energy of 14.6 eV into the scattering plane, as a function of the electron angle θ_k, for a momentum transfer $q = 0.9$ a.u. Dots: experiments [1], solid curves: two-centre FDCS, dashed curves: single-centre FDCS, dotted curves: M3DW results [1].

References

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