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Differential Cross Sections for Single Ionization of H_2 by 75keV Proton Impact

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Differential cross sections for single ionization of H_2 by 75keV proton impact

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Synopsis We have calculated Triply differential cross sections (TDCS) and doubly differential cross sections (DDCS) for single ionization of H_2 by 75 keV proton impact using the molecular 3 body distorted wave Eikonal initial state (M3DW-EIS) approach. Previously published measured DDCS-P (differential in the projectile scattering angle and integrated over the ejected electron angles) found pronounced structures at relatively large angles which were interpreted as an interference resulting from the two-centered potential of the molecule.

Fundamental quantum mechanical interactions at the atomic level can be studied by examining the results of charged particle collisions with atoms and molecules. One type of collision that has received considerable interest recently is charged particle collisions with diatomic molecules such as H_2. Since the two protons represent two different scattering centers, one question which immediately arises is whether or not one should see two-center interference effects similar to Young's double slit interference for light.

Very recently Alexander *et al* .[1] reported DDCS-P measurements for ionization of H_2 by 75keV proton impact which demonstrated significant structure directly in the projectile angular dependence and this structure was attributed to double slit interference.

Previous theoretical calculations treating H_2 as atomic H multiplied by a molecular interference factor [2] only predicted the observed structure when assumptions were made about the molecular orientation. In this work we employ the M3DW-EIS [3] method to see whether the structures in the experiment can be reproduced by a calculation that treats the target as a molecule ab initio. This method accounts for interference from first principles since any structure must result from the molecular wave functions used in the calculation (rather than being imposed on an atomic calculation through an interference factor). We will also investigate the TDCS to see what insight can be gained from the more differential level.

Figure 1 shows that the present M3DW-EIS results predict a structure almost identical to the experiment for 14.5 eV ejected electrons and a small structure for 34.6 eV ejected electrons. However, the magnitude of the M3DW-EIS cross sections were consistently lower than the data by a constant factor of 4.5.

We will show that the interference structure disappears when the ejected electron velocity matches the projectile velocity due to the strong final state interaction between the two particles.

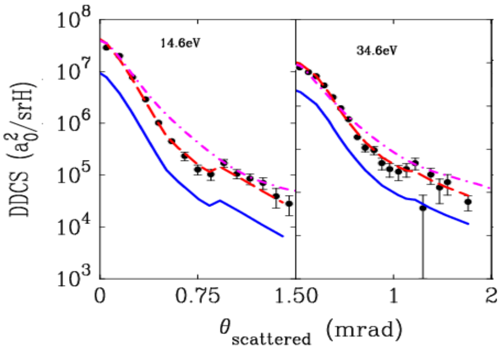

Figure 1: DDCS-P for ionization of a hydrogen molecule by 75keV proton impact as a function of projectile scattering angle. The energy of the outgoing electron is shown in each figure. Experimental results of Alexander *et al.* [1]. Theory: dash-dot atomic H cross sections times an interference factor [1], dash M3DW-EIS times 4.5. Solid M3DW-EIS.

References

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