Improved model for the interference effects
# in the ionization of H$_2$ by fast ions

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Synopsis A more precise description of the interference effects in the ionization of H$_2$ by fast ions is presented. The interference is due to the coherent emission of the electron waves from the vicinity of the two nuclei. The obtained results improve the previous ones mainly for perpendicular ejection of the electron relative to the projectile trajectory, where the experimentally observed secondary oscillations are reproduced.

Interference effects due to the two-center character of the target were observed in the ejected electron spectrum for the ionization of H$_2$ by fast ions more than a decade ago [1]. The oscillations observed in the differential cross section ratio H$_2$/2H as a function of electron velocity were analyzed theoretically using a simple plane wave description of the final state [2]. A dependence on the ejection angle of the interference pattern was predicted, which in principle was confirmed experimentally [3]. Other theoretical investigations were also published [4,5]. However, some discrepancies remained between the theoretical and experimental cross section ratios, mainly for 90^0 ejection.

In the present work we improve the previous calculations [2]. The two atomic amplitudes are calculated with a higher precision, and added up coherently. The obtained interference term has a more complex behavior, than predicted before. Our results are compared on Figure 1 to the previous theoretical cross section ratios, to the analytical formula deduced in [2] and to the experimental data. For the small ejection angle the obtained oscillations are in very good agreement with the experimental data and the CDW-EIS calculations [4], but have a higher frequency than the analytical formula's prediction. The main novelty of the present description may be observed at 90^0 – the model reproduces the secondary oscillations observed in the experiments, while the plane wave (PW) model [2] and the analytical formula predict a nearly constant ratio and the CDW-EIS calculations [5] give an increasing ratio as a function of velocity. It is somehow surprising the appearance of these secondary oscillations in a first-order approach. We explain this behavior with the modulation of the oscillations caused by the different distances between the detector and the nuclei by the oscillations originated from the different timing of the momentum transfer to the electron from the vicinity of the two nuclei. The disagreement between the present theory and the experiments for small electron velocities is due to the second-order interactions with the nuclei and to electron correlations, which are not taken into account in the present description.
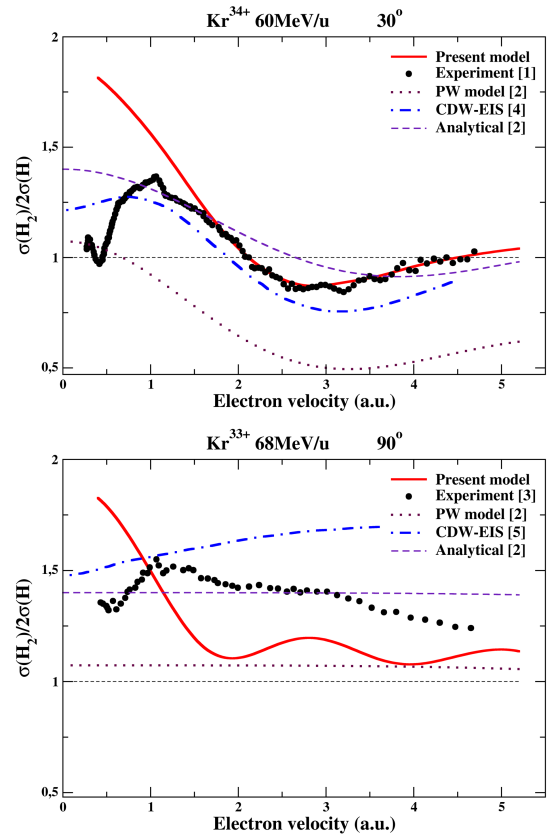
Figure 1. Calculated and experimental H$_2$/2H differential cross section ratios as a function of ejected electron velocity for different ejection angles.

References

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