Correlation between regions in the phase portrait of a hydrogen atom and the type of the products formed in a collision with a proton in one dimension: A classical perspective

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We have studied the relationship between the positioning of the initial conditions on the phase portrait of a one dimensional hydrogen atom and the outcome of a collision between a hydrogen atom and a proton in one dimension. Classical trajectories were generated to study the dynamics of the system and the relevant phase space of the problem was reduced to that of the electron (i.e. two dimensions) by driving the proton through the hydrogen atom at constant velocity.

Initial conditions (position and moment) of the electron were generated such that they were equally spaced along the phase portrait of a one dimensional hydrogen atom in its ground state. Hamilton's equations were then solved, numerically, using a variable order Runge–Kutta routine. After propagating each trajectory from a given initial inter–nuclear separation to a large final inter–nuclear separation, the outcome was identified as excitation, charge transfer or ionisation. This enabled us to systematically categorise the initial equally spaced points on the phase portrait of a hydrogen atom, based on the type of the final outcome and study their movement as a function of the initial inter–nuclear separation.

We have established that, at a given initial inter–nuclear separation, the phase portrait of a one dimensional hydrogen atom can be divided into patches such that all points in a patch lead to the same type of collision outcome. This provides a global picture of the origins of possible mechanisms of excitation, charge transfer and ionisation. These patches move clockwise along the phase portrait as the collision progresses, a movement that may be termed as "patch breathing" since they expand and contract during this excursion. We have identified 4 such patches for each of the above mentioned outcomes.

Based on the division of the phase portrait into patches, as indicated above, we propose a new, efficient method for generating the results of classical trajectory calculations for any given distribution of initial conditions. Using this method, we have reproduced the results generated by the Classical Trajectory Monte–Carlo method (which uses a micro–canonical ensemble of electronic initial conditions) for a collision between a hydrogen atom and a proton in one dimension.

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