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Identification of mechanisms of excitation, charge transfer and ionisation in classical proton–hydrogen atom collisions in two dimensions using divisions in phase space

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Thermal reactions are due to atomic and molecular collisions. Hence, a theoretical study of product formation in atomic collision processes constitutes a first step in understanding the detailed dynamics of chemical reactions. Quite often the simplest of such systems, viz. *bare nucleus–hydrogen atom* (three body) collisions, are studied in developing concepts associated with such processes and in testing new approximate theories. Such collisions lead to three types of outcomes, viz. excitation, charge transfer and ionization.

In the recent past attention has been focused in studying the said collision system using classical mechanics. In Classical Trajectory Monte Carlo method the quantum nature of the electron dynamics is incorporated by running a large number of trajectories. Trajectories are generated by numerically integrating the relevant Hamilton's equations. The dynamics of particles during the collision process can be studied in phase space. Such a study provides intriguing insights to the product formation process. In this context it is useful to examine such collisions in reduced dimensions. We have studied planner $H^+ + H(1s)$ collisions (where the electronic phase space is four dimensional) in the internuclear velocity range $v = 1.09 \times 10^6\ m\,s^{-1}(0.5\ a.u.)$ to $v = 6.56 \times 10^6\ m\,s^{-1}(3.0\ a.u.)$ in order to

device a method to identify different mechanisms of excitation, charge transfer and ionization based on division of the phase space and use it to identify different mechanisms.

At all velocities, we have established the existence of a finite number of regions in the electronic phase space, where the phase points in each region lead to the same outcome. The number of such regions associated with each outcome, viz. excitation, charge transfer and ionization, is distinct. Also, the extent of different regions leading to the same outcome is different in general. Each region represents a distinct mechanism of producing the associated outcome. Thus we have established a method to identify the mechanisms of product formation in $H^+ + H(1s)$ collisions in two dimensions and used it to recognise the mechanisms in that collision system. This method can be easily extended to other bare nucleus–hydrogenic atom/ion collisions.

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