Some effects in classical proton hydrogen atom collisions that originate due to dimensional restrictions

G Bandarage* and H S S Peiris
Department of Chemistry, The Open University of Sri Lanka, Nawala, Nugegoda

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 from a large internuclear separation, R_{in}, which is negative, to a large positive internuclear separation and then the outcome is determined. 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, viz. in one and two dimensions, in detail and the effects that originate due to such reduction in dimensions.

We have studied $H^+ + H(1s)$ collisions in one and two dimensions in detail in the internuclear velocity range $v = 1.09 \times 10^6\ \mathrm{m\,s^{-1}}(0.5\ \mathrm{a.u.})$ to $v = 6.56 \times 10^6\ \mathrm{m\,s^{-1}}(3.0\ \mathrm{a.u.})$. In the case of two dimensions, the impact parameter was kept at zero so that the nuclear motion is the same in both cases. The probabilities of all three types of outcomes oscillate as a function of R_{in}. These oscillations are counter intuitive and are an inherent feature of the collision process. They are not due to limitations in statistics. Consistently, the probability of ionisation is higher in the case of collisions in two dimensions compared to its counterpart in one dimension. Probability of excitation and charge transfer as a function of nuclear velocity, shows more structure in one dimension than in two dimensions. The difference in amplitudes of oscillations in the probability of excitation and charge transfer in one and two dimensions is more prominent than that with ionisation.

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*gband@ou.ac.lk Tel: 011-2822738