E1-29: Use of classical trajectory Monte Carlo simulations to study electron velocity distributions in 3-body breakup in ion- atom collisions

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Classical trajectory Monte Carlo simulations are widely used to study collisional ionization of atoms:

eg: $H(1s) + X^{n+} \rightarrow H^{+} + X^{n+}\ e,$

where X^{n+} is a bare nucleus of charge n. Here Newton's equations are solved for the motion of the particles and the quantum nature of the electron is incorporated by running a large number of trajectories to represent a collision event. This technique can produce experimentally measurable quantities and also provides interesting physical insights to the dynamics of collision processes.

Ionized electron produced in an ion-atom collision can be divided into 2 groups. One is produced early in the collision and involves a sudden mechanism. The other group is slowly pushed into the ionizing continuum and is affected by the nuclei for a longer period of time. Currently, there is much theoretical interest in the dynamics of these electrons, because of the 3- body nature of the interaction experienced by the electrons. Theoretically one can show that at 3 body breakup threshold, these electrons will have zero asymptotic velocity with respect to the saddle point in the nuclear Coulomb potential. However there are no theoretical predictions to the behaviour of these electrons above this threshold. Average velocity distributions of

these electrons at a higher energy for collisions involving H(1s) and H^+, He^{2+} and Li^{3+} ions were studied. Remarkable similarity was found between the distributions in H(1s) collisions with He^{2+} and Li^{3+}. The distribution was qualitatively different for the collisions involving H(1s) and H^+.