## Abstract

In the collisional dissociation of $H_3^+$ and $D_3^+$ into the Coulomb interacting channels of $H^+$+ $H^+$+$H^-$ and $D^+$+$D^+$+$D^-$ measured in triple coincidence, the results exhibit unique features when scrutinized from a center-of-mass energy partitioning perspective. Starting from the Wannier concept of the reaction zone boundary, classical and molecular simulations of the three Coulomb interacting fragments were undertaken with the goal of modeling the measured system energy partitioning. Starting from various configurations of dissociated $H_3^+$ and $D_3^+$, the simulations show that a bound $H^+$-$H^-$ or $D^+$-$D^-$ complex may form due to post-dissociation interactions. For short times, these complexes exhibit classical Keplerian-like orbits with each fragment maintaining its original physical characteristics. In order to identify and explore the properties of the time development of the three-body system's center-of-mass energy sharing, we use a generalized form of the Dalitz plot that highlights the time dependence of the three-body correlations with which we can then relate to experiment. Comparisons will be made between the experimental and theoretical results.

## Motivation

- We have measured the center-of-mass (cm) energy partitioning for the dissociation of $H_3^+$ and $D_3^+$ into the polar dissociation channel of $H^+$+$H^+$+$H^-$ and $D^+$+$D^+$+$D^-$
- In the experimental data interesting structures develop (Figure 13) when the energy sharing is plotted as a function of measured kinetic energy
- Conduct simulations of three-body motion:
  - Determine whether long-range Coulomb or short-range quantum interactions determine the measured energy sharing
  - Assess the influence of these interactions, we numerically calculate the trajectories and cm energy partitioning of the massive 3-body Coulomb systems

## Simulation Procedure

- Divide space into 2 zones (Figure 1)
  - Reaction Zone – Quantum Interactions
  - Coulomb Zone – Coulomb Interactions
- Focused on instantaneous three-body dynamics- Follow the trajectories of the three particles
- Numerically calculate the motion of $H^+$, $H^+$, $H^-$
  - Reasonable assumptions regarding initial geometry and energy partitioning
  - Classical Hamiltonian

$$H = \sum_{i=1}^{3}\frac{\vec{p}_i^{\,2}}{2m_i} + \sum_{i>j=1}^{3}\frac{q_i q_j}{2|\vec{r}_{ij}|}$$

  - Results in Figures 3-10
- Methodically probe influence of conserved quantities of total energy (T + U) and angular momentum

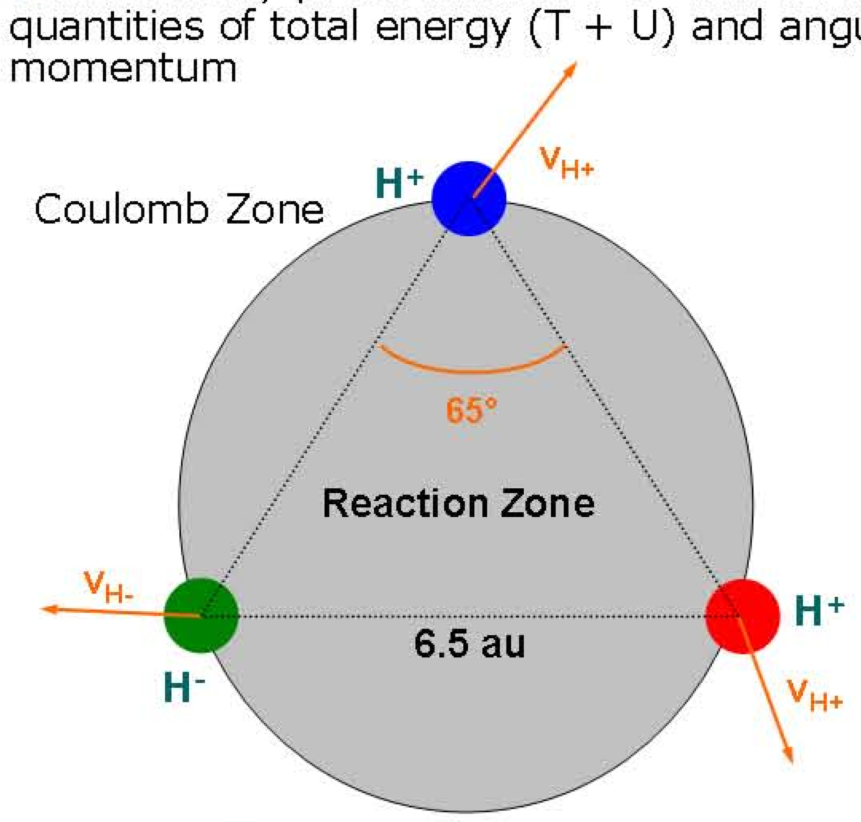


*Figure 1:* Reaction zone and initial geometry for following calculations

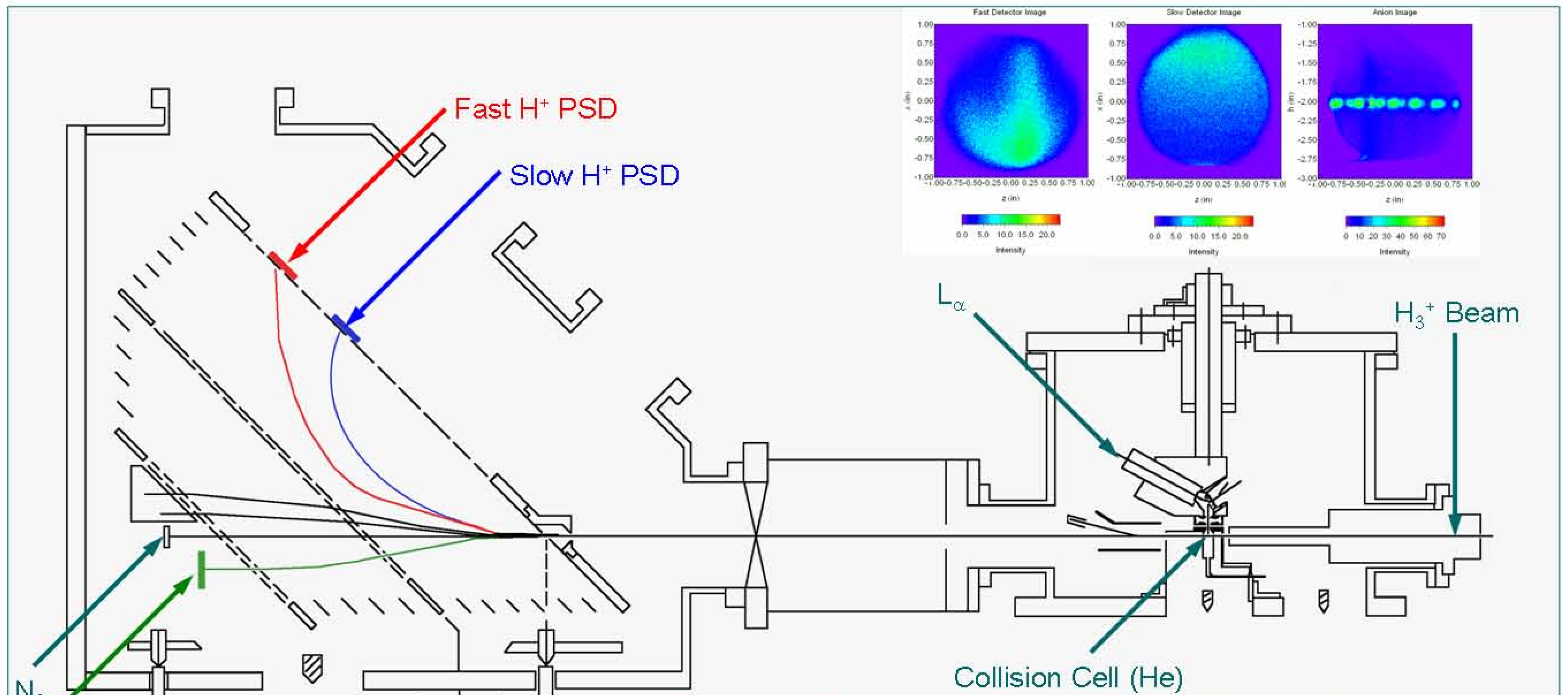


*Figure 2:* Experimental apparatus with inset detector images

## Results: Slightly Correlated

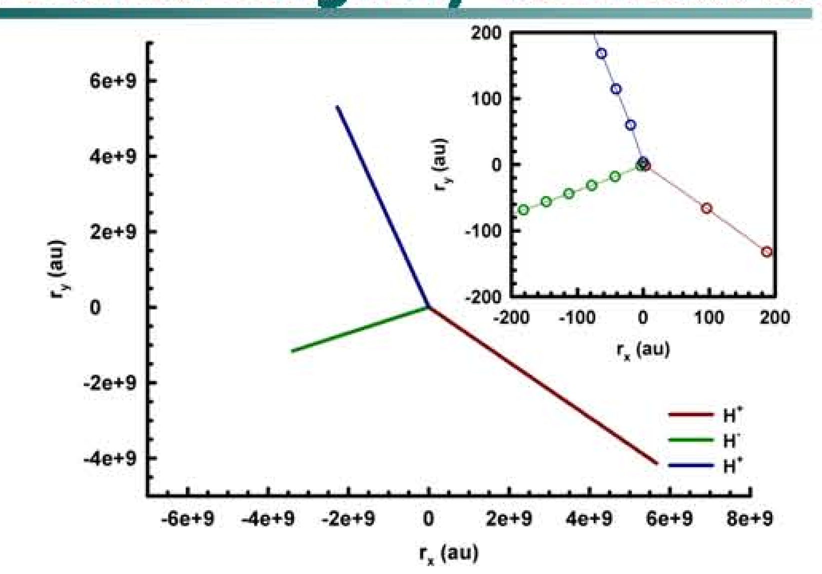

*Figure 3:* Trajectories in the three-body cm frame for $E_{Total}$ = 9.5 eV and j = 8

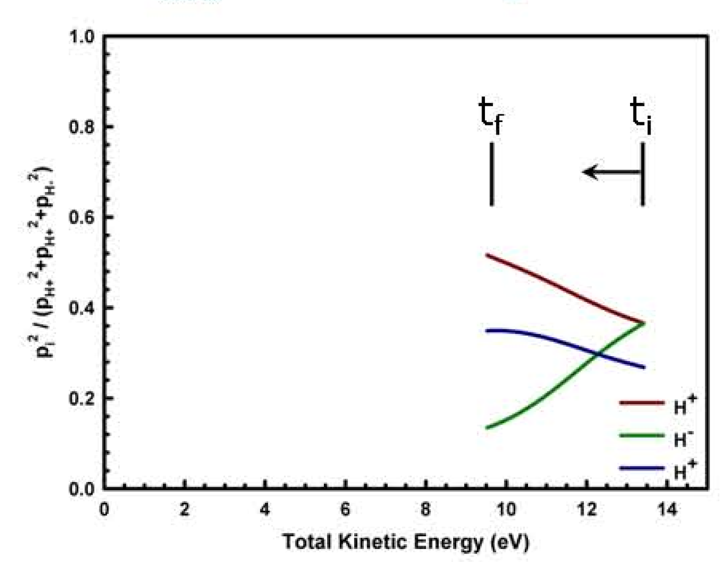

*Figure 4:* Energy sharing in the three-body cm frame for $E_{Total}$ = 9.5 eV and j = 8

## Results: Highly Correlated

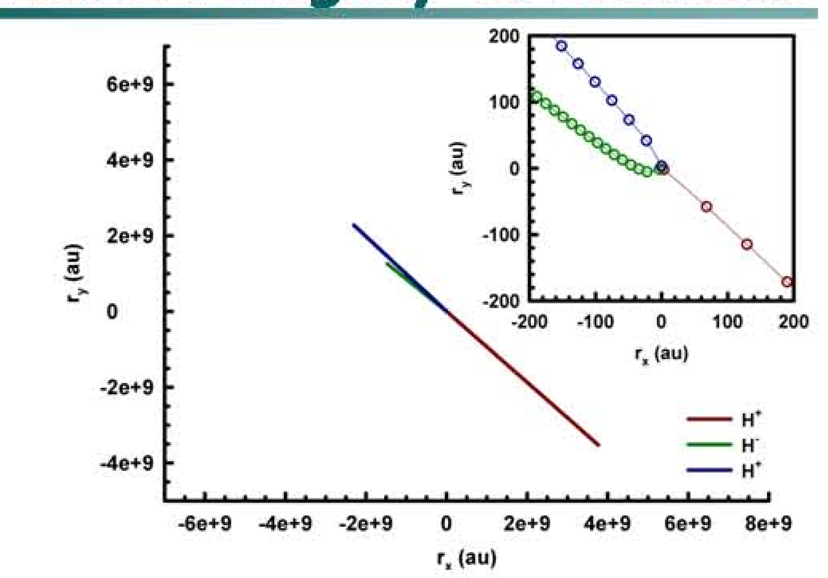

*Figure 5:* Trajectories in the three-body cm frame for $E_{Total}$ = 4.0 eV and j = 8

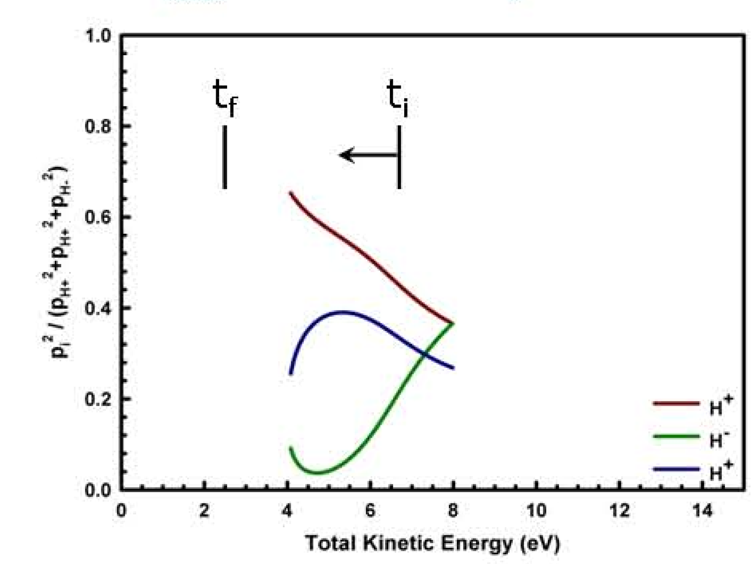

*Figure 6:* Energy sharing in the three-body cm frame for $E_{Total}$ = 4.0 eV and j = 8

## Results: Keplerian Bound

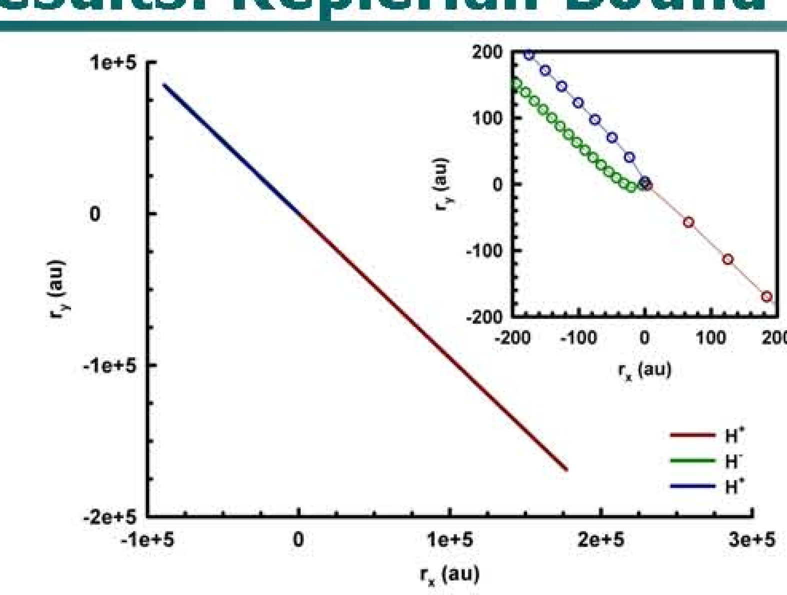

*Figure 7:* Trajectories in the three-body cm frame for $E_{Total}$ = 3.8 eV and j = 8

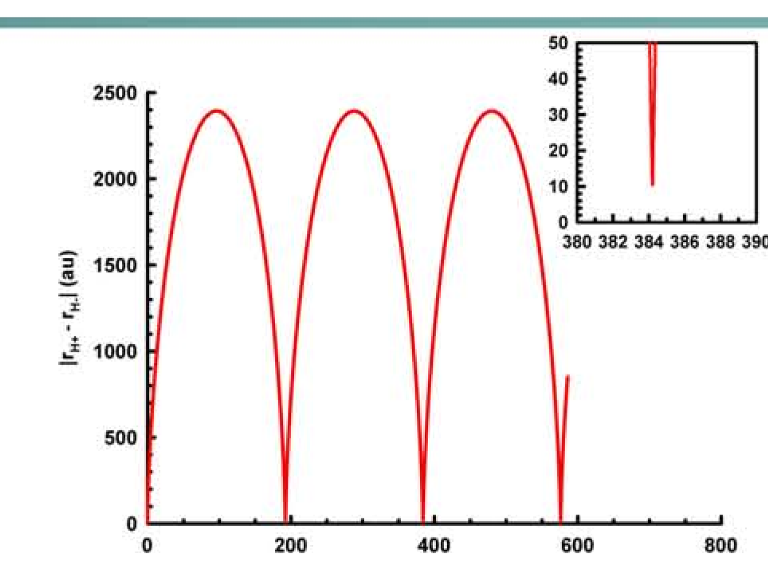

*Figure 9:* $H^+$ - $H^-$ Separation in the three-body cm frame for $E_{Total}$ = 3.8 eV and j = 8

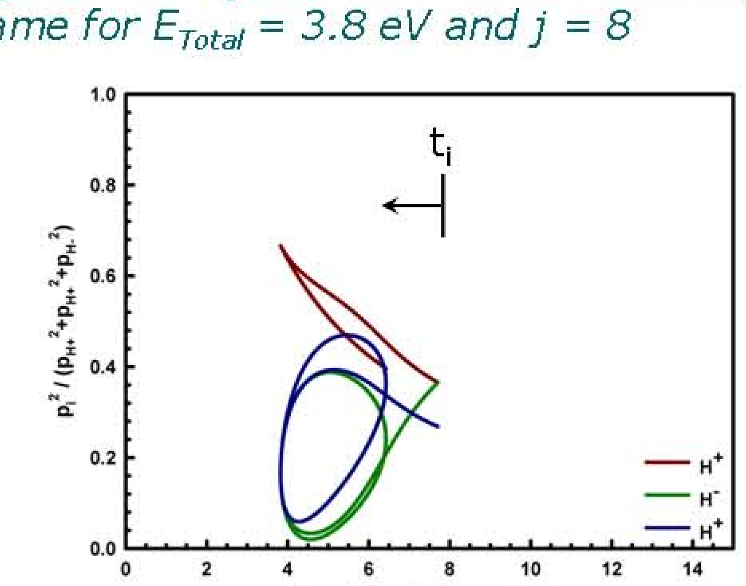

*Figure 8:* Energy sharing in the three-body cm frame for $E_{Total}$ = 3.8 eV and j = 8

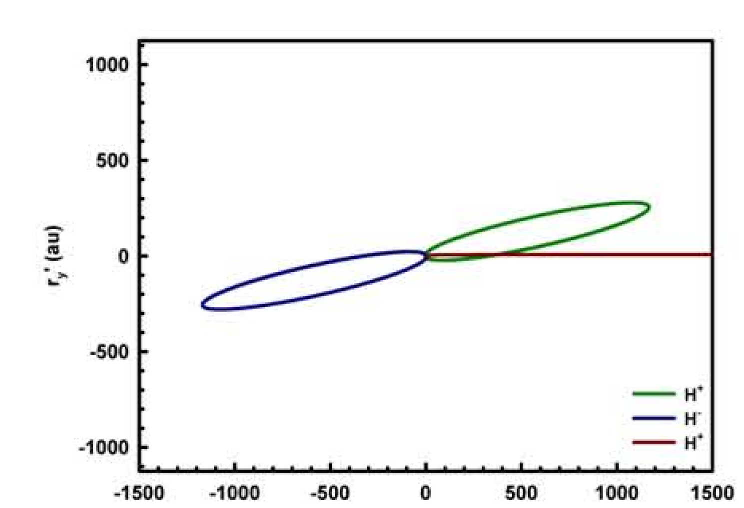

*Figure 10:* Trajectories in the bound $H^+$-$H^-$ frame for $E_{Total}$= 3.8 eV and j = 8

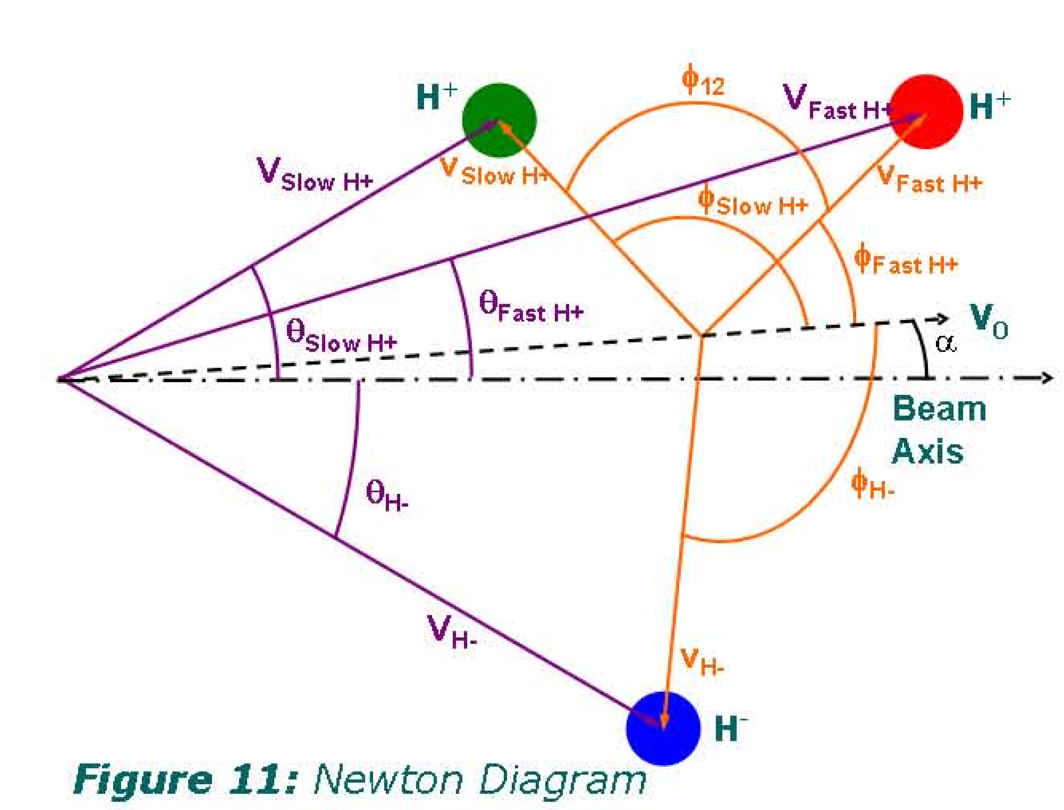

*Figure 11:* Newton Diagram

## Experiment

- Duoplasmatron source produces a 4 keV $D_3^+$ or $H_3^+$ beam
- Photon detector to monitor interaction intensity ($L_\alpha$) with neutral particle detector
- Energy analysis with two-stage parallel plate analyzer (Figure 2)
- Three WSZ position-sensitive detectors with timing signal facilitates energy analysis and triple coincidence measurement
- Data analyzed on an event-by-event basis, transforming from the lab to cm frame (Figure 11 and Figure 12)

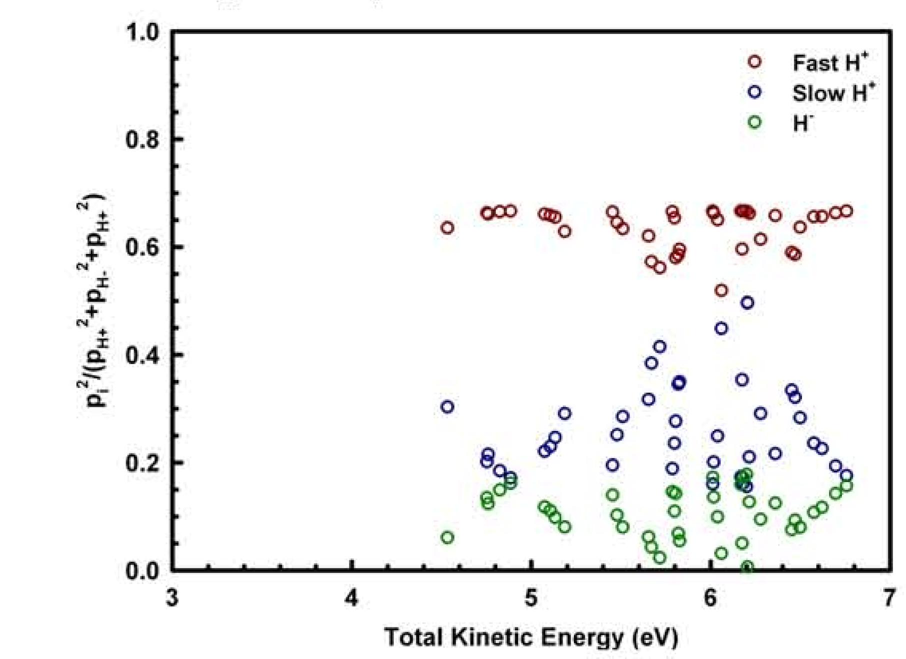

*Figure 12:* Measured $H^+$,$H^+$,$H^-$ energy partitioning emphasizing "fluted" patterns

## Discussion

- Due to the size and complexity of the three-body parameter space, we compare trends and structures between simulations and experiment
- Figure 13 compares the time dependent energy sharing in Figure 8 with experiment
- Highlighted simulation results is signature of $H^+$-$H^-$ bound system dissociating at maximum separation freezing two body dynamics

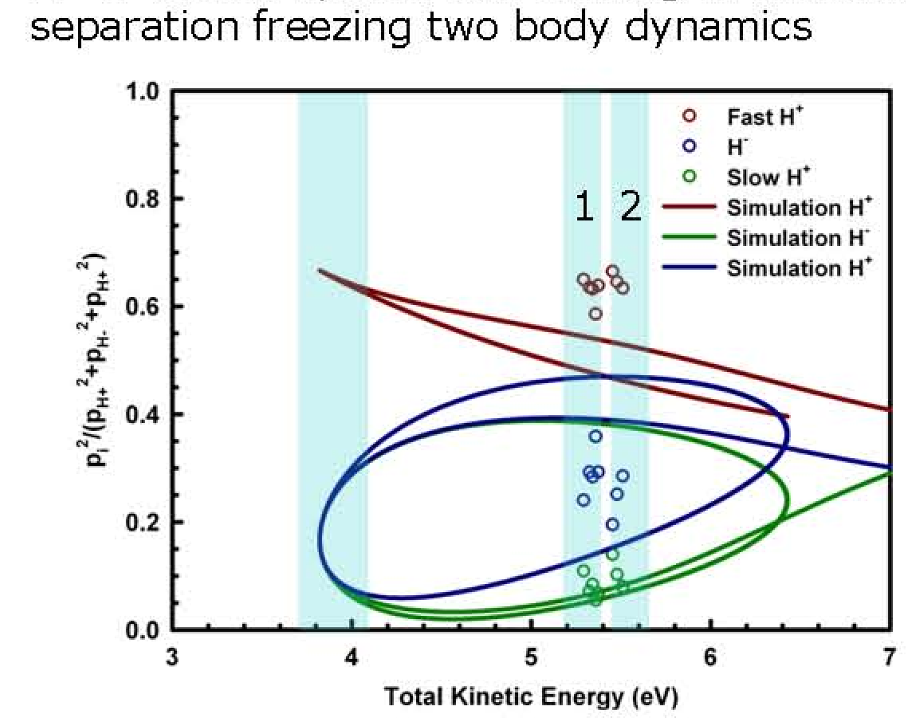

*Figure 13:* Comparing 2 "flutes" in experiment data with simulation results

## Acknowledgements

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