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State-selective charge exchange in collisions of multiply charged ions with H_2

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INTRODUCTION & AIM

Charge exchange processes play a key role in many astrophysical environments and are largely responsible for emission lines produced by electronic cascades following ion–neutral collisions. Such interactions occur in comets, planetary atmospheres, the heliosphere, astrospheres of stars, supernova remnants, and highly ionized regions of the interstellar medium [1-3].

Molecular hydrogen (H_2), the most abundant molecule in the Universe, governs much of the chemistry of the interstellar medium [4]. Over the past decades, charge exchange in ion–H_2 collisions has been extensively investigated experimentally across a wide range of impact energies, focusing on total and state-selective cross sections as well as cascade-induced emission spectra.

We present a five-body CTMC approach for ion–H_2 collisions that improves upon the traditional microcanonical description. Two hydrogenic distributions are implemented to achieve a more accurate H(1s) radial representation, extending the electronic distribution of H_2 to larger distances and providing a more realistic target model.

METHOD

The hydrogenic ECTMC and ZCTMC models improve upon the microcanonical description by yielding a more spatially extended electronic density. In both approaches, the H(1s) radial distribution is constructed as a linear combination of microcanonical distributions, using the nuclear charge (Z) or the ionization potential (E) as expansion parameters (see Ref. [5] for details).

The H_2 molecule is initially modeled as two independent hydrogen atoms bound by a Morse potential adjusted to the experimental vibrational ground state. At the initial stage, each electron is bound to its parent nucleus, while electron–electron and electron–other-nucleus interactions are neglected. These interactions are gradually activated during the collision once an electron reaches the continuum, ensuring a smooth transition in the Hamiltonian.

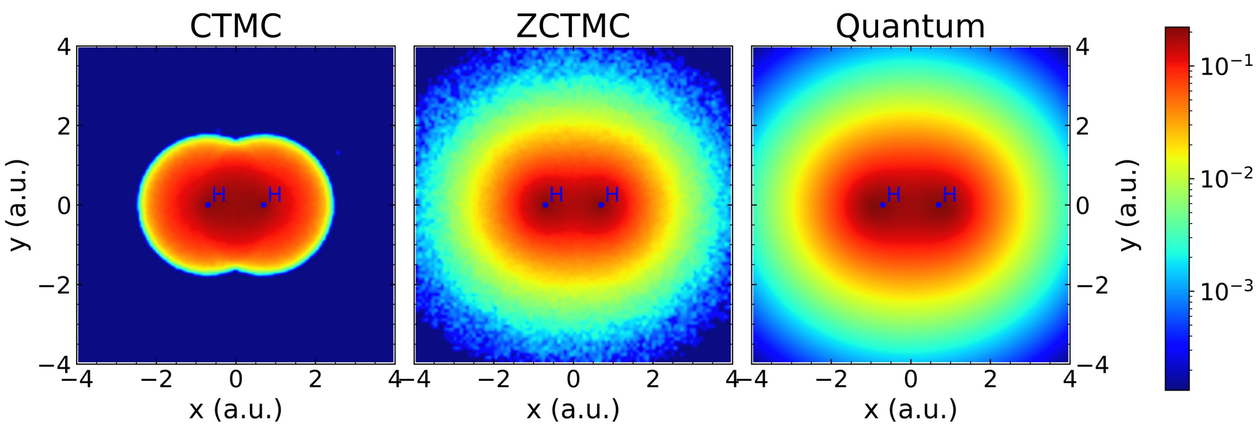

Figure 1: Logarithmic electronic densities in the *xy* molecular plane for H_2.

In **Figure 1** shows the electron density in the molecular plane on a logarithmic scale. Compared to the standard microcanonical model, ZCTMC yields a more spatially extended and realistic electronic distribution.

The simulation is terminated once the projectile leaves the interaction region. The relative energy of each electron with respect to the projectile, E_p is then evaluated to identify capture events. Then, classical principal quantum number n_c is obtained by

$$E_p = -\frac{Z_p^2}{2n_c^2},$$

These classical n_c values are mapped onto the corresponding quantum level (n,l) using the Becker–MacKellar [6] relation.

$$[n(n-1)(n-1/2)]^{1/3} \leq n_c < [n(n+1)(n+1/2)]^{1/3},$$

$$l \leq \left(\frac{n}{n_c}\right) l_c \leq l+1,$$

where l_c is the classical angular momentum $\boldsymbol{r}$ x $\boldsymbol{p}$ the captured electron.

The (n, l) state-selective capture cross section is defined as:

$$\sigma_{n,l} = \frac{N_{cap}(n,l)}{N_{tot}} \pi b_{max}^2$$

RESULTS & DISCUSSION

We benchmark the present method by analyzing n-resolved, state-selective nondissociative single–electron capture (SEC_{nd}) for Ne^{9+} and O^{6+} projectiles, for which recent COLTRIMS experimental data from the Lanzhou group are available [7,8].

Based on the experiments, only reactions of the following type are considered:

$$A^{q+} + H_2 \longrightarrow A^{(q-1)+}(n,l) + H_2^+,$$

where A is the projectile element and q its charge state.

Figures 2 and **3** show the SEC_{nd} cross sections into the n levels for Ne^{9+} and O^{6+} projectiles, respectively, colliding with H_2, as a function of the binding energy difference $Q = E_i - E_f$. Here, E_i and E_f denote the binding energies of the active electron in the initial ground state of the target and the final excited state of the projectile ion.

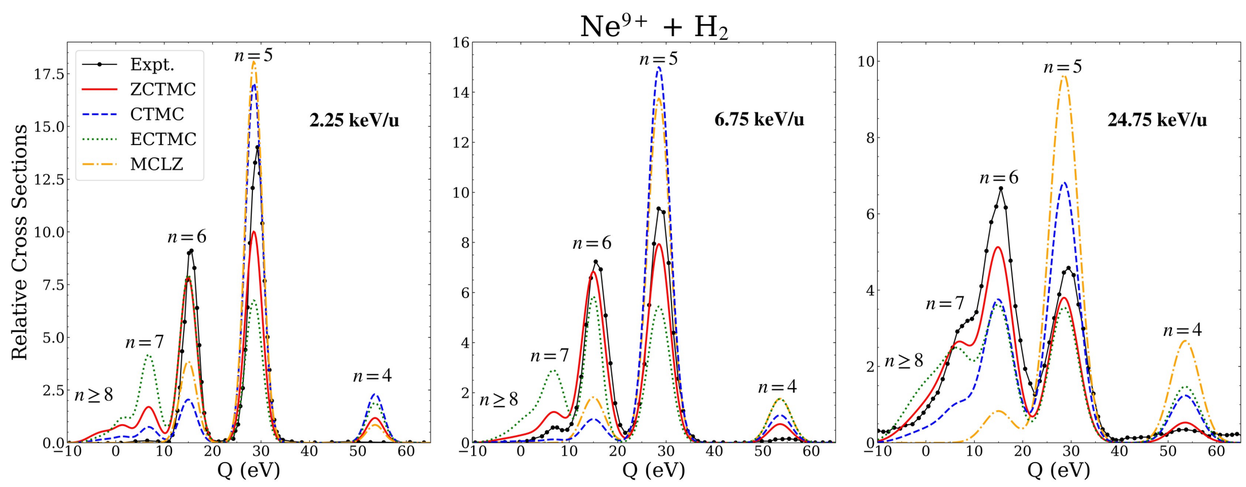

Figure 2: SEC_{nd} Q spectra for Ne^{9+} collisions on H_2 . The theoretical predictions of the ZCTMC model are contrasted to those provided by the ECTMC and CTMC methods. The MCLZ results and the experimental data are those reported in Ref. [7]

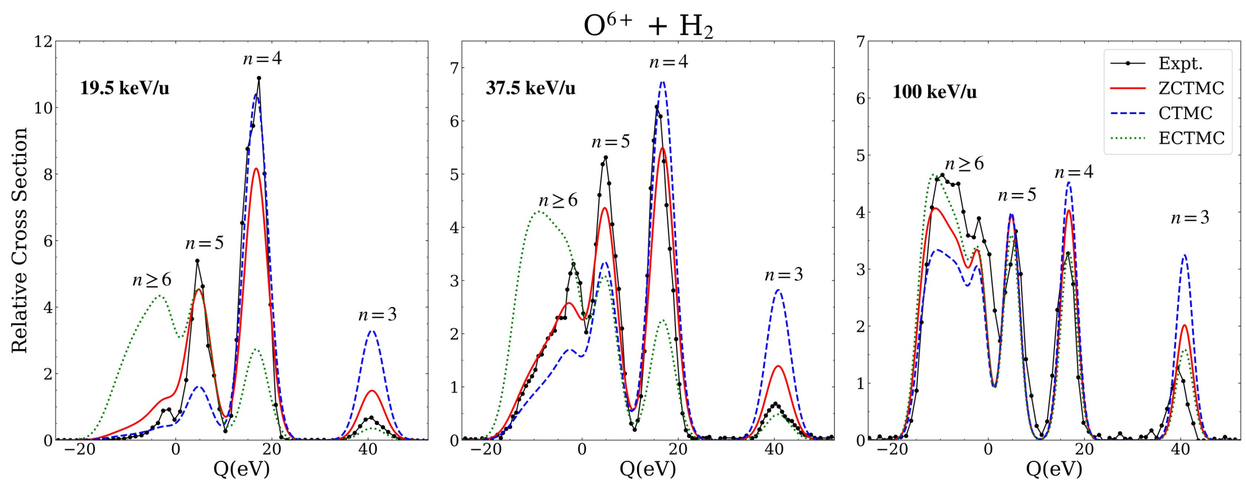

Figure 3: SEC_{nd} Q spectra for O^{6+} collisions on H_2 . The theoretical predictions of the ZCTMC model are contrasted to those provided by the ECTMC and CTMC methods. The experimental data are those reported in Ref. [8]

CONCLUSION

The ZCTMC model introduced here for H_2 has been benchmarked against recently reported state-selective experimental data for Ne^{9+} and O^{6+} projectiles at intermediate-to-low impact energies. Overall, the results indicate that ZCTMC provides the closest agreement with the experimental measurements. Notably, and in contrast to the CTMC, ECTMC, and MCLZ approaches, ZCTMC successfully reproduces the experimentally observed shift of n_{max} over the explored impact-energy range.

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