Charge Exchange Cross Sections in Collisions Between H^+ and Ar^{2+}, and Ar^{3+} and H. A Classical Treatment

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The classical trajectory Monte Carlo (CTMC) model, which calculates numerous individual particle trajectories based on randomly chosen initial atomic states, is a well-established classical approach for modeling atomic collisions [1]. In this work, we implemented the 3-body CTMC method with three variations of the model to determine the charge exchange cross sections for two collision systems: $H^+ + Ar^{2+}$ and $Ar^{3+} + H$. We conducted calculations for impact energies ranging from 1 keV/amu to 100 keV/amu. In all cases, the many-electron target atom was simplified to a one-electron atom, treating the projectile ion as a single particle. The differences between the models lie in their treatment of the additional electrons in the target. In the first case, the Coulomb force acts between the colliding particles, and we calculate the effective charge of the valence electron using Slater's rules [2]. In the second approach, a central model potential is employed to describe the interaction between the active target electron and the target core [3,4]. The third model is a three-body quasi-classical trajectory Monte Carlo (QCTMC) model, which incorporates some quantum features of the collision system by adding the Heisenberg correction term to the standard classical Hamiltonian to mimic the Heisenberg uncertainty principle [5,6].

We provide a detailed comparison and analyze the similarities and differences in our theoretical data.

References

[1] K. Tőkési and G. Hock, Nucl. Instrum Meth. Phys. Res. B**86**, 201 (1994).

[2] Slater, J. C. Phys. Rev. **36**, 57 (1930).

[3] R.H. Garvey, et al., Phys. Rev. A**12**, 1144 (1975).

[4] K. Tőkési and Á. Kövér, J. Phys. B **33,** 3067 (2000).

[5] I. Ziaeian, K. Tőkési, J. Phys. B: At. Mol. Opt. Phys. **55**, 245201(2022).

[6] I. Ziaeian and K. Tőkési, Sci. Rep. **11**, 20164 (2021).