Ionization, total and state selective charge exchange cross sections in fusion related collision systems

K. Tőkési^{1,2}

¹Institute for Nuclear Research (ATOMKI), Debrecen,4026, Hungary ²Centre for Energy Research, Budapest, Hungary <u>tokesi@atomki.hu</u>

The standard three-body classical trajectory Monte Carlo (CTMC) model is a well-known classical treatment for modelling atomic collisions [1]. But due to the lack of quantum features in the standard model, the CTMC model is not able to describe accurately the cross sections mostly at lower impact energies when the quantum mechanical characteristic is dominant. Therefore, we developed a three-body quasi classical trajectory Monte Carlo (QCTMC) model taking into account quantum feature of the collision system, where the Heisenberg correction term is added to the standard classical Hamiltonian of the collision system to mimic the Heisenberg uncertainty principle [2-10].

We present ionization, total and state selective charge exchange cross sections in collisions between fully stripped ions with Hydrogen atoms at the impact energies between 5-200 keV/amu by using CTMC and QCTMC models. We found that our QCTMC model remarkably improves the obtained cross sections, especially at lower projectile energies. Our results are very close and are in good agreement with the previously obtained quantum-mechanical results. Our model with simplicity can time efficiently provide accurate results where maybe the quantum mechanical ones become complicated. Therefore, our model should be an alternative way to calculate accurate cross sections providing the same results as the quantum-mechanical approaches [2-10].

We also present total and energy and angular differential cross sections for single-ionization and single charge exchange in a collision between singly charged lithium and sodium with ground-state helium and nitrogen atoms. For sake of simplicity, the considered collision systems are treated as three-body problems. The helium and nitrogen atomic targets are described within the single active electron approximation using a Garvey-type distance-dependent model potential where only the ground-state outermost electron is involved in the collision dynamics as an active electron while the other bound electrons are considered inactive [11,12]. The interactions between the projectile and target system are described by the Garvey-type potential. The scattering problem is solved within the frame of the classical trajectory Monte Carlo (CTMC) [1].

We found that the classical treatment of the collision problem describes reasonable well both the total and differential cross sections. Our present CTMC results are in good agreement with available theoretical and experimental data [13].

References

- [1] K. Tőkési and G. Hock, Nucl. Instrum Meth. Phys. Res. B86 201 (1994).
- [2] I. Ziaeian and K. Tőkési, Atoms 8 27 (2020).
- [3] S.J.A. Atawneh and K. Tőkési, Atoms 8 31 (2020).
- [4] I. Ziaeian and K. Tőkési, EPJD J. 75 138 (2021).
- [5] S.J.A. Atawneh and K. Tőkési, J. Phys. B: At. Mol. Opt. Phys. 54 065202 (2021).
- [6] S. J. A. Atawneh and K. Tőkési. Nucl. Fusion. 62 026009 (2021).
- [7] I. Ziaeian and K. Tőkési, Sci. Rep. 20164 (2021).
- [8] I. Ziaeian and K. Tőkési, Atomic Data and Nuclear Data Tables 146 101509 (2022).
- [9] S.J.A. Atawneh and K. Tőkési, Atomic Data and Nuclear Data Tables 146 101513 (2022).
- [10] S. J. A. Atawneh and K. Tőkési. Phys. Chem. Chem. Phys. 24 15280 (2022).
- [11] R.H., Garvey, C.H. Jackman and A.E.S Green 1975 Phys. Rev.A 12(4) 1144–1152
- [12] A.E.S. Green A 1973 Advances in Quantum Chemistry vol 7) ed. P.O. Löwdin (Academic Press) 221.
- [13] M Al-Ajaleen, A Taoutioui and K Tőkési, (2023), Physics and Controlled Fusion, in press