CLASSICAL DESCRIPTION OF H(1s) AND H*($n = 2$) FOR CROSS-SECTION CALCULATIONS RELEVANT TO CHARGE-EXCHANGE DIAGNOSTICS.

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Abstract

We introduce a classical trajectory Monte Carlo (CTMC) methodology, specially conceived to provide a more accurate representation of charge-exchange processes between highly chaged ions and H(1s) and H*($n = 2$). These processes are of particular relevance in power fusion reactor programs, for which charge-exchange spectroscopy has become a useful plasma diagnostics tool. To test the methodology, electron-capture reactions from these targets by C^{6+}, N^{7+} and O^{8+} are studied at impact energies in the 10-150 keV/amu range. The present results are found into be much better agreement with the quantal-mechanical results than the results of former formulations of the CTMC method.

Theoretical Method

We introduce an alternative CTMC model for H(1s) and H*(n=2) (hydrogenic-Z-CTMC) which provides a more accurate representation of the target system than the microcanonical ensemble, it follows the hydrogenic-E-CTMC spirit [1].

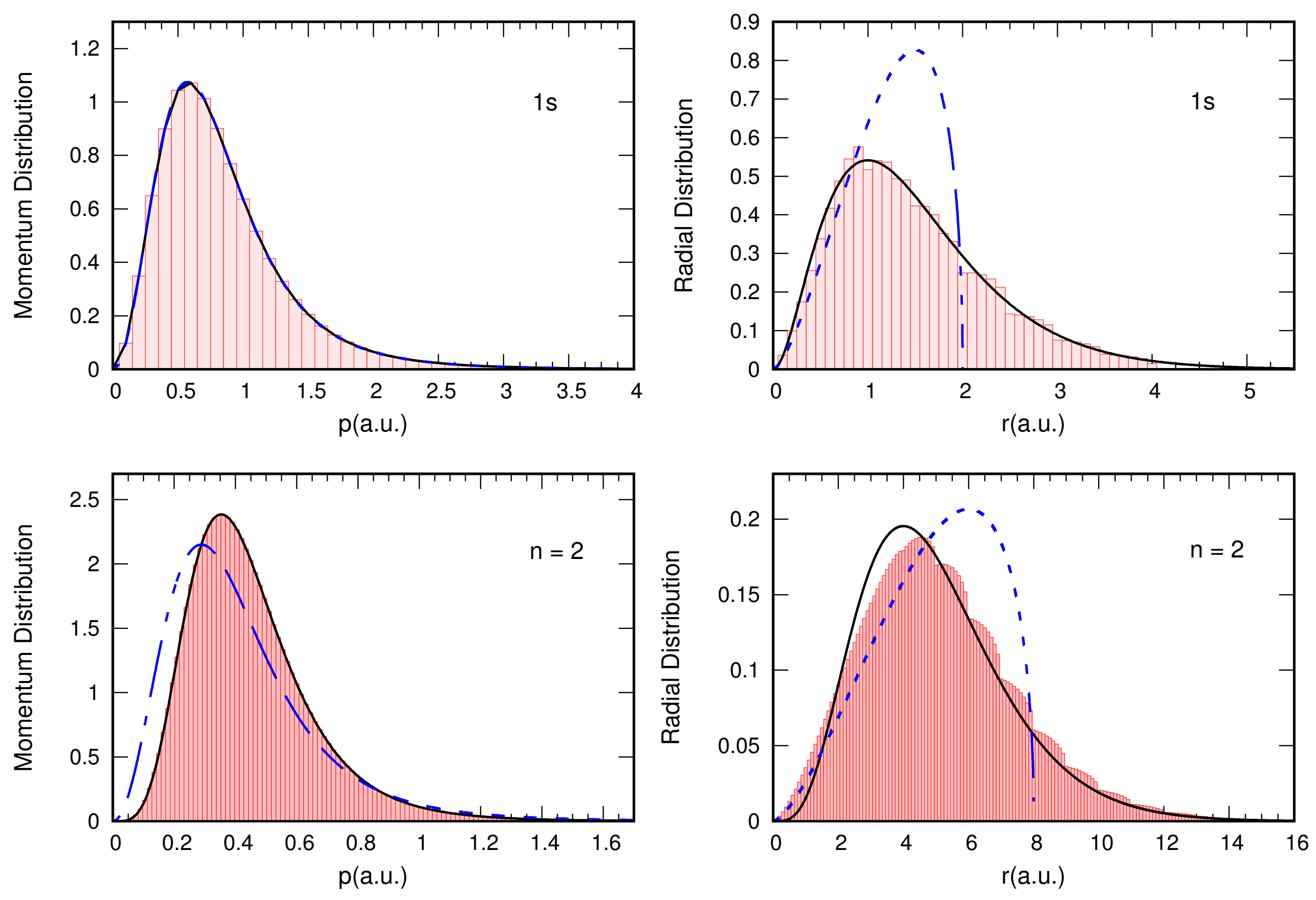
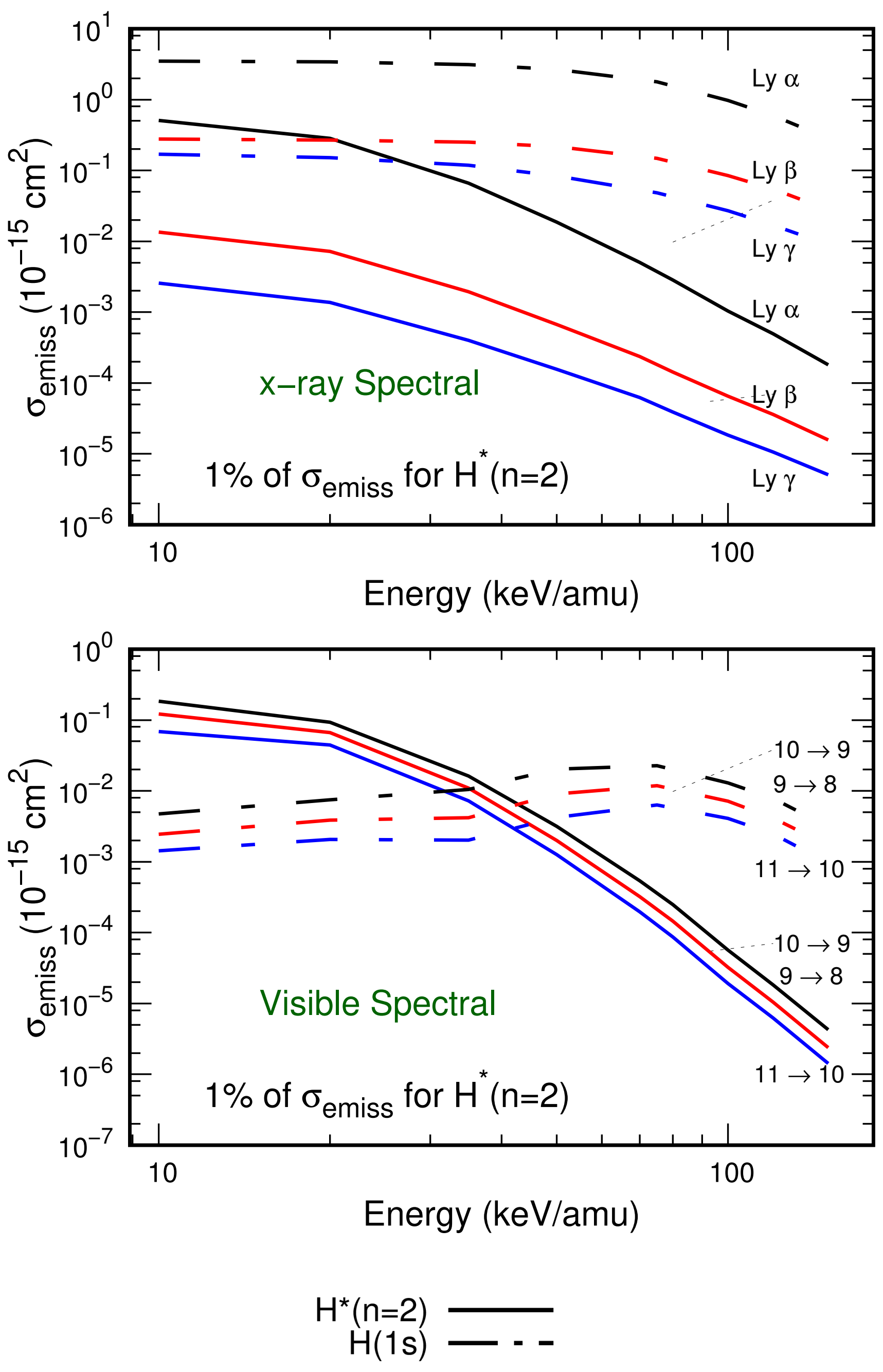


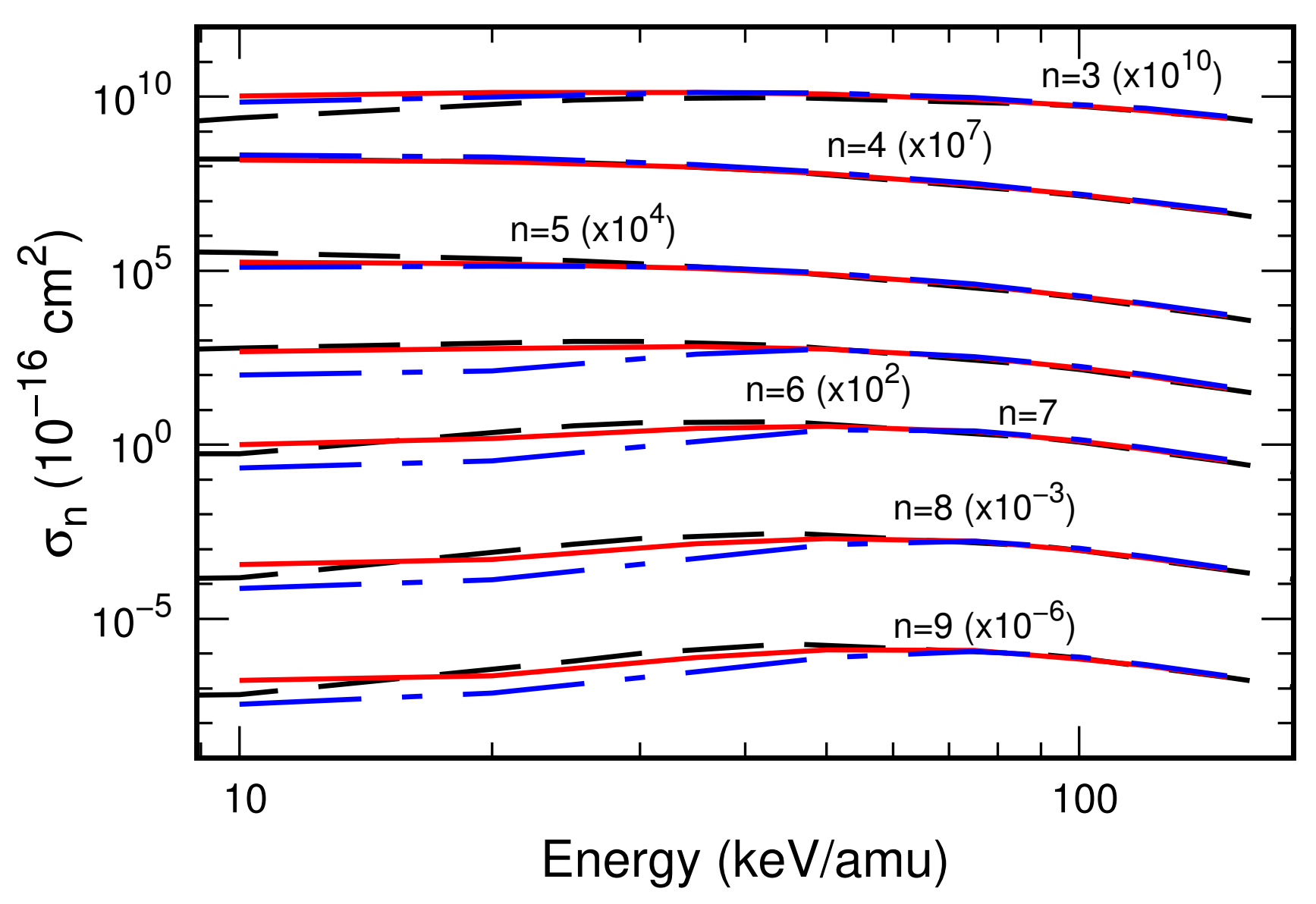
Fig. 1: Momentum and Radial distributions for 1s, 2s, and 2p orbitals. **Black-solid line**, **quantum mechanical** distributions; blue-dashed line, microcanonical distributions; and red columns present hydrogenic-Z-CTMC distributions.

While hydrogenic-E-CTMC proposes a discrete summation of microcanonical ensembles corresponding to different binding energies (V_{ion}) for the target electron, hydrogenic-Z-CTMC is achieved by considering different target nuclear charges (Z) while retaining the correct ionization potential for the target under consideration. Advantages of the hydrogenic-Z-CTMC methodology compared to the hydrogenic-E-CTMC is based on the fact that the most populated projectile n level in charge-exchange processes is given by the $\sqrt{13.6/V_{ion}}\ \ Z_p^{3/4}$ scaling law, a methodology based on set of microcanonical distributions involing different V_{ion} values is expected to lead to a wider overall n distribution [2]. For electron capture process, the states quantum relatives to the projectile are obtained according to the relationship derived by Becker and MacKellar [3].

Lines Emission Cross Sections of N^{7+} on H(1s) and H($n = 2$)



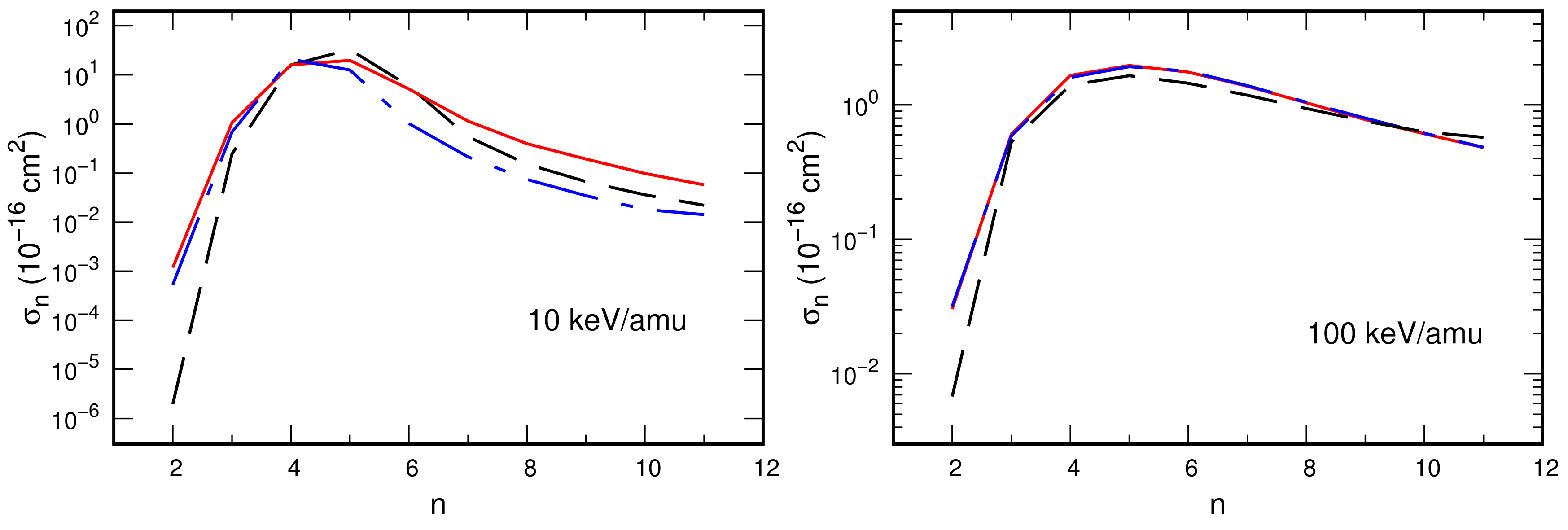
N^{7+} + H(1s)



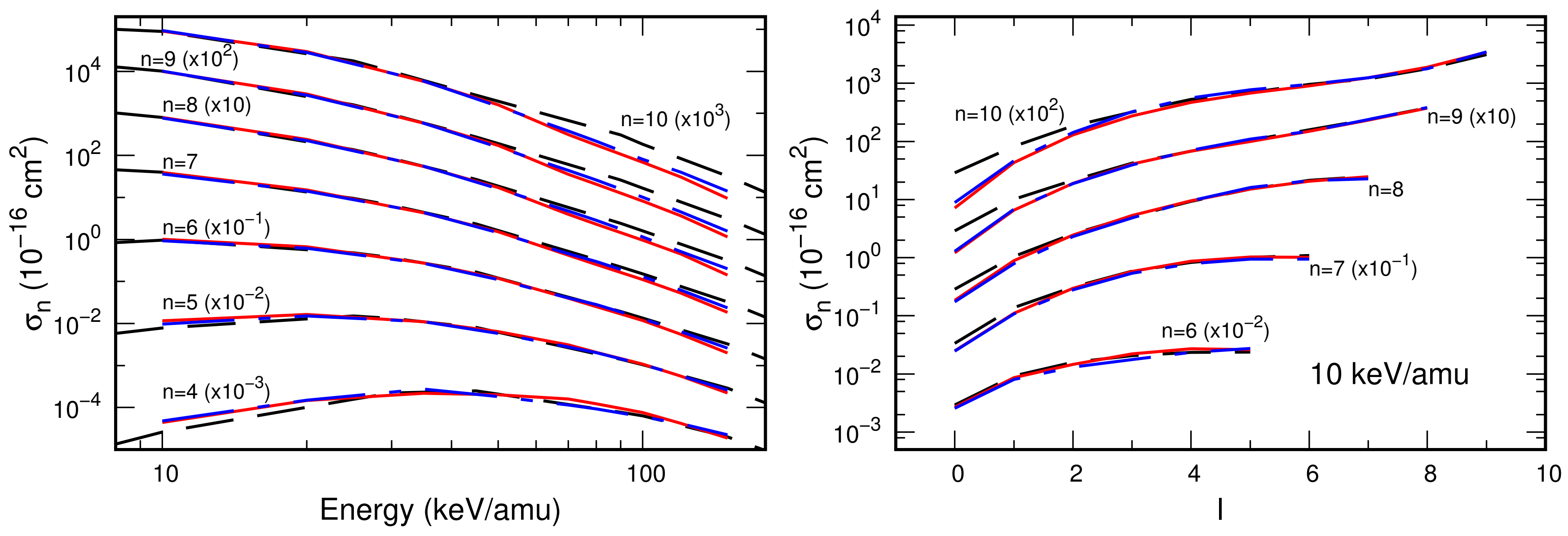
RIGHT n-state selective capture cross section as a function of the projectile energy N^{7+}.

DOWN State-selective electron-capture cross section for N^{7+} collisions on ground state H(1s) at collisions energies of 10 and 100 keV/amu.

━━━━ hydrogenic–Z–CTMC
━ ━ ╸ ━ microcanonical–CTMC
━ ━ ━ AOCC [4,5]



N^{7+} + H($n = 2$)



Conclusions

- State selective electron capture data provided by the present model were found in much better agreement with AOCC than those obtained by means of the standard microcanonical and the hydrogenic-E-CTMC methods.
- Present results show that charge exchange diagnostics that are based on the observation of visible transitions, demonstrate the dominant and crucial role that even a tiny fraction of H*($n = 2$) can have at low impact energies (ca 10 keV/amu).

References

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