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Reply to "Comment on 'Classical Description of H(1s) and H* (n=2) for Cross-Section Calculations Relevant to Charge-Exchange Diagnostics'"

N. D. Cariatore

Sebastian Otranto
Missouri University of Science and Technology, otrantos@mst.edu

Ronald E. Olson
Missouri University of Science and Technology, olson@mst.edu

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Reply to "Comment on 'Classical description of H($1s$) and H*($n = 2$) for cross-section calculations relevant to charge-exchange diagnostics'"

N. D. Cariatore,[1] S. Otranto,[1] and R. E. Olson[2]
[1]*IFISUR and Departamento de Física, Universidad Nacional del Sur, 8000 Bahía Blanca, Argentina*
[2]*Physics Department, Missouri University of Science and Technology, Rolla, Missouri 65401, USA*
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In reply to the Comment of Jorge *et al.* [Phys. Rev. A **93**, 066701 (2016)], we agree and reconfirm that the alternative classical trajectory Monte Carlo method (called hydrogenic-Z-CTMC) radial distributions for H*($n = 2$) we recently published are not stable in time. However, we show that such lack of stability which is more noticeable for H($2s$) than for H($2p$) is due to the initialization procedure employed and not to the hydrogenic-Z-CTMC method itself. A new set of completely stable hydrogenic-Z-CTMC calculations for H*($n = 2$) is introduced and found in very good agreement with standard microcanonical results reinforcing our previous findings. A second criticism of Jorge *et al.* concerning the number of components in hydrogenic-Z-CTMC with $n > 1$ for H($1s$) is shown not to have a significant impact on relative (n,l) populations in the final state.

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For more than five decades, the classical trajectory Monte Carlo (CTMC) method has provided theoretical insight for a wide range of atomic and molecular collision processes. Despite the fact that the method relies exclusively on Newton's physical laws to describe the collision dynamics well within the quantum-mechanical domain, the method has been systematically used on collision systems for which an accurate quantum treatment is still prohibitive in computational terms such as those involving highly charged ions. Moreover, it has provided complementary interpretations of processes for which accurate quantum treatments are feasible.

In a recent work [1], we have revisited one of the main limitations exhibited by the CTMC method for the hydrogen target, which is particularly relevant to charge-exchange diagnostics and the fusion plasma program. That is, the lack of the exponential decreasing behavior of the radial distribution in the microcanonical formulation of the CTMC method. During the last 35 years this problem has been tackled by different authors who proposed different phase-space functions which recovered the quantum-mechanical radial distribution for H($1s$) [2–4]. One of these is the denominated hydrogenic-E-CTMC which uses a discrete summation of microcanonical ensembles corresponding to different ionization potentials to reproduce the quantal radial distribution via a least-squares fitting procedure [3]. The main object of our study was the evaluation of an alternative hydrogenic-Z-CTMC method which employs different target nuclear charges in the discrete summation, allowing it to retain the proper ionization potential of the target. The motivation here stems from the limitations detected in the hydrogenic-E-CTMC method to describe recent recoil-ion momentum distributions in ion-atom collisions as well as charge-exchange processes either at low impact energies or involving highly charged ions. Initial studies were carried out on H($1s$), H*($2s$), and H*($2p$) targets and provided the relevance of excited hydrogen for the fusion plasma program. Interestingly, (n,l)-state-selective cross sections calculated for H*($n = 2$) with the hydrogenic-Z-CTMC model for C^{6+}, N^{7+}, and O^{8+} projectiles in the 10 keV/amu-150 keV/amu impact energy range were almost indistinguishable from those obtained with the standard microcanonical ensemble.

In their comment, Jorge *et al.* [5] criticize our methodology along two main lines: (i) our initialization procedure for H*($n = 2$), and (ii) they recall that the hydrogenic-Z-CTMC model is not physically correct even for H($1s$) and should not be used at all. In what follows we will address these two issues.

The classical phase-space distribution used in [1] can be expressed as follows:

$$\rho(r,p,n,l) = \sum_{i=1} \alpha_i \rho_0(r,p,Z_i,n,l).$$

The α_i coefficients were determined by means of a least-squares fitting procedure over the quantum-mechanical radial distribution for the (n,l) state. In our study we initialized the H*($n = 2$) target by sorting over the (n,l) quantum-mechanical momentum distribution which for H*($2s$) has a node that at $t = 0$ translates to the radial distribution. In their comment, Jorge *et al.* show that this node is washed out very fast as the system evolves provided that the Liouville equation is not satisfied ($[\rho_0(r,p,Z_i,n,l),H] \neq 0$). We have corroborated their statements. The nodal structures which at $t = 0$ a.u. are predicted in the momentum and radial distributions are rapidly lost. In Fig. 1, we show how the momentum and radial distributions for H*($2s$) and H*($2p$) evolve for much larger time intervals than those shown in their comment. These are more representative of the typical times considered in our simulations. We have performed tests within the time constraint allowed for this reply and found minor changes at the H*($n = 2$) cross-section level for different physically meaningful projectile incidence time lapses. This is possibly due to the fact that 75% of the H*($n = 2$) charge-exchange cross sections shown correspond to H*($2p$), and that this target is much more stable than H*($2s$) as can be inferred from Fig. 1. However, below in Fig. 2 we report the sensitivity of the H*($2s$) components of those cross sections by explicitly considering three different projectile incidence time lapses of 300, 450, and 600 a.u.

Provided that the genesis of the radial distributions' instability for H*($2s$) and H*($2p$) was not the hydrogenic-Z-CTMC method itself, i.e., the proposal of an expansion over distributions corresponding to different Z values, but our particular

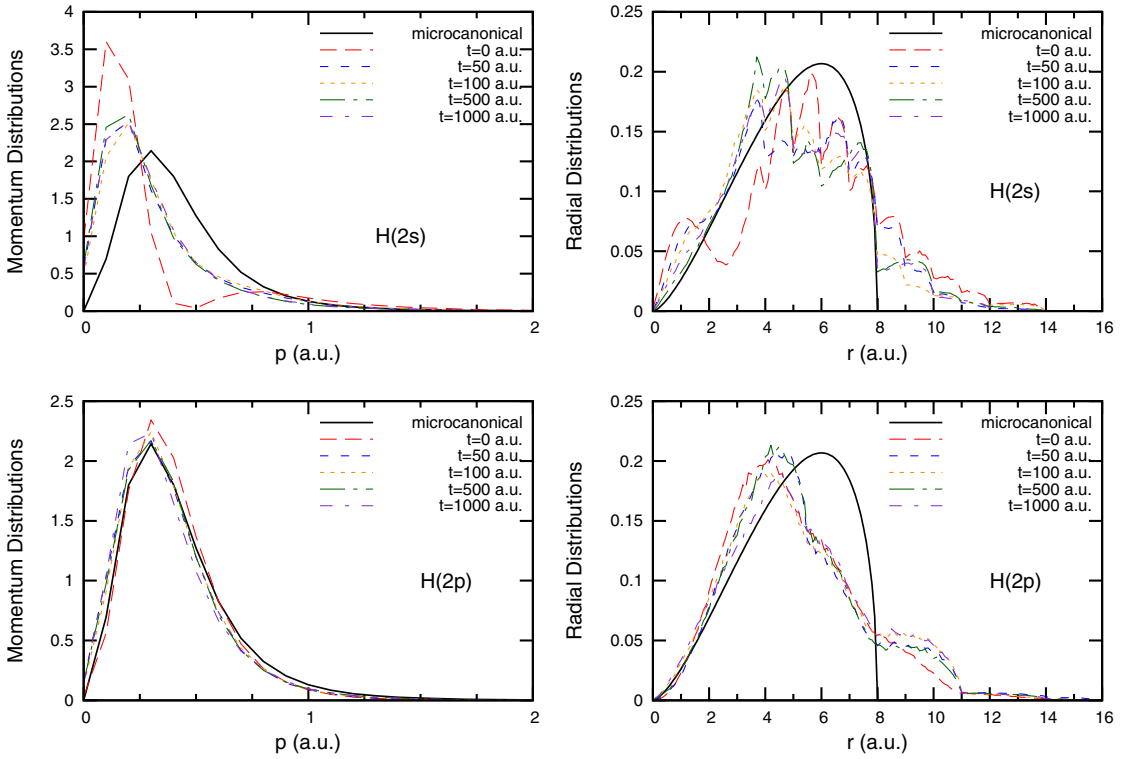

FIG. 1. Hydrogenic-Z-CTMC momentum and radial distributions for H$^*(2s)$ and H$^*(2p)$ as a function of time.

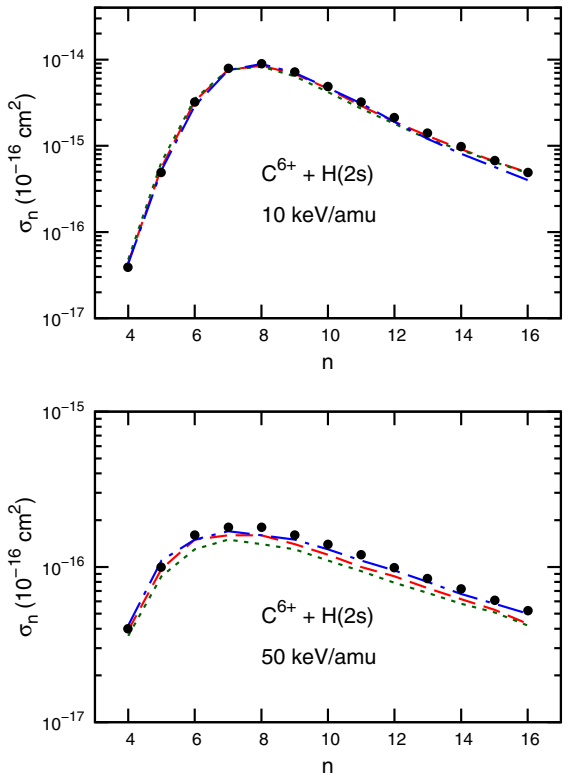

FIG. 2. Hydrogenic-Z-CTMC n-state selective charge-exchange cross-section sensitivity for 10 and 50 keV/amu C^{6+} collisions on H$^*(2s)$. Theories: black dots, results corresponding to Ref. [1]; red dashed line: projectile incidence time lapse of 300 a.u.; green dotted line: projectile incidence time lapse of 450 a.u.; blue dashed-dotted line: projectile incidence time lapse of 600 a.u.

choice of the $\rho_0(r,p,Z_i,n,l)$ distributions used which are not perfectly stable for $n=2$, we now present an alternative hydrogenic-Z-CTMC scheme to fit an effective H$^*(n=2)$ radial distribution built upon the quantum-mechanical radial distributions in a statistical proportion of 75% H$^*(2p)$ and 25% H$^*(2s)$. Results are shown in Fig. 3. By initializing the system using standard microcanonical ensembles $\rho_{\rm M}(r,p,Z_i)$, i.e., following a similar procedure to that used by the hydrogenic-E-CTMC, we reproduce the radial distribution without any possible chance of instability, provided that these

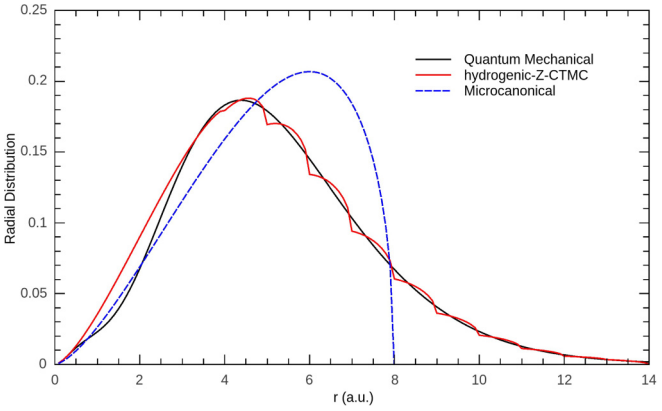

FIG. 3. Radial distribution for H$^*(n=2)$. The quantum-mechanical result is built upon the quantum-mechanical distributions for H$^*(2s)$ and H$^*(2p)$ by assuming relative contributions of 0.25 and 0.75 for each of them. The new hydrogenic-Z-CTMC method is initialized by means of microcanonical distributions providing a stable radial distribution.

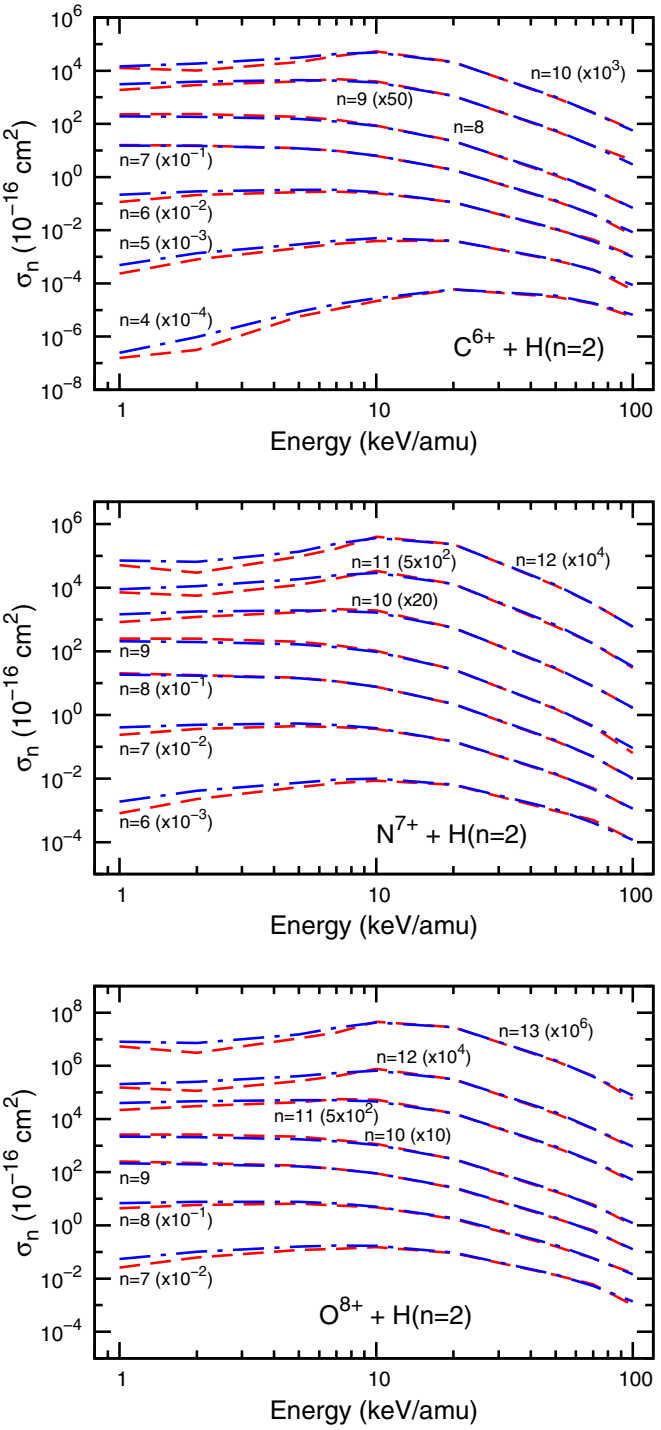

FIG. 4. n-state-selective capture cross section as a function of the projectile energy following C^{6+}, N^{7+}, and O^{8+} collisions on $H^*(n=2)$. Theories are shown by a blue dashed-dotted line for the new hydrogenic-Z-CTMC, and a red dashed line for microcanonical CTMC. Cross sections have been multiplied by factors in brackets to facilitate visualization.

microcanonical distributions satisfy the Liouville equation. The new hydrogenic-Z-CTMC scheme is then given by

$$\rho_{\rm new}(r,p,n) = \sum_{i=1} \alpha_i \rho_{\rm M}(r,p,Z_i).$$

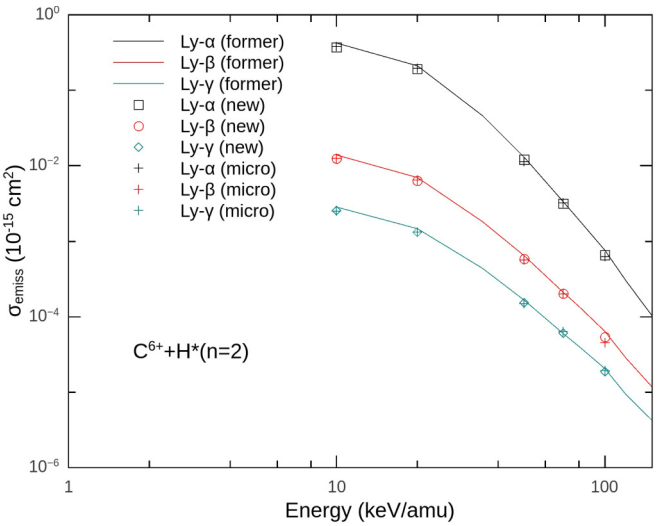

FIG. 5. Line emission cross sections in the x-ray spectral range as a function of impact energy for C^{6+} collisions on $H^*(n=2)$. The cross sections are reduced to 1% of their value to mimic the power reactor environment. Former results correspond to those published in Ref. [1].

We point out that the original hydrogenic-Z-CTMC formulation gets coincident with the new one for $H(1s)$.

In Fig. 4 we present the n-state-selective capture cross section as a function of the projectile energy following C^{6+}, N^{7+}, and O^{8+} collisions on $H^*(n=2)$ calculated with the new hydrogenic-Z-CTMC and are contrasted against the standard microcanonical CTMC results. As previously observed, the state selective cross sections are almost indistinguishable from those obtained with the simple microcanonical ensemble.

In Figs. 5 and 6 we perform a more exhaustive analysis of our models by revisiting the line emission cross sections corresponding to Lyman and visible spectral range following C^{6+} collisions on $H^*(n=2)$ that were shown in our article [1].

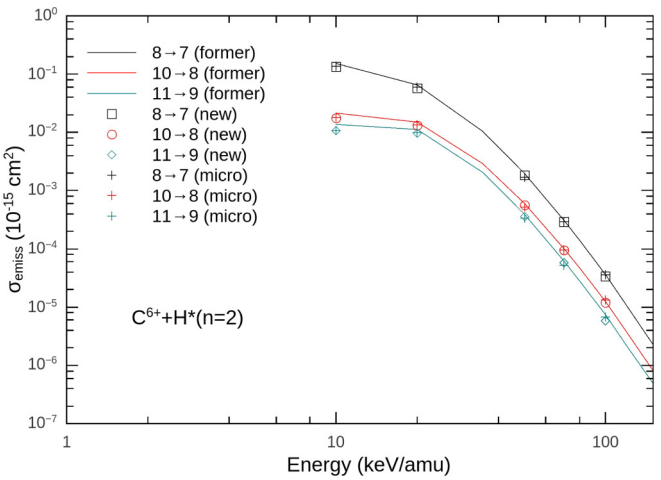

FIG. 6. Line emission cross sections in the visible spectral range as a function of impact energy for C^{6+} collisions on $H^*(n=2)$. The cross sections are reduced to 1% of their value to mimic the power reactor environment. Former results correspond to those published in Ref. [1].

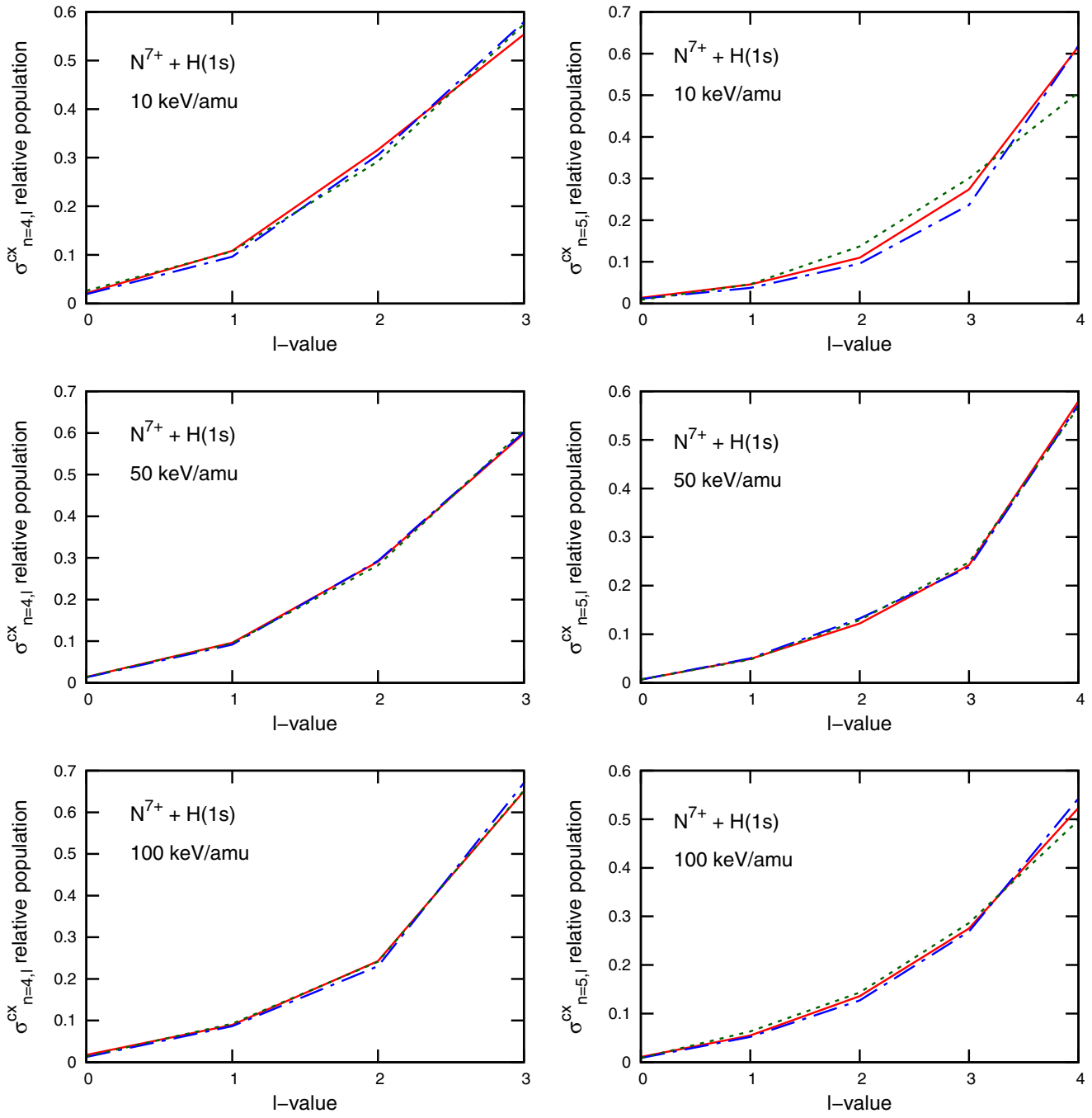

FIG. 7. $n = 4$ and $n = 5$ l-state-selective relative populations for 10, 50, and 100 keV/amu $N^{7+} + H(1s)$ collisions. Theories: red solid line: hydrogenic-Z-CTMC; green dotted line: hydrogenic-E-CTMC; blue dashed line: microcanonical CTMC.

These cross sections, which are reduced to 1% of their value to mimic the power reactor environment, are of potential relevance for the fusion reactor program and as such it is imperative to rule out any possible doubt on their reliability. In both figures, our new hydrogenic-Z-CTMC results are contrasted to our former results of Ref. [1] and to the results obtained using the microcanonical distributions. Very good agreement is obtained within the three models throughout the energy range explored of 10–100 keV/amu, reinforcing our previous statements that the $H^*(n = 2)$ target seems not to be sensitive to the initialization procedure studied which considers the correct ionization potential. Moreover, it clearly indicates that the charge-exchange cross sections obtained with the different methods are in agreement at the (n,l) level.

Now, we turn to the question about the eccentricities employed in our initialization procedure for the $H(1s)$ case. In Fig. 7 we consider the dominant $n = 4$ and $n = 5$ l-state-selective relative population for charge exchange following 10, 50, and 100 keV/amu $N^{7+} + H(1s)$ collisions. Provided that during the charge-exchange process the electron tries to preserve its orbital eccentricity [6], any flaw in the initial state angular momentum should translate to the

l-state-selective charge-exchange cross sections. From Fig. 7, we conclude that the relative populations of l values provided by the three models are all in good agreement with each other, clearly indicating that the hydrogenic-Z-CTMC initialization does not lead to any unphysical behavior as has been questioned.

In summary, no definite initialization procedure is available at this time that can completely mimic the quantum-mechanical phase-space distribution for hydrogen. Phase-space distributions built with the aim to correct the radial cutoff proper of the microcanonical distribution have at the same time strengths and limitations provided they are based on expansions in terms of different target nuclear charges or ionization potentials. Present results suggest that the hydrogenic-Z-CTMC model based on microcanonical expansions can be safely used to describe charge-exchange processes and its capabilities should be further explored, particularly on other target atoms.

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