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3D numerical calculation of electron capture cross sections in $Be^{4+} + H$ collisions.

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Synopsis Electron capture in Be^{4+} + H collisions is studied at collision energies between 1 and 100 keV/u, as a benchmark to discuss the accuracy of different theoretical approaches. Partial cross sections, obtained by solving numerically the time-dependent Schrödinger equation, are compared to the corresponding results from close-coupling and classical trajectory Monte Carlo calculations.

Collisions involving Be^{q+} ions are specially relevant because the first wall of ITER will contain Be, but experiments with these ions cannot be performed. In the present work, we have considered the electron capture reaction:

$$Be^{4+} + H(1s) \rightarrow Be^{3+}(n) + H^{+} \qquad (1)$$

in the energy range 1 keV/u $\leq E \leq$ 100 keV/u. We have calculated the partial cross sections by solving numerically the time-dependent Schrödinger equation with the Grid-TDSE package (GTDSE) [1]. At high velocities, we have also performed classical trajectory Monte Carlo (CTMC) calculations with the hydrogenic initial distribution, similar to those reported in [2].

In contrast to experimental data, which always include estimates of the uncertainties associated to the measurements, theoretical data do not present in general such uncertainties. In the last few years, several initiatives have encouraged data producers to include uncertainty estimates in their data; for instance, the International Atomic Energy Agency (e.g. [3]) has organized several workshops on this subject. In the present work, we have estimated the uncertainties of the GTDSE calculation by considering the convergence with the grid density and those of the CTMC calculation by the convergence of the cross sections with respect to the number of trajectories included in the calculation. At low energy, $E = 1$ keV/u, the molecular calculations of Harel *et al.* [4] indicate that the cross sections for populating the $n = 3$, 4 shells have converged with an absolute uncertainty of ± 0.3 Å^2, and our most precise GTDSE leads to cross sections within this range. As an illustration of the results at high E, we show in Fig. 1 the n-partial cross sections for reaction (1) at two collision energies, where it is clear the good agreement between the close-coupling atomic expansion (AOCC) and the GTDSE method at E = 30 keV/u. At E = 100 keV/u, the application of close-coupling methods is hindered by the need of representing transitions to very excited shells. The competition of the ionization reaction probably causes the unphysical increase of the AOCC cross section for $n > 5$, not shown by the GTDSE and CTMC results.

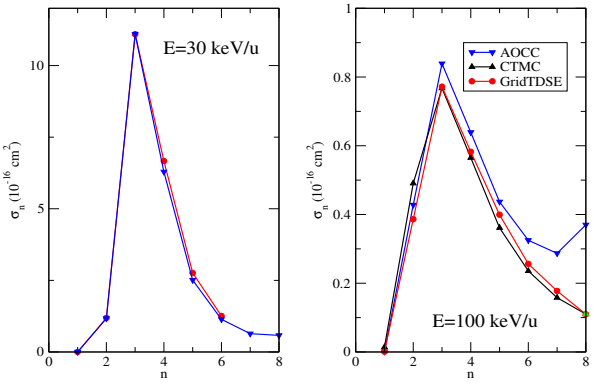

Figure 1. Comparison of state-selected capture cross sections calculated using an atomic expansion [5], the GTDSE method and the CTMC calculation at E =30 and 100 keV/u

References

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