Ionization and excitation of He by antiproton impact

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In the framework of the present STSM significant progress was achieved in the realization of the objectives fixed in the work plan.

A) Calculation of the stopping cross section: The starting point for the calculation of the stopping cross section of antiprotons in He gas target were the fully-correlated time-dependent two-electron wave functions calculated previously for the antiproton-He collisional system [1]. At fixed E_p antiproton energies and b impact parameters, from these wave functions the $P_{i\to f}(E_p, b)$ transition probability from the Ψ_i ground state to the Ψ_f final state was extracted. As final channels the single excitations, single ionization and double ionization were considered. From these probabilities the antiproton energy, and impact parameter dependent stopping power was calculated as

$$S(b, E_p) = \sum\!\!\!\!\!\!\int_f P_{i\to f}(E_p, b)\,[E_f - E_i]\,, \tag{1}$$

while the straggling as

$$T(b, E_p) = \sum\!\!\!\!\!\!\int_f P_{i\to f}(E_p, b)\,[E_f - E_i - S(b, E_p)]^2\,. \tag{2}$$

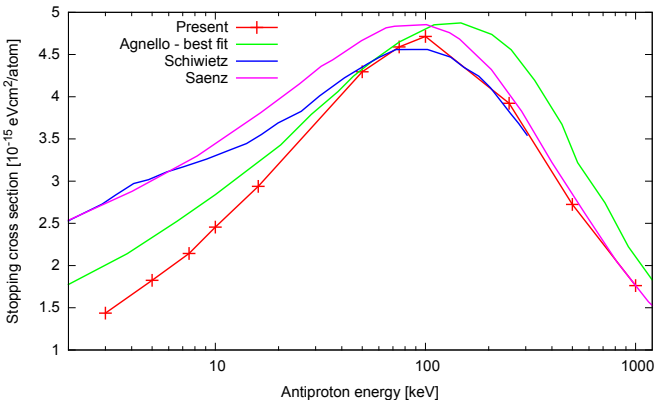

Figure 1: The present stopping cross sections compared to the experimental data [2] and to other theoretical data [3, 4]

From these, the stopping and straggling cross sections were calculated by performing the impact parameter integrations. During the present STSM the calculation of the stopping and straggling cross sections was implemented and the calculations were performed for antiproton impact energies ranging from 3keV up to 1MeV. The obtained fully-correlated two-electron stopping cross sections are shown in Figure (1) along with the experimental data of Agnello *et al* [2] and the theoretical predictions of Saenz *et. al* [3] and Schiwietz *et. al* [4]. At high antiproton energies the agreement between the theories and the experimental data is good, while at low antiproton energies notable discrepancies are present. Since the present results are based on fully-correlated two-electron *ab initio* calculations, they can provide a reference for approximate calculations. The results obtained during the STSM after further analysis will be prepared for dissemination in the form of an article.

B) Electron-electron correlations in the two-particle reduced density matrix (2RDM): From the available fully-correlated two-electron time dependent wave functions [1]

describing the antiproton He collision we have constructed the time-dependent two-electron density matrix (2RDM) $D_{1,2}(r_1, r_2; t)$. We have split the 2RDM into different parts:

$$\text{bound part: } D^{BP}_{1,2}(r_1, r_2; t) = \begin{cases} D_{1,2}(r_1, r_2; t) & \text{if } r_1 < r_{cut} \text{ and } r_2 < r_{cut} \\ 0 & \text{elsewhere} \end{cases}$$

$$\text{singly ionized part: } D^{SI}_{1,2}(r_1, r_2; t) = \begin{cases} D_{1,2}(r_1, r_2; t) & \text{if } r_1 > r_{cut} \text{ and } r_2 < r_{cut} \\ & \text{or } r_1 < r_{cut} \text{ and } r_2 > r_{cut} \\ 0 & \text{elsewhere} \end{cases}$$

$$\text{doubly ionized part: } D^{DI}_{1,2}(r_1, r_2; t) = \begin{cases} D_{1,2}(r_1, r_2; t) & \text{if } r_1 > r_{cut} \text{ and } r_2 > r_{cut} \\ 0 & \text{elsewhere} \end{cases}$$

and we have calculated the ionization probabilities as the integrated 2RDM inside these split regions. For a wide range of r_{cut} values the ionization probabilities calculated this way were in excellent agreement with the ionization probabilities calculated by the projection method used in [1]. This indicates that the outlined method for extracting the single and double ionization probabilities from the 2RDM is a robust one.

Next we have investigated how the two-particle correlation effects are influencing the calculated single and double ionization probabilities. In order to do this, we have calculated uncorrelated two-particle density matrix as $D^{UC}_{1,2}(r_1, r_2) = 0.5 D_1(r_1) D_1(r_2)$, where the single-particle density matrix wave calculated from the correlated two-particle density matrix as $D_1(r_1) = \int dr_2 D_{1,2}(r_1, r_2)$. We found that the single ionization probabilities calculated from $D^{UC}_{1,2}(r_1, r_2)$ are below the exact one, while the double ionization probabilities calculated from $D^{UC}_{1,2}(r_1, r_2)$ are above the exact one. This indicates that the single and double ionization probabilities calculated from single-particle densities (usually provided by density functional approaches) are always containing a notable amount of error due to the neglect of the two-particle correlation effects. It is worth noting that this error can be significantly reduced by following the procedure outlined in [5], but for this the prior knowledge of the fully-correlated ground state is required, which is not always available.

References

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[6] F. Lackner *et. al*, PRA **91** (2015) 023412.