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Antiproton helium collisions in time-dependent density functional theory

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Synopsis We have calculated total cross sections for single and double ionization in antiproton helium collisions over a range of impact energies. Several models for the incorporation of correlation have been explored in the context of time-dependent density functional theory.

Several models for single and double ionization in time-dependent density functional theory (TDDFT) are explored using antiproton helium collisions as a testbed. These models attempt to incorporate correlation effects through two mechanisms. The first pathway through which correlation enters these calculations is through approximation for the correlation potential v_c. The second and arguably more important mechanism by which correlation may be included is through the correlation integral I_c.

Two models for the correlation integral have been explored. The first of these models, the frozen correlation model (FCM), is completely new while the second is an adaptation of an earlier approximation for I_c in the context of laser interactions developed by Wilken and Bauer (WB) [1]. This was previously attempted by Henkel *et al* using a simplified WB model (sWB) [2].

Both of these models require knowledge of the (correlated) helium ground state two-particle density. An approximation for this function is generated using the multiconfiguration Hartree-Fock method (MCHF). This ground state is also used to generate an approximation for the correlation potential v_c.

Figure 1 presents a comparison of the results of FCM and WB models with the sWB as well as all experimental data available for the antiproton helium collision system. While all three of these models are in agreement at high impact energies their differences become apparent as we approach the peak in the experimental data around 80 keV. The differences between the results of the WB and FCM models offer clues to the importance of the explicit inclusion of the ionized final state for the determination of results.

The figure also demonstrates the differences between the full and simplified WB models. It can be seen that the full WB produces a reduction in single ionization over the sWB. It is not until one considers double ionization (not pictured here), where correlation effects become more important, that the full WB exhibit its true potential to out perform the sWB.

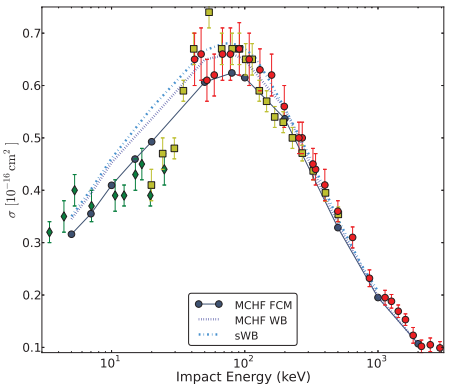

Figure 1. Comparison of single ionization total cross sections of FCM, WB and sWB [2] and experiment: ♦ [3], ■ [4], ● [5]

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