He^+-He collisions described within a time-dependent spin-density functional theory approach

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Synopsis Total cross sections for all electron transfer processes in the He^+-He collision system derived from exact-exchange, time-dependent spin-density functional theory calculations will be presented.

The He^+-He collision system is an interesting benchmark problem for atomic collision theory. If one wishes to obtain accurate results for all channels one is forced to employ a method that properly accounts for all three electrons present on target and projectile. At the same time, a direct solution of the many-electron Schrödinger equation constitutes a massive computational problem.

To properly describe both target and projectile electrons and the spin-polarized nature of the problem we treat the He^+-He system within the time-dependent spin-density functional theory framework making use of the exchange-only approximation. The (time-dependent) exchange potentials can then be determined by applying the Krieger-Li-Iafrate (KLI) approximation to the exact exchange [1, 2].

To be more precise, at each time step of the propagation of the spin orbitals the exchange potentials are calculated by feeding the spin-up and spin-down densities, $n_\uparrow$ and $n_\downarrow$, into the KLI functional $v^\sigma_{\mathrm{KLI}}[n_\uparrow, n_\downarrow]$, where $\sigma = \uparrow, \downarrow$ labels the spin projection. The two-center basis generator method is used for orbital propagation [3].

A variety of outcome processes are possible. These can be broadly categorized into those that involve one active electron:

$$\mathrm{He}^+ + \mathrm{He} \rightarrow \begin{cases} \mathrm{He}^+ + \mathrm{He}^+ + e^- & (p^{11}_{01}) \\ \mathrm{He} + \mathrm{He}^+ & (p^{10}_{01}) \\ \mathrm{He}^{2+} + \mathrm{He} + e^- & (p^{12}_{00}), \end{cases}$$

two active electrons:

$$\mathrm{He}^+ + \mathrm{He} \rightarrow \begin{cases} \mathrm{He}^+ + \mathrm{He}^{2+} + 2e^- & (p^{11}_{02}) \\ \mathrm{He}^{2+} + \mathrm{He}^+ + 2e^- & (p^{12}_{01}) \\ \mathrm{He} + \mathrm{He}^{2+} + e^- & (p^{10}_{02}), \end{cases}$$

and three active electrons:

$$\mathrm{He}^+ + \mathrm{He} \rightarrow \mathrm{He}^{2+} + \mathrm{He}^{2+} + 3e^- \quad (p^{12}_{02}).$$

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Transition probabilitites and total cross sections for these channels are calculated using the determinantal analysis method of [4]. Figure 1 displays the outcome probabilities (weighted by impact parameter) at 60 keV/amu impact energy. The two unphysical channels (p^{12}_{0-1} and p^{1-1}_{02}) with three electrons on the target or projectile are calculated as well, but not presented.

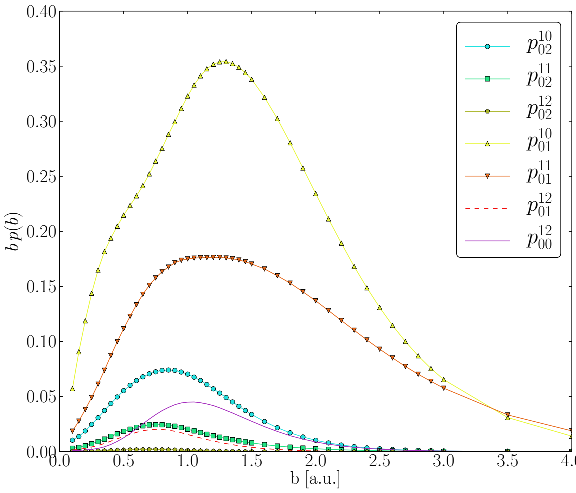

Figure 1. Impact-parameter-weighted probabilities for the seven physical outcome processes plotted as functions of impact parameter for 60 keV/amu He^+-He collisions.

Corresponding total cross sections over a range of impact energies will be presented and compared with measurements and previous calculations at the conference.

References

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