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 \(\nu_{\text{KLI}}[n_\uparrow, n_\downarrow]\), 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:

\[
\begin{align*}
\text{He}^+ + \text{He} & \rightarrow \begin{cases} 
\text{He}^+ + \text{He}^+ + e^- \quad (p_{01}^{11}) \\
\text{He} + \text{He}^+ \quad (p_{01}^{10}) \\
\text{He}^{2+} + \text{He} + e^- \quad (p_{00}^{12}),
\end{cases}
\end{align*}
\]

two active electrons:

\[
\begin{align*}
\text{He}^+ + \text{He} & \rightarrow \begin{cases} 
\text{He}^+ + \text{He}^{2+} + 2e^- \quad (p_{01}^{11}) \\
\text{He}^{2+} + \text{He}^+ + 2e^- \quad (p_{01}^{12}) \\
\text{He} + \text{He}^{2+} + e^- \quad (p_{02}^{10}),
\end{cases}
\end{align*}
\]

and three active electrons:

\[
\begin{align*}
\text{He}^+ + \text{He} & \rightarrow \text{He}^{2+} + \text{He}^{2+} + 3e^- \quad (p_{02}^{12}).
\end{align*}
\]

Transition probabilities 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 \((p_{01}^{12})\) with three electrons on the target or projectile are calculated as well, but not presented.

![Figure 1](image)

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