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Exact time-dependent Kohn-Sham potentials in electron-scattering processes

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Time-dependent density functional theory (TDDFT) is one of the most useful first-principles approaches to study the real-time many-body electron dynamics. However, the validity of its application to the electron-scattering processes has not been clear because of the lack of knowledge whether the current available exchange-correlation (XC) functional is reliable for such situations. In this study we have computed the exact time-dependent Kohn-Sham potential in the one-dimensional two-electron scattering system that models electron - hydrogen scattering. We will present the analysis of them and the idea how to refine their approximation.

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