

Potentials that Exactly Capture Correlated Electron and Ion Dynamics in Strong Fields

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The study of electron dynamics far from the ground-state is of increasing interest today in many applications: attosecond control and manipulation of electron and consequent ion dynamics, photovoltaic design, photoinduced processes in general. Time-dependent density functional theory is a good candidate by which to computationally study such problems. Although it has had much success in the linear response regime for calculations of excitation spectra and response, its reliability in the fully non-perturbative regime is less clear, although increasingly used. By studying some exactly-solvable models of charge-transfer dynamics and strong-field processes, we find that the exact correlation potential of time-dependent density functional theory develops stark features in time that are missed by the currently available approximations. We discuss these features and their implications for charge-transfer dynamics and time-resolved spectroscopy. In the second part of the talk, we broaden our focus to the description of coupled electron-ion motion. When the coupling to quantum nuclear dynamics is accounted for, we find additional terms in the potential acting on the electronic subsystem, that fully account for electron-nuclear correlation, and that can yield significant differences to the traditional potentials used when computing coupled electron-ion dynamics. We study such potentials for the phenomena of field-induced electron localization, and charge-resonance enhanced ionization, within the exact-factorization approach to coupled electron-ion dynamics.

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