NEW YORK CITY COLLEGE OF TECHNOLOGY
Physics Department
Center for Theoretical Physics

Capturing Correlated Electron and Ion Dynamics in Strong Fields

Presented by:

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Abstract

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 strongly non-adiabatic and spatially non-local features in time that are missed by the currently available approximations. We discuss these features and their implications for charge-transfer dynamics. 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.

Light refreshments will be served.