CFEL SCIENCE

SEMINAR

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ZOQ (bldg. 90), seminar room

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Multielectron dynamics in intense laser fields

Exposed to intense laser pulses, atoms and molecules exhibit highly nonlinear response such as above-threshold and tunneling ionization, high-order harmonic generation (HHG), and nonsequential double ionization. These have opened new research possibilities including ultrafast molecular probing, attosecond science, and extreme-ultraviolet nonlinear optics.

Theoretical description of atoms and molecules in intense laser fields is challenging. Direct solution of the time-dependent Schrödinger equation, though exact in principle, is unfeasible for multielectron systems beyond He [1-3] and H_2.

Here we present the time-dependent complete-active-space self-consistent-field (TD-CASSCF) method [4]. It introduces the concept of frozen-core, dynamical-core, and active orbital subspaces. The classification into the subspaces can be done flexibly, according to simulated physical situations and desired accuracy, and the time-dependent Hartree-Fock (TDHF) and the multiconfiguration TDHF (MCTDHF) approaches are included as special cases. This feature allows compact yet accurate representation of ionization dynamics in many-electron systems, bridging the huge gap between TDHF and MCTDHF methods.

We show and discuss the simulation results for the ionization dynamics and HHG in one-dimensional lithium hydride (LiH), LiH dimer [$(LiH)_2$], and beryllium (Be) models. The present method closely reproduces rigorous MCTDHF results if active orbital space is appropriately chosen. The TD-CASSCF method will open a way to the first-principle theoretical study of intense-field induced ultrafast phenomena in realistic atoms and molecules.

[1] K. L. Ishikawa and K. Midorikawa, Phys. Rev. A **72**, 013407 (2005).
[2] K. L. Ishikawa and K. Ueda, Phys. Rev. Lett. **108**, 033003 (2012).
[3] S. Sukiasyan, K. L. Ishikawa, and M. Ivanov, Phys. Rev. A **86**, 033423 (2012).
[4] T. Sato and K. L. Ishikawa, Phys. Rev. A **88**, 023402 (2013).

Hosts: Franz Kärtner and Shaobo Fang, CFEL