Time-dependent density functional theory in real time and real space: Application to electron dynamics in laser fields

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Electron dynamics in nanometer-sized molecules and nanostructured materials is an intrinsic process related to a number of interesting phenomena such as linear and nonlinear optical response, electrical conduction, and also chemical reaction. Despite their importance, theoretical understanding of electron dynamics is still in a juvenile stage. This is mainly due to the fact that it is difficult to treat the dynamical processes of a correlated many-electron system. Time-dependent density-functional-theory (TDDFT) is one of the promising theoretical approaches to reveal details of the electron dynamics. We have developed a computational method simulating the electron dynamics in real time and real space on the basis of TDDFT, and elucidated the dynamics in laser field.

I will first review the basic idea of TDDFT and show the computational results of photoinduced electric currents in ring-shaped molecules by circularly polarized laser pulse, high harmonic generation from C_{60}, and inhomogeneous electronic excitation by near-field radiation.

[1] "*Quantum Theory of the Electron Liquid*", G. F. Giuliani and G. Vignale, (Cambridge Univ. Press, 2005).

[2] "*Photoinduced electric currents in ring-shaped molecules by circularly polarized laser pulses*", K. Nobusada and K. Yabana, Phys. Rev. A **75**, 032518-1-032518-7 (2007).