Correlated many electron dynamics from different perspectives

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In this talk various approaches to the correlated quantum dynamics of electrons in atoms and molecules are discussed. We do so by solving the Time-Dependent Schrödinger Equation with first principle methods for several systems. The emphasis is on wave function based methods, especially Multi-Configuration Time-Dependent Hartree-Fock(MCTDHF). Selected applications, like the controlled manipulation of the electronic state of LiH, and the onset of thermalization of electrons in Na_8 clusters, serve to illustrate the opportunities and challenges of first principles electron dynamics. Also, the relation to Configuration Interaction based methods, and ansaetze to go beyond the fixed nuclei approximation are presented.

1] The Multi-Configuration Electron-Nuclear Dynamics Method, M. Nest, Chem. Phys. Lett. **472**, 171 (2009)
[2] Ultrafast electronic excitations of small sodium clusters and the onset of electron thermalization, T. Klamroth, M. Nest, PCCP **11**, 349 (2009)
3] Laser SteeredUltrafastQuantumDynamicsof Electrons in LiH,F. Remacle M. Nest, and R.D. Levine, Phys. Rev. Lett. **99**, 183902 (2007)