Real-time propagation of coupled Maxwell-Kohn-Sham systems

Based on a recent extension of time-dependent density functional theory to Quantum electrodynamics [1], we show first steps of an implementation of Maxwell's equations coupled to time-dependent Kohn-Sham equations. Our implementation utilizes the Riemann-Silberstein vector of the electromagnetic field which allows to write Maxwell's equations in a symplectic spinor representation similar to the Dirac equation. This spinor representation allows us to use standard unitary propagation techniques [2] developed for the solution of the Schroedinger equation. Our implementation in the real-space real-time code octopus [3] allows to propagate the Maxwell and Kohn-Sham systems with electrical dipole, magnetic dipole and electrical quadrupole couplings. As first application, we investigate dipole radiation characteristics and electromagnetic near-field effects for jellium spheres [4].

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$[2]$ A. Castro et al., J. Chem. Phys. \textbf{121} (2004).
$[3]$ X. Andrade et al., J. Phys. Cond. Mat. \textbf{24} (2012).
$[4]$ M. Brack, Rev. Mod. Phys. \textbf{65}, 677 (1993)