Real-time propagation of coupled light-matter systems

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Modern free electron lasers produce pulses on a timescale of femtoseconds and wavelengths of few nanometers. This experimental progress opens new frontiers for understanding the dynamics of molecules under extreme conditions. A particular challenge for theorists is the development of new theoretical and computational tools for the investigation of non-equilibrium dynamics of large coupled light-matter systems under such conditions. Here, the quantum nature of both the electronic and the photonic part cannot be omitted.

By solving the full relativistic quantum electrodynamics (QED) on a non-pertubative level as a lattice-field theory we investigate real-time dynamics of coupled electron-photon-systems. In the current work we present our first numerical results in this framework. Using the Riemann-Silberstein vector, we describe not only the electrons but also the photons with their wave function [1]. We show wave-packet dynamics for electrons and photons and investigate effects such as pair annihilation and Compton scattering in real-time. These solutions serve as exact numerical reference calculations for the construction of novel functionals in the recently established density-functional theory for QED [2].

In the non-relativistic limit, we present first steps of an implementation of Maxwell's equations coupled to time-dependent Kohn-Sham equations. Also here we utilize the Riemann-Silberstein vector of the electromagnetic field which allows us 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 [3] developed for the solution of the Schrödinger equation.

Our implementation in the real-space real-time code octopus [4] 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 [5].

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