Real-time propagation of coupled Maxwell-Schrödinger systems

René Jestädt, Heiko Appel, and Angel Rubio

The interaction of electromagnetic fields and matter play a prominent role in many processes in nature and technology. Examples include photosynthesis, photo-chemical reactions, or solar cells.
Most studies in the literature neglect the quantum character of the electromagnetic field and only classical electric and magnetic fields interacting with electronic many-body systems are considered.
A standard method to numerically solve the classical electromagnetic field in arbitrary geometries, and for external current and density sources is the Yee algorithm [1], which is based on a finite-difference discretization on a real-space mesh for the electric field and a shifted mesh in spacetime for the magnetic field. To simulate open systems with finite grid domains and to incorporate absorbing boundary conditions, Berenger introduced a method for a perfectly matched layer [2].
Since the Maxwell equations and have a symplectic structure and are first order in time, it is possible to transform them by using the Rieman-Silberstein vector [3] into a matrix spinor representation similar to the Dirac equation [4]. Such a spinor representation is advatageous for a coupled propagation of Maxwell's and Schrödinger's equations. In our present work we use unitary propagation techniques developed for the Schrödinger equation [5] in order to propagate the Rieman-Silberstein vector with perfeclty matched layer boundary conditions. We compare this novel way of propagating Maxwell's equations with the standard Yee algorithm.
Furthermore, in the stationary limit the Maxwell matrix spinor representation determines the eigenvalues and eigenmodes of classical electromagnetic fields for arbitrary geometry and matter distributions. These eigenvalues and eigenmodes are an essential input for a quantized description of the electromagnetic field. We use this mode description of the quantized field to develop correlation potentials for a time-dependent density functional theory formulation of quantum electrodynamics.

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