Kohn-Sham Approach to Cavity Quantum Electrodynamics

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Time-dependent density functional theory (TDDFT) has been successfully applied to a large variety of problems, such as studies of absorption spectra, excitation energies, or dynamics in strong laser fields. On the other side, many-body perturbation theory (MBPT) opens the possibility to construct approximations to every desired order of a 'weak' interacting system. Here, the drawback is a in general non-local interaction in space and time and it is therefore a demanding task to apply it to 'real' systems. Recently, we and our collaborators have generalized TDDFT to also describe electron-photon systems (QED-TDDFT) [1,2]. Here, matter and light are treated on an equal quantized footing.

The optimized effective potential (OEP), derived by inversion of the Sham-Schlüter equation, is a natural connection between local density-functional theory and MBPT. In principle, this variationally best local potential reduces the problem to solving a simple system of Kohn-Sham equations combined with the solution of the OEP integral equation. However, converging the full set of OEP equations is quite challenging and is in practice rarely tackled. The Krieger-Li-Iafrate (KLI) approximation reduces the integral equation to an analytically solvable one via a dominant orbital approximation.

In this work, we present the first numerical calculations in the framework of QED-TDDFT. We show exact solutions for fully quantized prototype systems consisting of atoms or molecules placed in optical high-Q cavities and coupled to quantized electromagnetic modes, both for model systems heavily used in Quantum Optics, as well as for real-space systems. We focus on the electron-photon xc-contribution by calculating exact Kohn-Sham potentials in real-space using fixed-point inversions and present the performance of the first approximated xc-potential based on an optimized effective potential (OEP) approach for a Jaynes-Cummings-Hubbard Dimer [3]. Furthermore, we extend the OEP and KLI approaches to the case of electron-photon interactions in quantum optics and quantum electrodynamics. Here an effective electronic interaction is transmitted via transversal photons. We present first static and time-dependent results for the OEP [3] and KLI approximations of the Rabi and 1D-hydrogen model and compare with the exact configuration-interaction solution and the corresponding exact Kohn-Sham potentials [2].

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