

Kohn-Sham Approach to Cavity QED: Exact vs. Approximate Effective Fields

Johannes Flick [1]
Camilla Pellegrini [2]
Michael Ruggenthaler [3,4]
Heiko Appel [1,4]
Ilya V. Tokatly [2,5]
Angel Rubio [1,2,4]

[1] Fritz-Haber-Institut der MPG, Berlin

[2] Nano-bio Spectroscopy Group/ETSF Scientific Development Centre, Departamento de Fisica de Materiales, Universidad del Pais Vasco UPV/EHU, San Sebastian

[3] Universität Innsbruck

[4] MPI for the Structure and Dynamics of Matter, Hamburg

[5] IKERBASQUE, Basque Foundation for Science, 48011 Bilbao

In the last decade, time-dependent density functional theory (TDDFT) has been successfully applied to a large variety of problems, such as calculations of absorption spectra, excitation energies, or dynamics in strong laser fields. 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.

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].

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[3] C. Pellegrini et.al., arXiv:1412.4530 (2014).