

Title:

Krieger-Li-Iafrate approximation to the optimized effective potential approach in density functional theory for quantum electrodynamics

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Abstract:

Many-body perturbation theory (MBPT) opens the possibility to construct approximations to every desired order of a 'weak' interacting system. 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.

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 a quite challenging procedure 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. It performs usually quite well for electronic systems.

In the present work, 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 [1] 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]

References:

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

[2] M. Ruggenthaler et.al., Phys. Rev. A 90, 012508 (2014).