Significance of vertex-corrections on the interface between non-equilibrium greens functions and time-dependent density-functional theory for cavity quantum electrodynamics

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With the consistent improvement of experimental and theoretical techniques for quantum electrodynamics on chemical scales, this novel connection presents in the mean-while a fascinating and realistic knob to modify chemical reactions using quantized transversal light interacting to matter. While the incorporation of the additional photonic contribution is straight forward in many-body perturbation theory, novel efficient reformulations such as quantum electrodynamic density functional theory suffer from the typical lack of sufficient functionals. This settings, makes the investigation at the interface between them a pivotal domain of interest, communicating between accuracy and efficiency and unraveling the impact of quantum nature. Within this work, we present different levels of approximations of the time-dependent optimized effective potential (TDOEP) for the interaction between matter and light. We do so, by setting the TDOEP in context to simplifications along the line of the time-dependent Krieger-Li-Iafrate approximation (TDKLI), classical Maxwell descriptions but also extension along the line of a consistent GW approximation. By discussion of computational feasibility and intrinsic physical drawbacks, we tackle the question which route is promising, paving the way for further developments. By comparison to exact results, we address the significance of vertex-corrections, emerging for resonant light-matter interaction. We will observe, that a sufficiently accurate photon-propagator can indeed capture the correct physical behavior for all reasonable light-matter couplings, implying that the vertex is indeed not of essential importance.

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