Optimized Effective Potential for Quantum Electrodynamical Time-Dependent Density Functional Theory

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Recently, we and our collaborators have extended time-dependent density functional theory (TDDFT) to electronic systems coupled to quantum electromagnetic fields [1, 2]. Merging electronic structure theory and quantum optics, the new QED-TDDFT formalism opens up to a first-principles description of the quantum dynamics of many-body electron-photon systems. Potential applications involve many areas of experimental interest (e.g. cavity and circuit QED, quantum computing, quantum plasmonics etc.), but require suitable approximations to the electron-photon exchange-correlation (xc) functional. Here, we construct the first approximation to such xc-functional by extending the optimized effective potential (OEP) approach to the photon-mediated electron-electron coupling. The (TD)OEP equation for the electron-photon system is derived in the form of the linearized (time non-local) Sham-Schlüter equation on the Keldysh contour. We illustrate the formalism with a simple yet non-trivial example, i.e. the two-site Hubbard model for the H_2^+ molecule coupled to one photon mode (the well-known Rabi model in quantum optics) from the weak to the ultrastrong coupling regime. The electron-photon (TD)OEP for the model clearly improves over the classical treatment of the electromagnetic field, providing a promising path for describing complex strongly coupled matter-photon systems.

[1] I. V. Tokatly, Phys. Rev. Lett. **110**, 233001 (2013).
[2] M. Ruggenthaler, J. Flick, C. Pellegrini, H. Appel, I. V. Tokatly and A. Rubio, Phys. Rev. A **90**, 012508 (2014).

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