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Light-matter coupling in density-functional theory for quantum electrodynamics (I)

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Recently, ground-state and time-dependent density-functional theory have been extended to include the interaction with photons from first principles. This so-called quantum-electrodynamical density-functional theory (QEDFT) treats light and matter on equal quantized footing and provides a bridge between high-energy physics, quantum chemistry, and quantum optics. QEDFT allows deriving numerically feasible approximations for a novel class of physical situations, where the matter and photon degrees of freedom are equally important. In the first part of this sequence of presentations, we illustrate the basic ideas of how light-matter coupled quantum systems allow for a reformulation in terms of the charge current (of the particles) and the vector potential (of the photons). To find reasonable approximations to the unknown functionals we introduce an auxiliary uncoupled Kohn-Sham system with effective potentials. For the standard situation of cavity QED, i.e. dipole coupling, we present first approximations to the resulting effective potential that take the explicit coupling to the photons into account. We conclude this part with an outlook on field-theory, multi-mode and free-space problems.

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