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Title: Electron-Photon Exchange-Correlation Functional in the Weak and Strong Light-Matter Coupling Regimes

Abstract: The intersection of quantum electrodynamics (QED) and density-functional theory (DFT) has opened up exciting opportunities in controlling quantum matter through light-matter coupling. This frontier, however, is beset with computational challenges, especially in the weak and strong coupling regimes. Building upon previous research, we present the results of nonperturbative QED functional in the long-wavelength limit, centered solely on the matter Hilbert space. This novel approach accurately reproduces QED's exact results in strong coupling, offering enhanced accuracy and computational efficiency. In this study, we present the results of this electron-photon exchange-correlation functional to facilitate QEDFT calculations in the weak and strong coupling regime, bridging the gap between quantum mechanics and quantum electrodynamics. Using this approach, we explore the energy and electronic density of polaritonic states, comparing our results with QED coupled cluster and optimized effective potential (OEP) calculations for a range of molecules and intermolecular interactions. Our findings shed light on the compatibility of this functional with practical applications and provide a promising avenue for exploring quantum matter control in light-matter coupling.