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

Thursday 2 June 2016 17:50 (25 minutes)

In the second part of our presentation of QEDFT, we illustrate effects that appear in the strong-coupling regime of matter with cavity photons. In particular, we show how Born-Oppenheimer surfaces are modified in the presence of the cavity, discuss photon bound states, and analyze polariton splittings in molecular absorption spectra. As illustrated in part (I), the density-functional approach to quantum electrodynamics is formally an exact framework. Here we show by inversion of the exact many-body solution of the time-dependent Schrödinger equation for a quantum dot system the exact time evolution of the effective potential of the Maxwell-Kohn-Sham system in QEDFT and analyze this in terms of a cavity Born-Oppenheimer approximation. We compare these exact results with the first approximate functional of QEDFT which is based on an optimized-effective-potential approach for the coupled matter-photon system. To go beyond model systems, we introduce a Riemann-Silberstein formulation of Maxwell's equations and present the first ab-initio real-time propagations of the coupled Maxwell-Kohn-Sham equations for molecular systems.

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