Ab-Initio Description of Photoinduced Processes Beyond Classical Maxwell Theory

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In common methods for the ab-initio description of photoinduced processes such as the visual process, photosynthesis or solar cells, typically the classical Maxwell's equations are employed to describe the propagation of light. The applicability of these equations has been demonstrated since decades for a wide range of physical phenomena and parameter regimes. However, considering the ultimate limit of single molecules interacting with a few photons, the classical description of the electromagnetic field does not suffice anymore. In this case the quantum nature of the electromagnetic field has to be taken into account and therefore existing ab-initio approaches have to be extended.
In the present work we face the question: Whether and what changes in the analysis and simulation of photoinduced processes by going beyond the classical Maxwell description. Here the idea of the exact factorization [Abedi et. al., Phys. Rev. Lett. 105, 123002], introduced for electron-nuclear problems, will be generalized to electron-photon systems, by considering the Maxwell-equations as Ehrenfest limit for quantum electrodynamics. We apply our novel approach to spontaneous and stimulated emission for atoms and molecules in optical cavities.

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