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CFEL-bldg. 99, seminar room IV

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Ab-initio non-relativistic quantum electrodynamics: Bridging quantum chemistry and quantum optics from weak to strong coupling

The creation of novel states of matter, e.g., by application of periodic driving or incorporation of matter into a strongly coupled cavity, is a vastly expanding field. Experimental advances allow the manipulation of chemical reactions and individual components. Theoretical investigations in this frame-work of non-relativistic quantum electrodynamics (QED) are however often treated in an ad-hoc approach, neglecting important constituents for qualitatively correct predictions.

By applying the Born-Huang expansion, we deduce an exact set of coupled equations for electrons on photonic energy surfaces and the nuclei on the resulting polaritonic energy surfaces. Since the photonic surfaces and the corresponding non-adiabatic coupling elements can be solved analytically, the resulting expansion can be brought into a compact form which allows us to analyze aspects of coupled nucleus-electron-photon systems in a simple and intuitive manner. Furthermore, we discuss structural differences between the exact quantum treatment and Floquet theory, highlight, by assuming that the relevant photonic frequencies of a prototypical cavity QED experiment are in the energy range of the electrons, how from this generalized Born-Huang expansion an adopted Born-Oppenheimer approximation for nuclei on polaritonic surfaces can be deduced. Furthermore, we bridge quantum chemistry and quantum optics and finally highlight numerically that simple few-level models can lead to physically wrong predictions, even in the weak coupling regime, and show how the presented derivations from first principles help to check and derive physically reliable simplified models.