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Exact factorization approach to coupled electron, ion and photon dynamics

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Whether perturbed away from the ground state, or driven by either classical or quantized light, the dynamics of molecules involves a complex interplay of electronic and nuclear motion taking place in a landscape of a multitude of Born-Oppenheimer potential energy surfaces. Yet, often one is interested in just one of the subsystems, either the electronic motion (e.g. in charge-transfer or ionization dynamics), or the nuclear motion (e.g. in chemical reactions), or the photonic system (e.g. in superradiance). Can one then define a Schroedinger equation for the subsystem of interest, in which the potentials contain all the coupling to the other subsystems exactly? This talk discusses the recent "exact factorization approach", which answers this affirmatively. The original theory was formulated for the electron-nuclear problem, for which I will present the formalism and some examples. I then extend this to the light-matter interactions in cavity-QED, finding the exact potential that drives the photonic dynamics. Open issues regarding the mathematical structure and numerical stability of the exact factorization equations will be raised.

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