Correlated electron-ion dynamics for resonant systems

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Quantum coherence between electronic and nuclear dynamics, as experimentally observed in organic semiconductors, is the object of an intense theoretical and computational effort. In particular, to simulate this kind of quantum coherent dynamics, I have introduced [1] a suitable numerical scheme based on Correlated Electron-Ion Dynamics (CEID). In this talk, I describe a further generalization of CEID [2] and its practical numerical implementation [3]. To illustrate the capability of this extended CEID scheme, I also present a detailed investigation of a model system which displays the electron-phonon analog of the optical Rabi oscillations. Finally, I discuss convergence and scaling properties of the extended CEID scheme along with its applicability to more realistic systems, e.g., the ultrafast nonradiative decay of photoexcited conjugated polymers [4].

[1] L. Stella *et al.*, J. Chem. Phys. **127**, 214104 (2007)
[2] L. Stella *et al.*, J. Chem. Phys. **134**, 194105 (2011)
[3] https://bitbucket.org/lstella/polyceid
[4] E.J. McEniry *et al.*, Eur. Phys. J. B **77**, 305–329 (2010)