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Far out-of-equilibrium dynamics and time-resolved spectra: the non-perturbative Boltzmann equation

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Ultrafast excitation and sub-picosecond probing of dynamics in materials have allowed for the discovery of a number of exciting and unexpected effects. A system evolving strongly out of equilibrium has a much larger amount of degrees of freedom compared to the same system evolving close to equilibrium. It is also often the complex interplay of out-of-equilibrium transport, scatterings within different quasiparticles and interaction with transient electromagnetic fields that generate the emergence of exciting phenomena. This implies that to fully grasp such dynamics it is often essential to theoretically treat all the possible involved dynamics and move away from perturbative treatments. This problem is extremely challenging. The full Boltzmann equation (different from its many approximations that go by the same name) can describe to a very high degree of precision scatterings (constructed as in the quantum Fokker-Planck equation), transport, and interaction with fields.

From the numerical point of view, the full Boltzmann equation (BE) is rather challenging, as it is a high dimensional problem. Transport and interaction with fields within the BE have been already addressed and very efficient numerical algorithms are available. The scattering term is however, if approached without approximations, a prohibitive task.

We developed a very efficient numerical algorithm that allows us to do full time propagation of the scattering term (as well as transport and interaction with fields) of the BE. [1-3] We can predict ultrafast dynamics in solids far from equilibrium (see figure). Interestingly the same machinery can produce spectra and time resolved spectra to a rather high precision. [4]

[1] F. R. Bagsican et al, Nano Lett. 20, 3098 (2020)
[2] M. Wais et al, Comput. Phys. Commun. 264, 107877 (2021)
[3] I. Wadgaonkar et al, Comput. Phys. Commun. 263, 107863 (2021)
[4] S. Dal Forno et al. manuscript

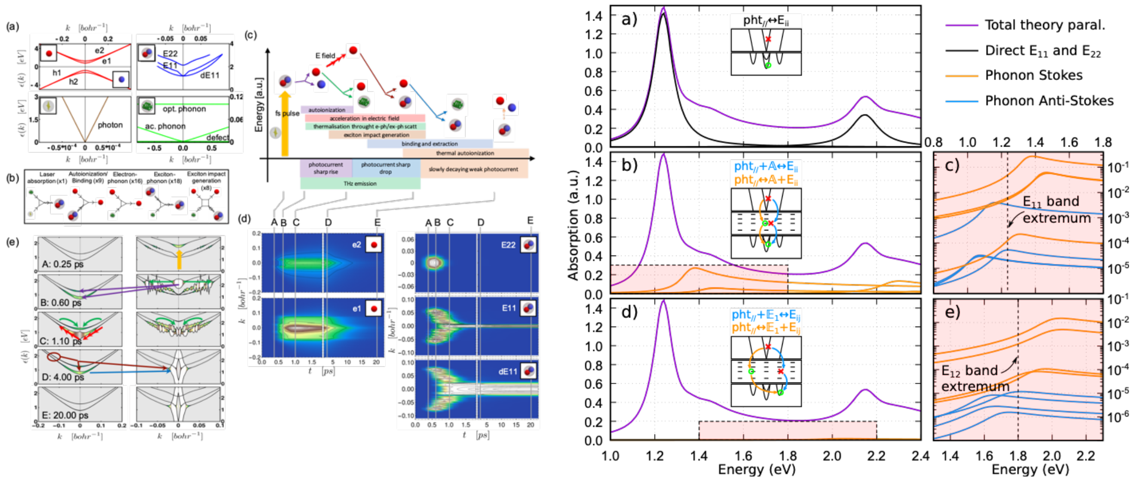

Figure 1 : (Right) Simulation of ultrafast dynamics in carbon nanotubes with the inclusion of 52 scattering channels and electric field. [1] (Left) Optical absorption spectra of carbon nanotubes. [4]