SFB 767
Seminar

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P 602

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Spatiotemporal evolution of inhomogeneous wave packets

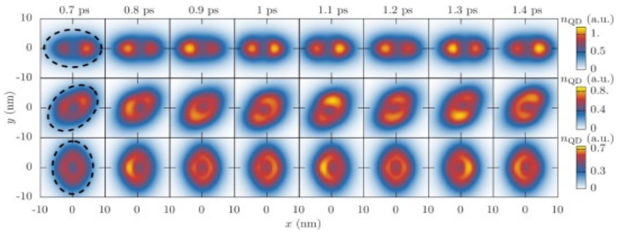

Fig. 1: Spatiotemporal dynamics of the charge which is captured by emission of optical phonons from a travelling wave packet into a differently oriented 0D potential (sketched as dashed line)

Inhomogeneous electronic wave packets describe a nanometric localization of electrons (obtainable, e.g., by near field spectroscopy) [1]. Their evolution could describe travelling electrons and may thus be important in several fields, e.g., in quantum information as flying qubits [2]. The initial localization is made possible by the presence of strong interstate coherences, but may be lost during the evolution due to both coherent and incoherent phenomena, i.e., a coexistence of different group velocities and the scattering mechanisms, respectively. A proper description of the evolution of nanometric wave packets must catch the interplay between coherent and dissipative dynamics: For this purpose, we employ the (off-diagonal) density matrix formalism and account for scattering mechanisms by alternative Markov approaches [3,4], which are able to combine accurate predictions, flexibility and computational feasibility (despite the presence of the off-diagonal density-matrix elements). With these treatments, we examine different nanodevices to show different phenomena associated with an initial confinement: (i) in conventional parabolic materials, a scattering-induced loss of spatial shape due to the so-called scattering nonlocality and scattering-induced diffusion [5]; (ii) in metallic nanotubes, a shape-preserving dispersionless propagation (up to micrometers also at room temperature) [6]; finally, (iii) in 2D TMDC monolayers embedding 0D confinement potentials (obtainable, e.g., by means of strain [7] or gating [8]), a spatial control of the nontrivial spatiotemporal dynamics of the charge, which is captured in the 0D potential from the travelling wave packet due to electron-phonon scattering [9] (see Fig. 1).

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