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Phonon-induced dynamics of electrons and excitons in solids driven out-of-equilibrium by strong laser pulses: an Ab-Initio approach

Ultra–fast optical spectroscopy [1] is a powerful tool for the observation of dynamical processes in several kind of materials. The basic time–resolved optical experiment is the so-called pump-probe: a first light pulse, the pump, resonantly triggers a photo-induced process. The subsequent system evolution can be monitored, for example, by the time–dependent transmission changes of a delayed probe pulse. The pump pulse photon energy, spectral width and peak intensity creates a certain density of electron-hole pairs in a more or less localized region of space. After the creation of the initial carrier density the time evolution of the single–particle and many–particle excitations is now governed by a non-trivial interplay between electron–electron scatterings and energy relaxation [2, 3]. Dephasing will be driven by different phenomena. One of the most important is the energy transfer to the atomic motion in form of phonon excitations [2]. In this talk I will present a novel approach based on the merging of Non-Equilibrium Green's function theory [4] and Density Functional Theory[5] to treat static electronic correlations [6] and dynamical phonon–mediated relaxation[7, 8] following the pump excitation. I will discuss key theoretical and methodological aspects showing how the full memory dependence of the electron–phonon kernel can be turned in an efficient iterative procedure [8]. I will also show that the present theory successfully describes two kind of paradigmatic experiments: the time–resolved absorption of solid GaAs and the time–resolved two–photon photoemission of bulk Silicon. I will also predict that a strong laser pulse resonant with the first bound exciton of bulk h–BN will cause its collapse due the combined effect of the Pauli blocking and intra–band screening [8].

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