Phonon-induced quantum diffusion in semiconductors

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Semiclassical-transport modeling strategies —grounded on the neglect of carrier phase coherence— have been successfully employed for the investigation of new-generation semiconductor nanodevices [1]; they are however unable to properly describe space-dependent ultrafast phenomena, in which quantum effects play a central role. To this aim, several approaches —ranging from phenomenological dissipation/decoherence models to quantum-kinetic treatments— have been proposed. In particular, a conceptually simple as well as physically reliable quantum-mechanical generalization of the conventional Boltzmann theory has been recently put forward [2]. The latter preserves the power and flexibility of the semiclassical picture in describing a large variety of scattering mechanisms; more specifically, employing a microscopic derivation of generalized scattering rates based on a recent reformulation of the Markov limit [3], a Lindblad-like density-matrix equation has been derived, able to properly account for space-dependent ultrafast dynamics in semiconductor nanostructures.

Primary goal of this contribution is to discuss and further expand the preliminary study of scattering-induced quantum diffusion in GaN-based nanomaterials reported in Ref. [4]; To this aim, as physical system we consider an effective one-dimensional GaN-based nanostructure, whose main energy-dissipation/decoherence mechanism is carrier-LO phonon scattering. In our simulated experiments we have chosen as initial condition a single-particle density matrix corresponding to a gaussian carrier distribution both in space and momentum, namely

$$\overline{n}(z) \propto \frac{e^{-\frac{z^2}{2\overline{\Delta}_z^2}}}{\sqrt{2\pi}\,\overline{\Delta}_z}\ , \qquad \overline{n}(p) \propto \frac{e^{-\frac{p^2}{2\overline{\Delta}_p^2}}}{\sqrt{2\pi}\,\overline{\Delta}_p}\ , \qquad (1)$$

where $\overline{\Delta}_z$ describes the degree of spatial localization of our initial state, and $\overline{\Delta}_p = \sqrt{m^* k_B T}$ describes the thermal fluctuations of our carrier gas.

Goal of our simulated experiments is to investigate the non-local character of the proposed Lindblad scattering superoperator, and to compare it with the well-known and widely employed relaxation-time approximation.

Figure 1 displays the sub-picosecond time evolution of the spatial carrier density obtained in the absence of carrier-phonon coupling (upper panel), via the proposed Lindblad scattering superoperator (central panel), and via the relaxation-time model (lower panel). As we can see, compared to the scattering-free case (upper panel), both Lindblad and relaxation-time treatments give rise to a speed up of the diffusion process, and the effect is more pronounced in the relaxation-time case (lower panel). This scenario is fully confirmed by analyzing the effective spatial-distribution width λ as a function of time reported in the upper panel of Fig. 2.

Finally, our simulated experiments have shown that the failure of the relaxation-time model becomes particularly severe for quasielastic scattering processes; this conclusion is fully confirmed by the results reported in the lower panel of Fig. 2, where, in order to mimic the quasielastic limit, the LO-phonon energy has been reduced to 20 meV.

REFERENCES

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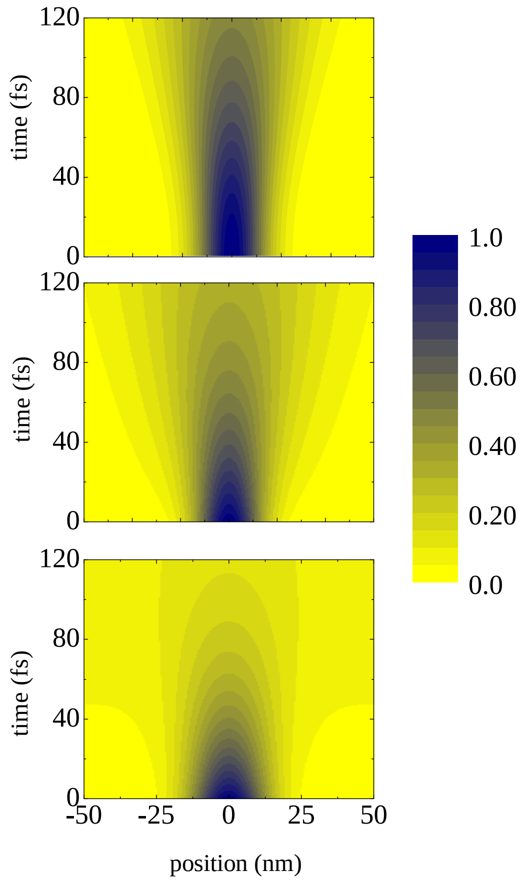

Fig. 1. Room-temperature quantum-diffusion dynamics in a GaN bulk system obtained in the absence of carrier-phonon coupling (upper panel), via the proposed Lindblad scattering superoperator (central panel), and via the relaxation-time model (lower panel): sub-picosecond time evolution of the spatial carrier density corresponding to the initial distribution in (1) with $\overline{\Delta}_z = 10\,\mathrm{nm}$ (see text).

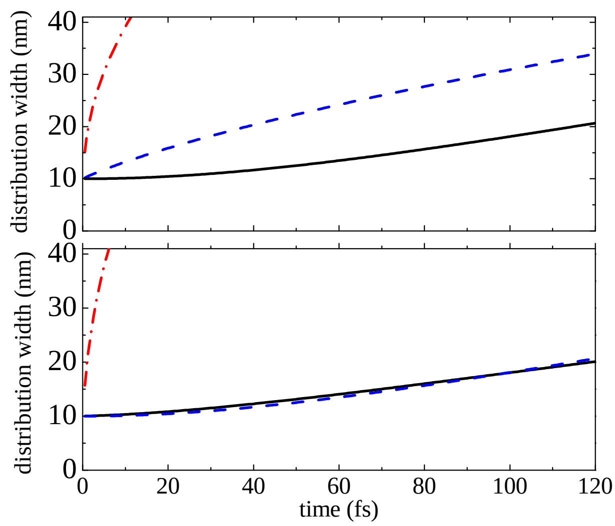

Fig. 2. Effective spatial-distribution width λ as a function of time for a LO-phonon energy of $80\,\mathrm{meV}$ (upper panel) and $20\,\mathrm{meV}$ (lower panel). Here, the scattering-free result (solid curve) is compared to the corresponding results obtained adopting as scattering models the Lindblad superoperator (dashed curve) as well as the relaxation-time model (dash-dotted curve) (see text).