P:22 Lindblad-based Markov approach to spatiotemporal quantumdynamics of wave packets in nanostructures

F Lengers, R Rosati, T Kuhn and D E Reiter

Universität Münster, Germany

The ultrashort time and length scales involved in carrier dynamics like carrier capture or ultrafast and highly localized optical generation inside a nanostructure call for a suitable quantum mechanical treatment of the dynamics. Fully quantum mechanical treatments like quantum kinetic approaches [1] describe these processes very well, but are limited to low-dimensional systems or systems with suf- ficiently high symmetry as well as rather short times. Those limitations result from the computational complexity as well as from instabilities due to interference phenomena of the dynamical variables. Those problems call for a suitable approximation scheme. We here introduce a Lindblad single- particle (LSP) equation of motion, which is obtained by a proper tailoring [2] of the superoperator provided by a recently introduced Markov approach [3,4]. Although in general nonlinear, the latter is still able to preserve the positivity of the density matrix in any circumstance, in contrast to conven- tional Markov approximations [4].

In this contribution we will discuss the dynamics of traveling wave packets in a semiconductor quan- tum wire with an embedded quantum dot under the influence of carrier-light, carrier-carrier and carrier-phonon interaction. During the local optical excitation localized electron and hole wave pack- ets are generated. Because of the spatial localisation, the description of the wave packet dynamics in the density matrix formalism includes both occupations of the quantum wire states and coher- ences between the states, i.e. diagonal and off-diagonal elements of the density matrix. The excited electron and hole wave packets then travel along the quantum wire with velocities depending on the respective effective masses and excess energy of the optical pulse whilst being subject to interac- tions. These interaction processes lead to transitions between the quantum wire states, which affects both occupations and coherences. When an embedded quantum dot inside the quantum wire is present the carrier-phonon interaction leads to capture processes into the localized states. We study the carrier capture using the LSP approach and compare it to a quantum kinetic (QK) approach. We show that the essential features of the carrier capture process are well described by the LSP approach (Fig. 1, left panel) when compared to the QK approach (Fig. 1, right panel) while the computational complexity is greatly reduced.

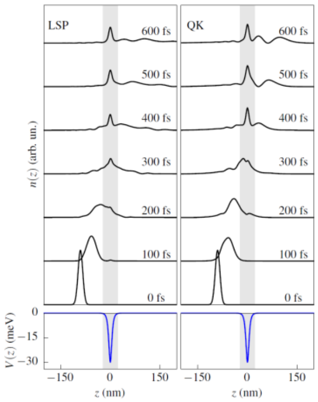

Figure 1: Comparison of electron density dynamics. The solid lines in the two upper panels show the dynamics when carrier-phonon interaction is considered within the Lindblad based approach (LSP, left panel) and the quantum kinetic approach (QK, right panel). The quantum dot is described by the potential depicted in the two lower panels.

[1] D. Reiter et al., Phys. Rev. B 75, 205327 (2007).
[2] R. Rosati et al., submitted.
[3] D. Taj et al., Eur. Phys. J. B 72, 305-322 (2005).
[4] R. Rosati et al., Phys. Rev. B 90, 125140 (2014).

P:23 Impact of the gate and external insulator thickness on the static characteristics of ultra-scaled silicon nanowire FETs

D Logoteta[1], N Cavassilas[1], M Pala[2], A Cresti[3] and M Bescond[1]

[1]Aix-Marseille Université, France, [2]Université Paris-Saclay, France, [3]Université Grenoble Alpes, France

The geometries routinely considered for the numerical simulation of nanoelectronic devices within quantum self-consistent models do not result in a realistic description of the electrostatic potential in the insulator covering the access regions. The thickness chosen for this latter is indeed tipically too small with respect to the decay length of electric field and the gate is modeled with thickless stripes, preventing any account for fringe fields. More realistic geometries are considered only in the framework of simpler transport models, in order to provide semianalytical descriptions of parasitics [1], [2], [3] or perform extensive explorations of the design parameter space [4], [5].

We propose a full quantum simulation study focusing on gate-all-around ultra-scaled silicon nanowire field effect transistors (NW FETs), aimed to investigate the impact of extending the simulation domain so as to include a larger part of the gate electrode and of the insulator enveloping the source and drain extensions.

Our simulation approach relies on an effective mass Hamiltonian fitted on tight-binding band structure computations [6] and is based on the self-consistent solution of the transport equations within the non-equilibrium Green's function formalism and of the Poisson equation. The electron scattering with acoustic and optical phonons is taken into account within the self-consistent Born approximation.

The geometries compared in this study are sketched in Fig. 1. The geometry A is the simplest and most widely used one, in which the gate corresponds to a wrapping surface belonging to the boundary of the simulation domain. On the contrary, the geometry B models the gate as a three-dimensional shell; the value of 5 nm set for its thickness has been verified to guarantee a reasonable stabilization of the results against any further increase. In order to investigate the interplay with different degrees of quantum confinement and short channel effects, we consider NW FETs with two different transversal crosssections (2x2 and 5x5 nm^2), gate lengths (5 and 10 nm) and gate underlaps (0 and 3 nm).

Our results highlight deviations between the two models both in the subthreshold region and at large gate overdrives. As illustrated in Fig. 2 and in the top panel of Fig. 3, accounting for the fringe field of the gate in the B arrangement can dramatically improve the electrostatic integrity and consequently the subthreshold swing with respect to the A case. This effect is particularly pronounced in the wider and shorter devices, as a consequence of the less effective gate control. In the narrower devices, due to the weaker pinning in the doped source region, at large overdrive the gate fringes can induce a sizeable bottom shift in the lowest subband with respect to the A case (bottom panel of Fig. 3). This effect, stronger in the ballistic regime and quite weakly dependent on the gate length, results in an increase of the current in the B arrangement with respect to the A one. The overall impact on the estimation of the device performance for several representative configurations is summarized in Table1, which indicates that the $I_{ON}=I_{OFF}$ ratio computed with the A geometry can suffer from large underestimations as compared to the results obtained with the B geometry.