Time-resolved Quantum Transport in Open Systems: Phase Versus Real-Space Methods

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Introduction

Density matrix based simulation methods can offer great insights into the time-resolved quantum charge carrier transport in nanoscale devices with open boundaries such as tunneling diodes, multigate FETs or 2D material based transistors. The most widely applied methods are based on the Wigner Transport Equation (WTE) and have been in use for the analysis of transient carrier transport phenomena for almost 40 years now. Results are consistent with those obtained by using non-equilibrium Greens function (NEGF) methods, though the latter continues being plagued by extreme computational demands in the transient case. More recently, however, our research has shown that studying the density matrix directly in real space can provide several advantages. As such, a comparison of the strengths and limitations of the phase space and real space methods is given here.

Phase space based methods

The preference for the WTE and similar methods such as quantum Liouville-type equations (QLTE) naturally follows from the ease of distinguishing between in- and outgoing waves when setting up the necessary inflow boundary conditions. The wealth of research conducted over the years encompasses the use of a variety of discretization methods, including the finite volume method visualized in Fig. 1, efficient finite element methods and Monte Carlo sampling [1]. Results can be obtained for a variety of devices such as resonant tunneling diodes (Fig. 2) and gate-all-around FETs (Fig. 3). Nevertheless, the conventional discretization methods approach their limits when applying such continuum models onto devices just few atoms in dimension [2] (see Fig. 4).

Real space based methods

While the already mentioned discretization methods can also be applied onto the von Neumann equation, the real space formulation naturally lends itself to the use of atomistic models such as tight-binding Hamiltonians [3]. If inserted into an equation of motion along with the density operator defined in terms of field operators, a density matrix formalism in second quantization can be obtained that retains the atomistic description appropriate for nanoscale devices (Fig 1). Instead of the arbitrarily chosen computational grid used with the WTE, the density matrix elements are defined on the same lattice points as those of the Hamiltonian that is used. The resulting equation of motion can not only reproduce results obtained by the WTE (Fig. 2 and Fig. 3), but also account for otherwise hard to include effects, such as varying lattice spacings [3], nonparabolic band structures or rapid change in device geometry (Fig. 4).

Discussion

The WTE provides an easy to implement and efficient model that is applicable to numerous devices. However, while numerical challenges must still be addressed, the real-space method seems to be the more capable method for bridging the gap between established atomistic methods (NEGF) and time-resolved models (WTE).

References

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[3] M. Pech, A. Abdi, and D. Schulz, "Density matrix based transport in heterostructure devices utilizing tight-binding approaches," *SISPAD 2024*.

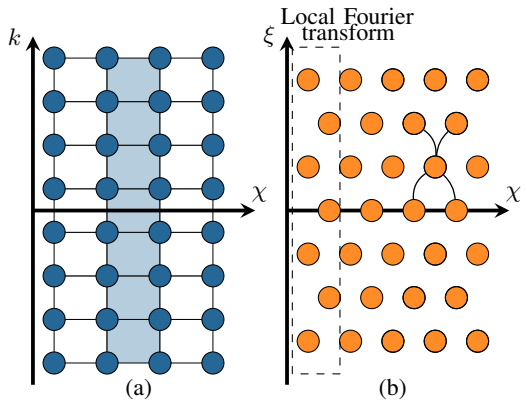

Fig. 1. The schematic representation of the Wigner function discretized by a finite volume scheme is shown in (a) with the blue circles representing the locations at which the Wigner function is defined. By nature of the discretization scheme, the blue shaded area connects the vectors to its left and right and needs to be integrated over, possibly introducing a numerical error in the case of discontinuities. With the real space formulation shown in (b), the density matrix elements are defined on the same lattice sites as the Hamiltonian and discontinuities can easily be taken into account. The resulting grid does not have to be uniform within the device, thus allowing for spatially varying lattice distances as the Fourier transform is only needed at the contacts as is indicated in (b).

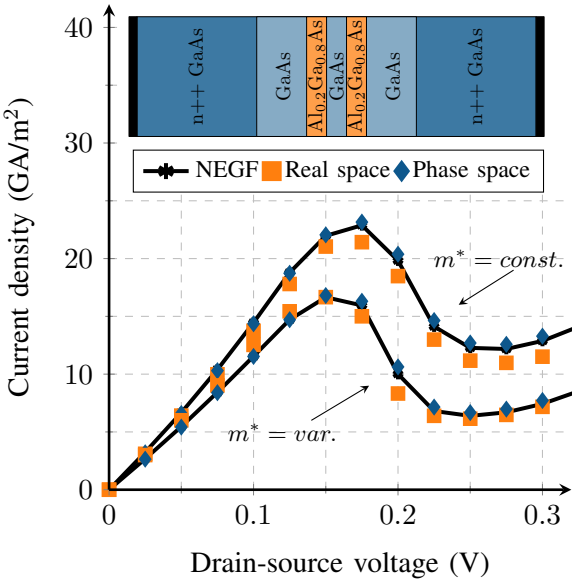

Fig. 2. The current densities from the NEGF method, the WTE solved in phase space and the tight-binding density matrix solved in real space [3] all agree well with each other for the flatband simulation of a GaAs/AlGaAs resonant tunneling diode with spatially constant (upper graphs) and spatially varying (lower graphs) effective masses. Additionally, the higher sparsity of the real space system matrix leads to faster computation times and lower memory requirements.

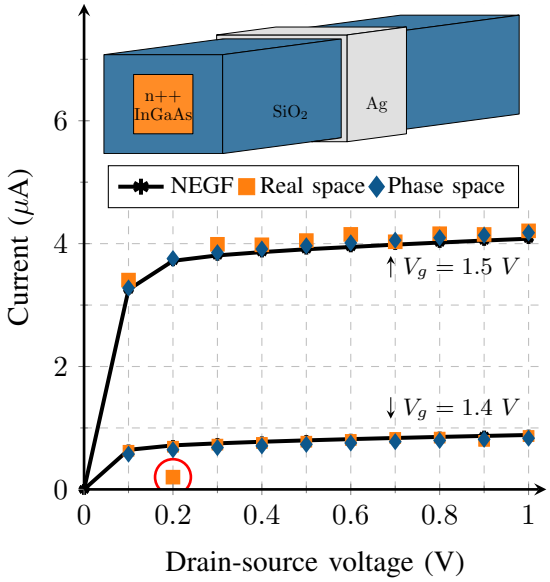

Fig. 3. For gate-all-around FETs the previously mentioned approaches can be combined with the mode-space approximation [2]. The self-consistent results from the real space formulation are in good agreement with the other methods for both gate voltages V_g, except for one bias point where convergence issues are apparent (circled red), requiring further improvements of the boundary conditions.

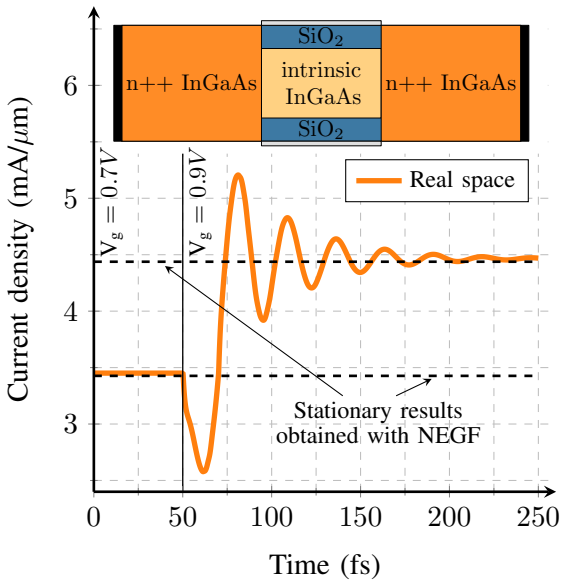

Fig. 4. A constriction in the dual-gate FET leads to strongly varying coupling terms at the interface [2] and coupling between the modes. As such, the real space method is better suited for these problems and no solution using the WTE could be obtained. At $t = 50$ fs, the gate voltage V_g is switched from 0.7 V to 0.9 V. As it can be seen, the self-consistent current density perfectly converges from its initial state to the reference result for $t \to \infty$.