Incorporation of the Tight Binding Hamiltonian into Quantum Liouville-type Equations

A. Abdi, M. Pech, and D. Schulz
Chair for High Frequency Techniques, TU Dortmund, Friedrich-Wöhler-Weg 4, 44227 Dortmund, Germany
e-mail: alan.abdi@tu-dortmund.de

***Abstract*— A novel numerical approach is introduced and validated for the determination of the statistical density matrix based on the Tight Binding Hamiltonian included in a Quantum Liouville-type equation. Besides the main advantage that the atomic structure is taken into account, a transport model results which, unlike the conventional Wigner equation, does not involve any loss of information in the domain of the density matrix.**

Introduction

For the analysis of quantum mechanical transport, well-known models such as the Wigner Transport Equation (WTE), the Non-Equilibrium Green Function (NEGF) method or Quantum Liouville-type Equations (QLTE) have been developed. However, the use of a Tight Binding (TB) Hamiltonian as an addition for these models allows an atomistic view and thus considers the electronic structure of the materials used. The solution of the QLTE in combination with the TB Hamiltonian results in a density matrix defined on lattice points. On this basis computationally efficient algorithms can be realized.

Model

After incorporating the TB Hamiltonian into the Von-Neumann Equation (VNE) and applying the center of mass transformation, a transport equation for the density matrix in center mass coordinates χ and ξ results. As a consequence, a staggered grid formulation appears as depicted in Fig. 1 on which a formalism in the phase space can be established. For this purpose a transformation based on a set of plane wave functions with wave numbers k is carried out in ξ-direction for both sub-grids arriving at a QLTE [1]. The orthogonality of the basis is mandatory. With this resulting staggered grid formulation, all of the density matrix information is contained in the transport equations [2]. The transport equations obtained are related to a formalism presented by Mains and Haddad [3], where the transformations chosen for each sub-grid are different. Unfortunately, the latter model leads to negative carrier densities and requires the use of a scattering model while this is not the case for the proposed approach.

Discussion

Special attention needs to be paid with regard to boundary conditions. In χ-direction the inflow and outflow concept is applied onto both grids [2], whereas in ξ direction a Complex Absorbing Potential (CAP) is applied [4]. A resonant tunneling diode (Fig. 2) is now acting as a test device. In the flat band case, the model (referred to as TB-QLTE) shows good agreement with the results obtained from the NEGF method as it can be seen from Fig. 3 and 4. Combining the TB Hamiltonian with the QLTE seems to be a promising approach and shall be further investigated.

References

[1] L. Schulz, B. Inci, M. Pech, and D. Schulz, *Subdomain-based exponential integrators for quantum Liouville-type equations*, Journal of Computational Electronics **20**, 2070-2090 (2021).

[2] W. Frensley *Boundary conditions for open quantum systems driven far from equilibrium*, Review of Modern Physics **62**, 745 (1990).

[3] R. Mains, and G. Haddad *An Accurate Re-formulation of the Wigner Function Method for Quantum Transport Modeling*, Journal of Computational Physics **112**, 149-161 (1992).

[4] L. Schulz, and D. Schulz, *Complex Absorbing Potential Formalism Accounting for Open Boundary Conditions Within the Wigner Transport Equation*, Ieee Transactions on Nanotechnology **18**, 830 - 838 (2019).

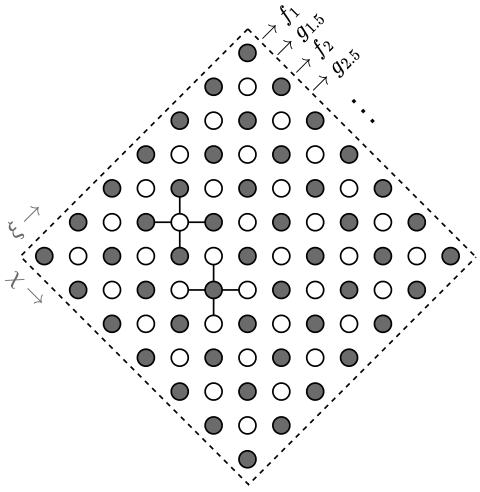

Fig. 1. Illustration of the staggered grid composed of the two subgrids (f-black and g-white) in the center-of-mass coordinates χ and ξ. The circles stand in for the elements of the density matrix. The coupling between the two grids is indicated for two grid points. When not at the boundary each element couples to four neighboring elements.

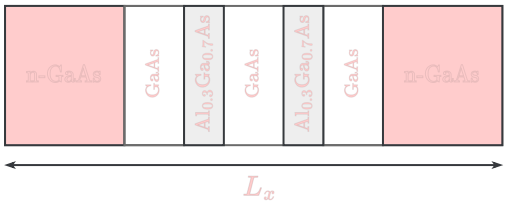

Fig. 2. Structure of a AlGaAs/GaAs resonant tunneling diode with a width of L_x=152 nm, barriers of 3.38 nm width and a quantum well of 4.5 nm width. The contacts are n-doped with a concentration of N_D=2 $*$ 10^{18} cm^{-3}. A spatially constant effective mass distribution with the effective mass of GaAs is assumed.

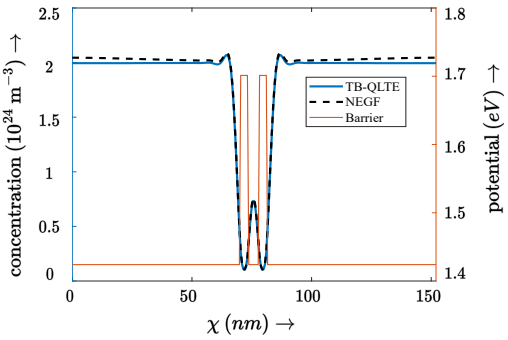

Fig. 3. The electron density from the use of TB-QLTE for one of the both grids is shown as a function of the coordinate χ. For the equilibrium case, the results are compared to those obtained from the NEGF method. The results agree very well. For the k-discretization $N_k = 200$ values were considered.

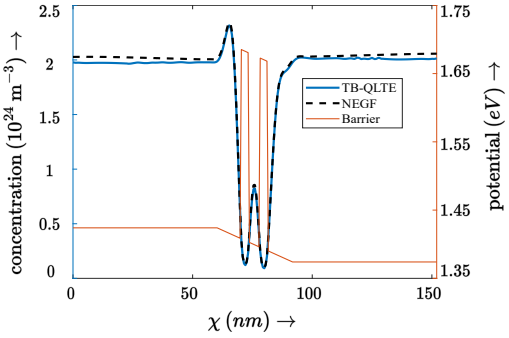

Fig. 4. The electron density from the use of TB-QLTE for one of the both grids is shown as a function of the coordinate χ with an applied voltage of 0.05 V. The results are compared to those obtained from the NEGF method. At this point it should be mentioned that the CAP has a considerable influence on the results, so it is important to choose a suitable parameter set for it. Further investigations with regard to the CAP and the boundary conditions will be presented.