Subdomain Algorithm for the Numerical Solution of the Liouville-von-Neumann-Equation

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For the numerical simulation of quantum electronic devices sophisticated methods are desirable. The numerical solution of the Wigner Transport Equation (WTE) is preferable for engineering applications [1,2,3]. On the one hand, transient effects can be analyzed in a straightforward manner. On the other hand, scattering mechanisms can be implemented in detail. Unfortunately, conventional methods utilized for a numerical solution of the WTE tend to pose problems [2].

To begin with, the conventional discretization schemes cannot adequately include coherent effects resulting in an overestimation of the diffusion effect [4] as these are based on upwind difference schemes. Furthermore, by the utilization of these schemes, the drift operator is not interacting with the inflow boundary conditions, whereas this is a prerequisite [2]. Additionally, the drift operator represents a highly oscillating function, when considering heterostructure devices, leading to a worse convergence behavior with respect to the Fourier integrals. As a result, large computational errors are subject to these drawbacks.

In order to address these aspects, an approach based on the formulation of an exponential operator combined with the finite volume discretization technique has been developed for the numerical solution of the Liouville-Von-Neumann-Equation (LVNE) in center-mass coordinates, χ and ξ [5]. On the basis of the discretized diffusion operator with regard to the ξ-direction, a transformation of the statistical density matrix is carried out allowing a definition of the inflowing and outflowing waves. With regard to the continuity conditions at the interfaces, the real space formulation is preferable.

Here, a concept is proposed allowing the utilization of arbitrary basis functions as well as allowing the application of a subdomain approach for a highly efficient solution of the LVNE. Indeed, when an orthogonal set of exponential functions is applied to form the transformation matrix, the WTE is formally obtained from the discretized equation and, therefore, the corresponding advantages with regard to the implementation of scattering mechanisms can be preserved. Furthermore, the conventional coupling between the discretized real space and the discretized phase space can be effectively avoided. Along with this procedure more flexible and efficient solutions are enabled.

The approach is verified with the numerical simulation of a simply structured resonant tunneling diode (RTD) on the basis of the AlGaAs/GaAs material system as demonstrated in Fig.1-6. Finally, a novel approach for a highly efficient solution of the LVNE combined with an in-depth analysis with regard to the WTE is presented.

[1] J. Weinbub et al., Appl. Phys. Rev., doi: 10.1063/1.5046663 (2018)

[2] D. Schulz et al., J. Quantum Electron., 8700109, doi: 10.1109/JQE.2015.2504086 (2016).

[3] W. R. Frensley, Phys. Rev. B., 1570, doi: 10.1103/PhysRevB.36.1570 (1987).

[4] C. Carey et al., Appl. Math. Modelling, doi: 10.1016/0307-904X(93)90048-L (1993).

[5] K. Khalid et al., Trans. Nanotechnol., doi: 10.1109/TNANO.2017.2747622 (2017)

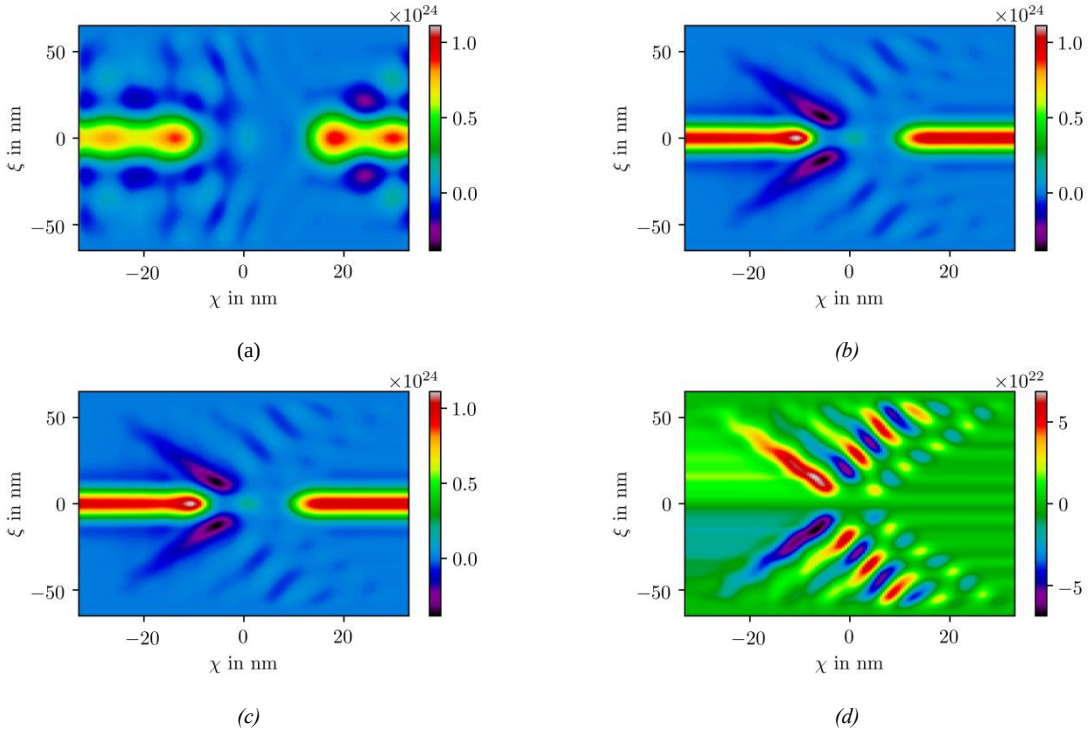

Fig.1: Real part of the statistical density matrix for the RTD for the non-equilibrium case shown for an external bias of -0.15V and for different subdomain dimensions. For the demonstration an exponential basis is applied so that the expansion coefficients are inherently linked with the values of the discretized Wigner function. The discretized statistical density matrix obtained for the use of N=250 basis functions is depicted in (c), which corresponds to the full set of basis functions, whereas the subdomain dimensions N=10 and N=50 are shown in (a) and (b), respectively. As apparent from the numerical solution in (b), N=50 basis functions are sufficient for a convergence of the statistical density matrix. As a consequence, the number of basis functions can be drastically reduced in comparison to standard methods. The computation time as well as the computational resources can be effectively reduced. The imaginary part of the statistical density matrix obtained from the subdomain solution is shown in (c).

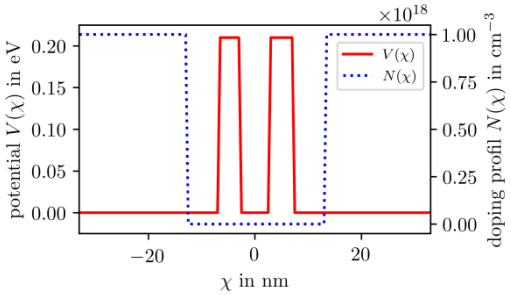

Fig.2: Conduction band diagram V and doping concentration N of the RTD.

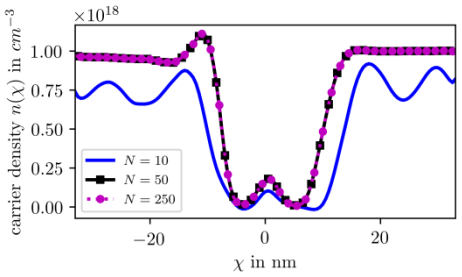

Fig.3: Carrier densities calculated from the values of the corresponding statistical density with regard to different subdomain dimensions N as shown in (a), (b) and (c).