A phenomenological method to reduce NEGF simulation from 3D to 1D for lateral translation invariant systems

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ABSTRACT

In this work we present a methodology for calculate the current-voltage characteristics of devices within the Non-equilibrium Green's Function Formalism (NEGF). The methodology is valid for lateral translational invariant (TI) systems in the direction perpendicular to the transport direction. The calculation of a 3D system is reduced to a 1D. One essential feature of the method is that it allows the use of the recursive algorithm for the reduced 1D retarded Green G^R and lesser $G^<$ matrices for block triangular Hamiltonians. It is exact for ballistic systems. However, for system with photon/phonon interactions, the approximations reside between the Kadanoff-Baym ansatz [1] and the exact 3D methodology. For elastic scattering the method is explicit current conserving. However, for inelastic scattering conditions needs to be supplied to ensured current conservation. Application to a pn junction will be presented.

INTRODUCTION

Simulation of current voltage characteristics of semiconductor devices has mainly used Drift-Diffusion (DD) based simulators. Commercial 2D simulators for 3D space invariant systems were realisable by the 80s. This is possible as the DD equations are not energy resolved and are essentially model a density charge fluid with drift and diffusion currents. With the increase of computational power 3D simulations were possible for several hundred microns systems using DD. However, even today, three dimensional (3D) NEGF simulations of devices are almost prohibited for relatively large systems. For the case of space invariant system, simulation of 3D system requires the simulation of a number of copies of 1D system (uncoupled mode), of a coupled set of 1D systems. This is possible for narrow systems as nanowires or even Finfets. However, for large cross-sections or bulk-like devices these methods prohibitive and larges copies of 1D systems deed to be simulated (see QCLasers). A method presented in ref [2] allowed for the reduction of 3D to 1D for TI system. Even if approximated, the method is ingenious, however the reduced 1D system required the calculation of the full NEGF matrices i.e. the equations are not suitable for the use of the recursive algorithm [3].

MODEL AND CONCLUSION

The method proposed here projects the 3D NEGF problem to an equivalent 1D NEGF problem. The method assumes that the retarded scattering self-energy Σ^R is a function of $E-E_t$, where E is the carrier total energy and Et the transversal energy. The resultant 1D equations are the same Keldysh equations (for G^R and $G^<$) as the standard NEFG and therefore the recursive algorithm can be used. However, the scattering self-energies needs to be renormalized to the 3D weight. In addition, the Keldysh equations [4] do not contain E_t and therefore the 3D problem is reduced to the calculation of a pure 1D problem. The 1D $G^<$ needs to be renormalized and integrated to produce the 3D density and current. This means that a large 3D problem of µm size may be considered. The methodology is current conserving for elastic scattering (or phase breaking scattering). For inelastic scattering the method needs further refinements to ensure current conservation. The method would be applied to calculate the current voltage characteristic of a GaSb *n-p* junction diode. Ballistic, Dissipative and recombination limited current would be studied.

REFERENCES

[1] Quantum Statistical Mechanics. L. P. Kadanoff and G. Baym. (New York : W. A. Benjamin, Inc., 1962.)

[2] R. Lake and S. Datta, *Non-equilibrium Green's-function method applied to double-barrier resonant-tunnelling diodes*, Phys. Rev. B **45**, 6670 (1992).

[3] A. Svizhenko et al *Two dimensional quantum mechanical model of nano-transistors*, Journal of Applied Physics, vol. 91, no. 4, pp. 2343-2354 (2002).

[4] L. V Keldysh, *Diagram technique for non-equilibrium processes*, Sov. Phys. JETP ***(*20*)**, P.* 1018*, (*1965)