

NANOELECTRONIC DEVICE SIMULATION BASED ON THE WIGNER FUNCTION FORMALISM

Hans Kosina

TU Vienna, Institute for Microelectronics, A-1040 Vienna, Austria

Modeling of electronic transport in mesoscopic devices requires a theory describing open, quantum-statistical systems driven far from thermodynamic equilibrium. Especially when the device is operated at room temperature, scattering processes due to electron-phonon interaction can play an important role. To treat this mixed coherent/dissipative regime several quantum transport formalisms are available. In this work the Wigner function formalism is considered. Early numerical solutions of the Wigner equation were obtained by the finite difference method, assuming simplified scattering models based on the relaxation time approximation [1]. For realistic device simulations, however, comprehensive scattering models are required. This can be achieved by solving the Wigner equation by means of Monte Carlo techniques [2]. At present scattering is treated semi-classically by including a Boltzmann scattering operator. The limitation of the approximation will briefly be discussed. Since the Wigner function reduces to a classical distribution function for sufficiently smooth potentials, this method allows for a seamless link of quantum regions and extended classical regions. The Monte Carlo technique developed for the solution of this kinetic equation is based on an interpretation of the Wigner potential operator as an generation term for numerical particles. Details on the algorithm for particle generation and subsequent particle annihilation are presented. Including a multi-valley semiconductor model and a self-consistent iteration scheme, the described Monte Carlo simulator can be used for routine device simulations. Applications to single barrier and double barrier structures will be presented. Fig.1 shows the quantum ballistic currents through a single-barrier structure computed using Wigner Monte Carlo and a numerical Schrödinger equation solver. Good quantitative agreement between the two numerical techniques is achieved. The quantum ballistic current is higher than the classical one due to tunneling.

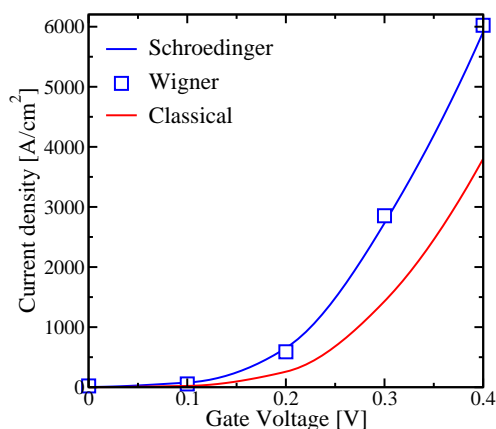


Figure 1: Normalized ballistic currents calculated classically and quantum mechanically.

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[1] W.R Frensley, Rev.Mod.Phys., 62, 745 (1990).

[2] H. Kosina, M. Nedjalkov, and S. Selberher, J. Computational Electronics 2, 147 (2003).