ADVANCED TRANSPORT MODELS FOR NANODEVICES

Lecturer: Hans Kosina, Institute for Microelectronics
Technical University of Vienna, Austria

SUMMARY

Coherent transport in mesoscopic devices is well described by the Schroedinger equation supplemented by open boundary conditions. When electronic devices are operated at room temperature, however, effects of scattering need to be included for a device model to be realistic. Frequently used formalisms for this mixed coherent-dissipative transport regime are based on the Wigner function and on Non-equilibrium Green's functions. This presentation gives a review on the Wigner function method. Starting with an introduction to the Wigner function formalism, treatment of the electron-phonon interaction within this formalism is then studied in more detail. Derivation of the reduced single-particle Wigner function, the weak interaction limit, and the semi-classical limit are discussed. As a quantum transport model suitable for numerical device simulation we consider the single-particle Wigner equation including a semi-classical scattering operator. After transforming this kinetic equation to a path-integral form, the Monte Carlo method for solving integral equations is applied. Several particle models assigned to the quantum transport problem are discussed. The development of Monte Carlo algorithms and the corresponding particle models is complicated by the fact that, as opposed to the semi-classical case, the integral kernel is no longer positive. This so-called negative sign problem requires the introduction of new numerical techniques in order to obtain stable Monte Carlo methods. Particle models are presented which interpret the potential operator as a generation term of numerical particles of positive and negative statistical weight. The problem arising from the generated avalanche of numerical particles is thereby solved by a suitable particle annihilation algorithm. The Monte Carlo method is finally applied to resonant tunneling diodes. Comparison with other numerical simulation techniques verify the accuracy of the Wigner function-based device model. The effect of scattering on current-voltage characteristics and internal distributions is shown. Since the quantum Monte Carlo method gradually turns into the semi-classical Monte Carlo method when the potential variation becomes sufficiently smooth, the method is inherently suitable for the simulation of quantum regions embedded in extended classical regions.