Wigner-Boltzmann Particle Simulations: Methods and Applications

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Abstract

Computational tools for simulation of electronic devices bring to the semiconductor industry a considerable reduction of the development costs. The classical era of device simulation in terms of charge transport and electrical behavior can be characterized by the keywords 'Boltzmann equation' and 'Silicon'. However, the nano-era of semiconductor devices involves novel materials and architectures, along with a number of novel phenomena which must be taken into account. While some of them can be described in classical terms, others, being dominant at nanometer and femtosecond scales, require multi-dimensional quantum description capable of taking into account both, purely coherent processes such as quantization and tunneling, as well as phase breaking processes of interactions with the lattice.

The aim of this project is threefold: (i)Upgrade of the in-home VMC particle simulator to a multi-dimensional, parallel, self-consistent, stationary/transient ensemble Monte Carlo routine with statistical enhancement. According to the road-map for VMC this is a necessary step for a further expansion of the simulator towards complex physical models imposed by novel materials and structures. (ii)Development of a two-dimensional particle quantum simulator based on the WIgner ENSemble (WIENS) union. (iii)Further development of WIENS as a union of theoretical and numerical approaches and algorithms for particle simulation of quantum phenomena in nanostructures. The evolution principle is the common linking element for these activities. The single-particle simulator VMC accounts for most cubic semiconductors. The material modules related to band structures, phonon scattering models, and alloy compositions will be adopted directly by the ensemble counterpart. The quantum simulator is built as an extension of the two-dimensional ensemble routine re-utilizing the models for boundary conditions, particle evolution, and estimators for physical averages. The algorithms and parameter settings of WIENS are used consistently with the particle generation-annihilation scheme to construct the Wigner part of the code. The classical and Wigner simulators are applied for simulation of actual devices where Boltzmann or quantum-dissipative conditions of transport dominate the device behavior. The work on WIENS continues to address still open physical and numerical issues related to the Wigner picture of statistical mechanics, which are resolved by theoretical analysis and numerical experiments. An idea is pursued for the cases where the transport is close to coherent or is determined by processes of dissipation. Under the assumption that the Wigner function in the considered limiting case is known, we theoretically and numerically investigate the equation for the corresponding correction. The approach involves an interface with other numerical methods which are efficient in providing the limiting solution. Active collaboration with groups from the home and international institutions is envisaged.