The Non-Equilibrium Green Function Approach to Quantum Transport in Nano-Structures

J.R. Barker
College of Science and Engineering, University of Glasgow, Glasgow G12 8LT, Scotland, UK
e-mail: john.barker@glasgow.ac.uk

MANUSCRIPT

The Non-Equilibrium Green Function (NEGF) formalism was established 50 years ago [1-3] to describe non-equilibrium quantum statistical mechanics in open systems [4-6]. Clever algorithm development [7-10] and the wide availability of powerful computer technology has made the technically complex NEGF formalism a practical simulation tool for studying transport in nanostructured devices. The central concept is the 8-dimensional Green Function $G[r, t; r', t']$ that describes the quantum mechanical probability amplitude for a carrier to propagate from a position $r$ at time $t$ to another position $r'$ at time $t'$ within a many-body interacting system that is driven out of thermal equilibrium by applied fields. $G$ is rarely calculated directly, instead we may compute physically interesting properties such as the charge density, current density and local density of states in computationally efficient schemes. NEGF theory is a highly technical formalism [1-6] because the need to establish a non-equilibrium many-body perturbation theory leads to consideration of four different types of coupled Green functions. The general case is reviewed and we show the connection with semiclassical Boltzmann transport theory. Our main focus is on stationary systems where the Green functions depend on two position coordinates and energy. Four different Green functions are required: we consider the retarded and advanced Green functions $G^R(r, r'; E), G^A(r, r'; E)$, (describing the dynamical states and quantum dynamics) and the so-called lesser and greater Green Functions $G^<$($r, r'; E$), $G^>$($r, r'; E$) (correlation functions that pick up the mainly statistical or thermodynamic properties). A simple picture is developed of the basic NEGF simulation methodology. Useful visualisation techniques are described based on the quantum hydrodynamic velocity field. We start with the projection algorithms [7-10] that reduce the computational domain to a finite device region at the expense of introducing a self-energy correction that takes account of coupling to the leads/contacts/environment. Criteria are then developed for choosing between full complexity 3D spatial modelling versus the lower dimensional modal decomposition method in confined nanostructures [11-12]. NEGF methods are particularly useful in quasi-ballistic systems where the complexity of the self-consistent electrostatic architecture of the device (including atomistic treatment of the scattering on individual impurities and surface/interface roughness) may be incorporated non-perturbatively [13-15]. Non-ballistic nanostructures [16] are now becoming of interest for which many-body self-energy models are required to describe both elastic and inelastic scattering. Examples include gate-all-around (GAA) silicon nanowire (SNW) devices (Fig.1) that are non-ballistic because: (i) the electron-phonon interactions [18, 19] are enhanced by confinement effects and (ii) long-range remote phonon scattering from interfacial regions. Self-energies are generally non-diagonal [17] and this renders the standard Green function algorithms intractable. To reduce the numerical complexity many adopt approximations to the electron-phonon self-energies. We review important self-energy models including: electrostatic [20], Hartree, exchange and correlation, carrier-phonon/plasmon. We examine the errors created by common approximations to self-energies that arise from the diagonality approximation or violation of the requirements for physical causality [21] and we
discuss a strategy for efficient accurate numerical calculation.

REFERENCES


Fig. 1. Schematics of a nano-scale transistor.
Channel dimensions: 2.2nm X 6 nm [21]