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

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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 $G[\mathbf{r},t;\mathbf{r}',t']$ that describes the quantum mechanical probability amplitude for a carrier to propagate from a position $\mathbf{r}$ at time t to another position $\mathbf{r}'$ 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 semi-classical 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 $G^R(\mathbf{r},\mathbf{r}';E)$, $G^A(\mathbf{r},\mathbf{r}';E)$, (describing the dynamical states and quantum dynamics) and the so-called *lesser* and *greater* Green Functions $G^<(\mathbf{r},\mathbf{r}';E)$,$G^>(\mathbf{r},\mathbf{r}';E)$ (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

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discuss a strategy for efficient accurate numerical calculation.

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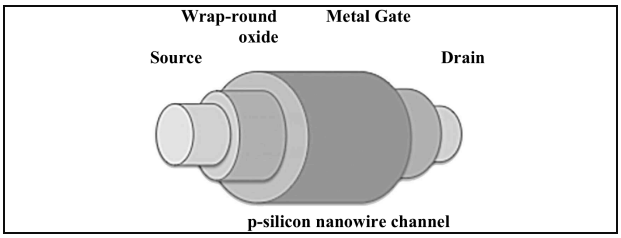

Fig. 1. Schematics of a nano-scale transistor. Channel dimensions: 2.2nm X 6 nm [21]