

R-matrix Theory and Equivalent Model for Nanoscale Device Simulation

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INTRODUCTION

Continual technological innovations have made it possible to create metal-oxide-semiconductor field-effect-transistors (MOSFETs) with the channel length down to sub-30 nm. Detailed computational studies are now a necessity to predict the transport characteristics and to accelerate the development of future ultra-small MOSFETs with novel structures and materials. The non-equilibrium Green's function (NEGF) formalism [1]–[3] provides a suitable theoretical framework for such studies. The NEGF method, however, requires substantial computational demand, which makes computations very challenging for three dimensional (3D) device structures. We have been developing computationally efficient approaches based on the R -matrix theory [4], [5]. The purpose of this paper is to give a brief review on our recent progress in developing the R -matrix theory of quantum transport within the effective-mass [6]–[8] and the tight-binding models [9], [10], and the equivalent transport model for atomistic simulation [11], [12].

R-MATRIX THEORY

Effective-Mass Model

As a simple illustration of some important aspects of the R -matrix theory of quantum transport, let us consider an open system, i.e. a MOS device channel, described by a single-particle effective-mass Hamiltonian, $H = -(\hbar^2/2m^*)\nabla^2 + V$. Because of the coupling between the channel and the electrodes, H is not Hermitian over the internal region, and can be decomposed as $H = \tilde{H} - \mathcal{L}$. Here \mathcal{L} is the Bloch boundary operator [13] and the remaining \tilde{H} is a Hermitian operator describing a closed system. The retarded Green's function, $G(E) = (E - H + i0)^{-1}$,

can be written from the Dyson's equation as

$$G = \tilde{G} - \tilde{G}\mathcal{L}G, \quad (1)$$

where $\tilde{G}(E) = (E - \tilde{H})^{-1}$ is the Green's function for the closed system. We now introduce the surface basis functions $\{|v\rangle\}$ as the subband eigenfunctions associated with confinement in the contact planes, and calculate the matrix elements of the Green's functions;

$$G_{v\mu} = \tilde{G}_{v\mu} - \frac{\hbar^2}{2m^*} \sum_{v'} \tilde{G}_{vv'} ik_{v'} G_{v'\mu}. \quad (2)$$

Here $G_{v\mu} = \langle v|G|\mu\rangle$, $\tilde{G}_{v\mu} = \langle v|\tilde{G}|\mu\rangle$, and k_v are the wavevectors in the leads. Equation (2) suggests that the surface components of G can be calculated from the R -matrix, $R_{v\mu} \equiv \tilde{G}_{v\mu}^{-1}$. As shown in Ref. [7], $R_{v\mu}$ provides all the necessary information for the NEGF simulation.

Since the R -matrix is defined through the Green's function of a closed system, it can be calculated in the form of spectral (or basis) expansion, similar to the contact block reduction (CBR) method [14]. For the R -matrix theory, we can make use of the

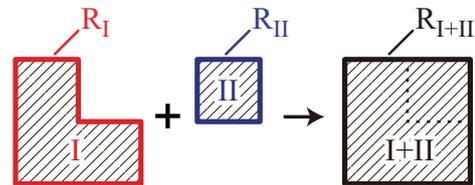


Fig. 1. Schematic diagram of the R -matrix propagation. The new R -matrix R_{I+II} is obtained by adding a device element II to the previously constructed element I. The next step will be started from the device element I+II.

[†]The definition of the R -matrix here differs by a constant factor from the conventional one.

propagation algorithm [15], which greatly reduces the numerical burden [7]. We first split the device into a set of small closed subsystems. We then start with an arbitrary element and “grow” the device by adding all other elements one by one (see Fig. 1). This avoids large matrix operations because the device elements can be chosen to be simple in a sense that the matrix size of the corresponding Hamiltonian is small.

Tight-Binding Model

In the effective-mass model, the localized nature of the boundary operator \mathcal{L} leads to the R -matrix propagation algorithm. The tight-binding (TB) model can be treated exactly in the same way with the only modification that \mathcal{L} should be replaced by the coupling part of the TB Hamiltonian [9]. The R -matrix in the TB model is defined as $R = \mathcal{P}\tilde{G}\mathcal{P}$, where \tilde{G} is the Green’s function for the closed device and \mathcal{P} is the projection operator to the atomic orbitals in the device. We can propagate this R -matrix through a set of the device elements, which can be a single atom or a cluster of atoms, and obtain all the necessary information for the NEGF simulation [9].

EQUIVALENT TRANSPORT MODEL

Although the R -matrix propagation technique can effectively manage the computation burden, atomistic simulation in realistic nanostructures with thousands of atoms requires substantial computation resources, especially for modeling inelastic scattering processes. We have recently proposed the equivalent model (EM) which allows the above computational limitations eliminated [11].

The EM utilizes a small number of the Bloch states in the energy window of interest to construct

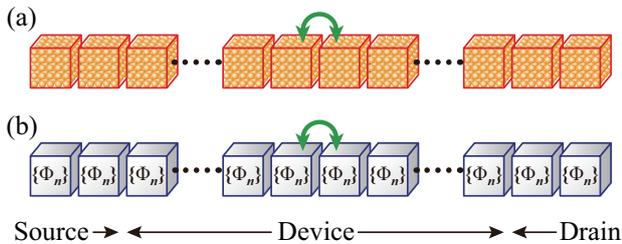


Fig. 2. Schematic diagram of an ideal nanowire (a) in the tight-binding picture and (b) in the basis representation. The cuboids represent the unit structure of the nanowire.

a set of basis functions $\{\Phi_n\}$, which reproduce all the scattering states of the TB model within the energy window. Neglecting contribution outside the energy window, we replace the original huge set of the atomic orbitals with $\{\Phi_n\}$, and obtain a low-dimensional EM in the basis representations (see Fig. 2). Numerical tests for Si nanowires of a few nm width have confirmed that accurate atomistic transport simulation can be performed using $\sim 1\%$ of the total number of atomic orbitals [11]. This greatly reduces computational burden and allows inelastic scattering to be incorporated.

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