Efficient solution algorithm of non-equilibrium Green's functions in atomistic tight binding representation

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INTRODUCTION

With the shrinking dimension of electronic devices, quantum transport attracts increasing interest. The non-equilibrium Green's function (NEGF) formalism [1] provides a very general framework for quantum transport, but it is numerically expensive when applied on atomistic tight binding representations. So far, computational burden (in memory and CPU time) limits the maximum diameter of nanowires that are solvable within atomistic NEGF to about 8nm. Several methods are developed to reduce the numerical costs. However, these methods are either limited to effective mass model [2] or to small cross-sections perpendicular to the transport direction [3]. In this work, it is demonstrated how to apply the concept of low rank approximation [4] to the NEGF method in atomistic tight binding representation. Using this method, transport in a 12nm squared Si nanowire is solved.

METHOD

All electrons are represented in atomistic multi band tight binding models. If a device consists of several millions of atoms, tight binding descriptions yield millions of electronic states. Only a small fraction of these states contribute to charge transport. In this method, the NEGF equations of the tight binding Hilbert space of rank N are transformed into a Hilbert space of rank n that is spanned by only these relevant states. The maximum achievable speed up is given by $(n/N)^3$ and the maximum reduction of required memory by $(n/N)^2$.

First, the energy dependent contact self-energies are calculated within the transfer matrix method of [5] and folded into the device Hamiltonian to represent an open system through the nonhermitian Hamiltonians $H(E)$ for each considered energy E. For every $H(E)$, those n right sided eigenstates are calculated that have eigenvalues closest to E. These eigenstates represent the n columns of a rectangular transformation matrix T (N rows and n columns). The NEGF equations are transformed by T into the smaller Hilbert space and solved therein.

RESULTS

The new method is demonstrated in a squared Si nanowire with 5nm diameter in a $sp^3d^5s^*$ tight binding representation [5] that is small enough such that the exact solution can be computed. Actually, 10% of the original matrix rank is sufficient to reliably solve the transport problem as shown in Figs. 1-4: Figure 1 shows the density through the center in Fig. 2. Figure 2 shows the small deviation in electron density; Figures 3 and 4 show the transmission for valence and conduction band of both cases. Both electron density and transmission can be reproduced with 10% of the matrix rank. The observed speed up factor of 8 is effectively limited by the solution of the eigenvalue problem. Nevertheless, the reduced problem rank allows solving NEGF equations beyond common computational limitations: Figures 5 and 6 show the transmission for a 12nm cross-section nanowire in the same tight binding representation, when the matrix rank is reduced down to 10%. This calculation was done on only 288 CPUs in 2200 minutes, whereas an exact calculation is a task for high-end supercomputers and has not been attempted.

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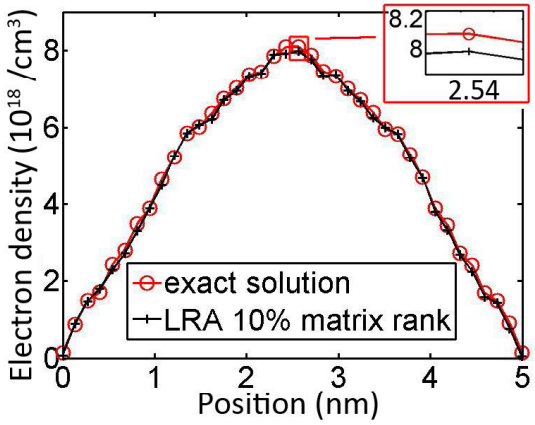

Fig. 1. Electron density through the center in Fig. 2, of the exact NEGF calculation (circle) and of NEGF calculations with 10% of the original matrix rank.

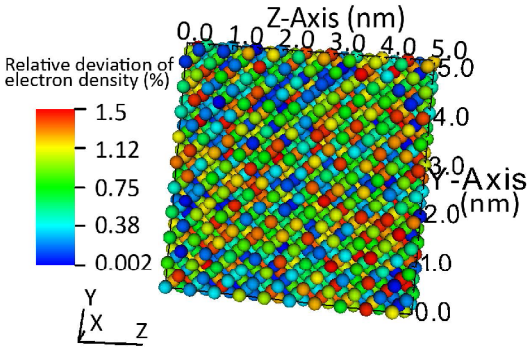

Fig. 2. Relative deviation in electron density in a squared, 5nm diameter Si nanowire of the exact NEGF calculation and of NEGF calculations approximated with 10% of the original matrix rank. Transport is along the x-axis.

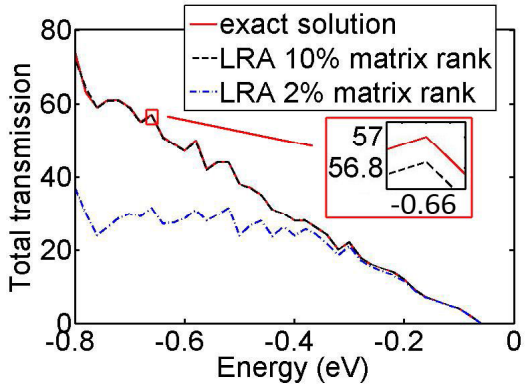

Fig. 3 Total transmission of the exact NEGF calculation (solid) and of NEGF calculations with reduced matrix rank for the valence band of the 5nm diameter Si nanowire in Fig.2.

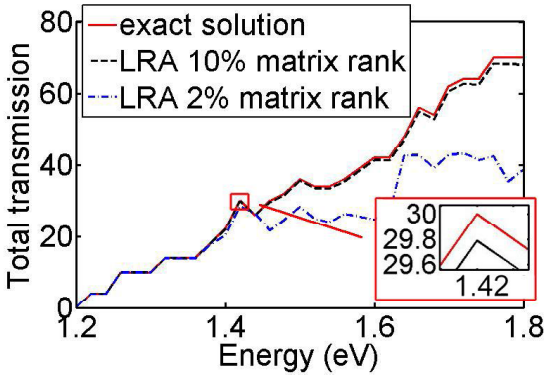

Fig. 4 Total transmission of the exact NEGF calculation (solid) and of NEGF calculations with reduced matrix rank for the conduction band of the 5nm diameter Si nanowire in Fig.2.

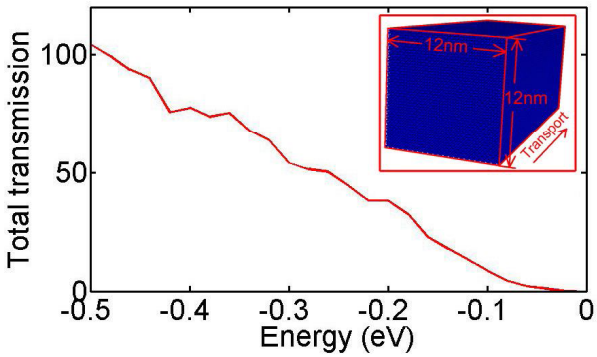

Fig. 5. Total transmission calculated with 10% of the original matrix rank for the valence band of a 12nm diameter Si nanowire. The inset shows the schematic of the nanowire.

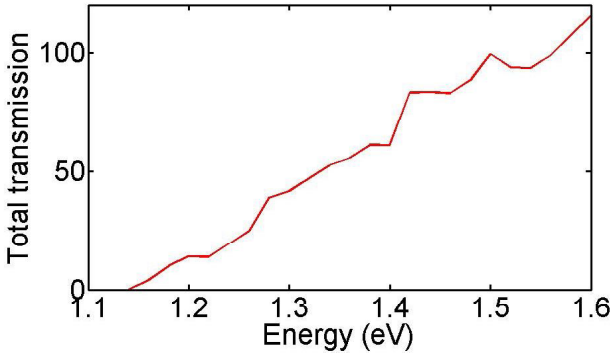

Fig. 6. Total transmission calculated with 10% of the original matrix rank for the conduction band of the 12nm diameter Si nanowire.