# Efficient solution algorithm of non-equilibrium Green's functions in effective mass approximation

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## INTRODUCTION

The non-equilibrium Green's function (NEGF) method is widely accepted as the most general method for realistic quantum transport. However, the NEGF method suffers from a large computational burden: it requires matrix inversions and matrix-matrix multiplications which scale cubically with the matrix rank. Several methods have been implemented to overcome this burden [1-3], but these methods either require very specific transport geometries or they are limited to coherent transport only. In this work, it is demonstrated how the concept of low rank approximation [4] can be applied to solve electronic NEGF equations in an effective mass representation. In this way, Green's functions and self-energies are solved without loss of accuracy, but with a fraction of the original computational costs.

## METHOD

Electrons are given in a single band effective mass Hamiltonian. Different materials are considered with different conduction band offsets and spatially varying effective masses.

All NEGF equations are transformed from their real space representation of rank $N$ into a Hilbert space of rank $n < N$ which gives a maximum possible speedup of $(n/N)^3$.

In the first step of this method, electrons are represented in spatial Eigen function representation with $N$ homogeneously distributed spatial grid points. The $n$ Eigen states $\Phi_i$ of the smallest $n$ Eigen energies of the device dependent Hamilton operator with Neumann boundary conditions in this real space represent the $n$ columns of a rectangular transformation matrix $T$ ($N$ rows and $n$ columns). This matrix $T$ transforms operators of the real space into a reduced Hilbert space $H1$ (similar to Ref.[5]). In the second step, the position operator $x$ is transformed via $T$ and $T^\dagger$ into the space $H1$ and its Eigen vectors $\varphi_j$ are calculated therein. The Eigen values of these Eigen vectors define a new real space $H2$ on which the local scattering self-energy for inelastic scattering on acoustic phonons is defined (in self-consistent Born approximation following Ref.[6]). Once the NEGF equations are solved in $H2$, observables are transformed back into the original real space of dimension $N$. Note that the NEGF equations are solved exactly, when $n = N$.

## RESULTS

Figure 1 shows a comparison of $I$-$V$ characteristics of 40nm GaAs/$Al_{0.3}Ga_{0.7}As$ resonant tunneling diode attached to a homogeneous 40nm GaAs layer calculated with the full rank ($n = N$), with 10% ($n = 0.1\ N$) and 3.75% ($n = 0.0375\ N$) of the original matrix rank, respectively. Here, the original matrix rank is $N = 160$. The matrix rank can be reduced down to 10% without loss of the predictive power of the NEGF method for the $I$-$V$ characteristics. The same is true for the electron density as shown in Fig. 2 at the resonance voltage $V$ = 0.14V. Energy resolved data that is vital for device analysis is also correctly predicted with only 10% of the original matrix rank. This can be seen by the comparison of Figs.3 and 4 which show the energy and spatial resolved density $n(z, E)$ at resonance bias. Deviations of $n(z, E)$ in Fig. 4 can only be found in details of the interference pattern. In a preliminary code prototype, calculations with 10% of the original matrix rank are **150 times faster** than calculations with the full rank.

Financial support by China Scholarship Council (No.2009601231) is acknowledged. Computational resources from nanoHUB.org and support by National Science Foundation (NSF) (Grant Nos.

EEC-0228390, OCI-0749140) are acknowledged. This work was also supported by the Semiconductor Research Corporation's (SRC) Nanoelectronics Research Initiative and National Institute of Standards & Technology through the Midwest Institute for Nanoelectronics Discovery (MIND) and SRC Task 2141.

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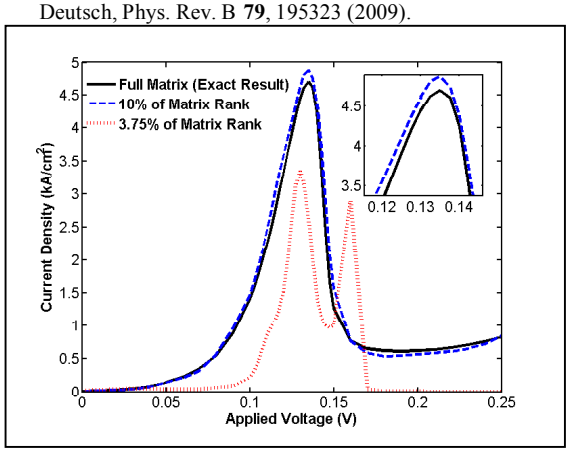


Fig. 1. Current voltage characteristics of the GaAs/$Al_{0.3}Ga_{0.7}As$ resonant tunneling diode described in the main text. The NEGF results were calculated using the full matrix (exact result) as well as only 10% and 3.75% of the matrix rank.

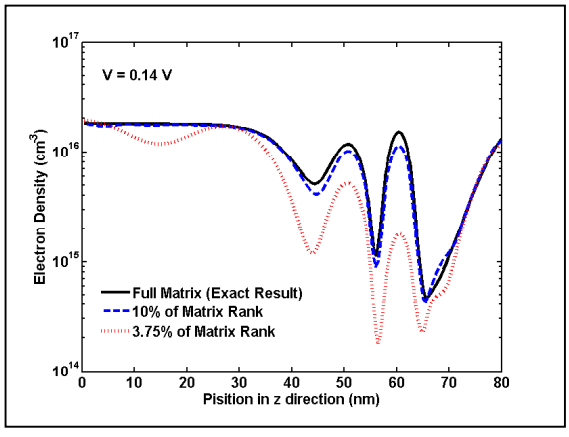


Fig. 2. Electron density of the GaAs/$Al_{0.3}Ga_{0.7}As$ resonant tunneling diode described in the main text at a voltage of $V$=0.14V. The NEGF results were calculated using the full matrix (exact result) as well as only 10% and 3.75% of the matrix rank.

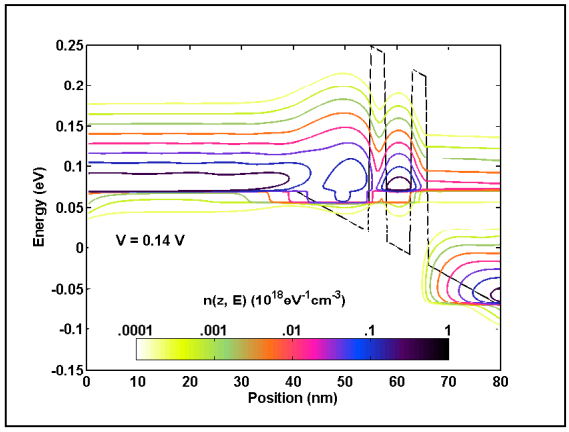


Fig. 3. The exact spatial and energy resolved electron density of the device in Fig.2.

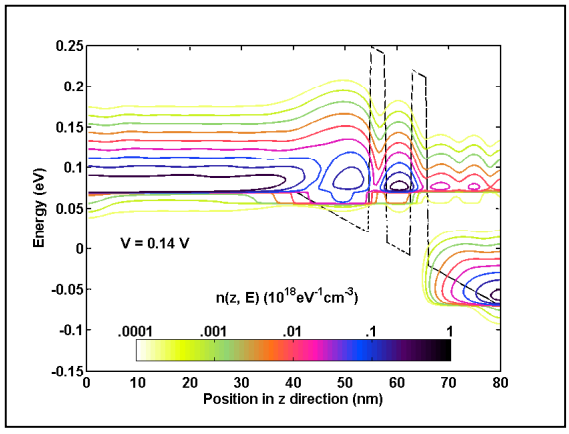


Fig. 4. The spatial and energy resolved electron density of Fig.2 when the NEGF equations are solved with only 10% of the original matrix rank.