Low Rank Approximation Method for Efficient Green’s Function Calculation of Dissipative Quantum Transport

Lang Zeng,1,2,3 a) Yu He,2,3 Michael Povolotskyi,3 XiaoYan Liu,1 Gerhard Klimeck,2,3 and Tillmann Kubis3 b)

1) Key Laboratory of Microelectronic Devices and Circuits, Institute of Microelectronics, Peking University, 100871, P. R. China
2) School of Electrical and Computer Engineering, Purdue University, West Lafayette, USA 47907
3) Network for Computational Nanotechnology, Purdue University, West Lafayette, USA 47907

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In this work, the low rank approximation concept is extended to the non-equilibrium Green’s function (NEGF) method to achieve a very efficient approximated algorithm for coherent and incoherent electron transport. This new method is applied to inelastic transport in various semiconductor nanodevices. Detailed benchmarks with exact NEGF solutions show 1) a very good agreement between approximated and exact NEGF results, 2) a significant reduction of the required memory, and 3) a large reduction of the computational time (a factor of speed up as high as 150 times is observed). A non-recursive solution of the inelastic NEGF transport equations of a 1000 nm long resistor on standard hardware illustrates nicely the capability of this new method.

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I. INTRODUCTION

Modern semiconductor devices have reached such small dimensions that carrier confinement, interference effects and tunneling play an equally important role as incoherent scattering, momentum and energy relaxation do.1–4 The non-equilibrium Green’s function (NEGF) method is among the most widely employed methods to describe carrier dynamics in open quantum systems. In fact, the NEGF method is applied to a constantly growing variety of systems ranging from phonon transport,24–25 spin transport,26–28 electron dynamics in metals,19–23 organic molecules,17–19 and fullerenes,14–15 and semiconductor nanostructures.29–31 Unfortunately, the basic NEGF equations are numerically cumbersome and extremely time demanding to solve. Therefore, several different approximations for particular devices and situations have been developed to reduce the numerical costs. The recursive Green’s function method reduces the peak numerical burden to a device dependent sub-block matrix of the system’s hamiltonian, and the computational cost scales linearly with the number of blocks but cubically with the block size.24,25 It is widely used for the simulations with one transport direction such as FinFET,2–4 and nanowire structures.26 Mode space approaches in similar wire structures as well as the newly developed Equivalent transport mode method separate the transport direction from transverse confinement directions thus reducing the block size in each layer.26–28 All these methods usually require a clear distinction between the transport direction and transverse degrees of freedom. When this distinction gets blurred, as in the case of incoherent scattering, their numerical efficiency drops significantly. A very efficient method to solve ballistic NEGF equations is the contact block reduction method (CBR).29–31 However, this method does not offer self-consistent incoherent scattering capability. Niche applications of the NEGF method have used sophisticated Wannier and Wannier Stark functions to represent the transport problem in the presence of many incoherent scattering mechanisms.32–33 This specific basis representation, however, is custom made for quantum cascade lasers and superlattices.

In this work, the low rank approximation (LRA) method is adapted to the NEGF equations of electrons in semiconductors in the presence of inelastic scattering on phonons. This method is an extension of the “basis reduction method” of Greck et al.35–37 The concept of low rank approximation is inherited from data modeling in control theory,37 machine learning,38 signal processing,39 bioinformatics39 for microarray data analysis etc. In the framework of NEGF, the transport problem is transformed from the original basis representation, i.e. in this work real space in effective mass hamiltonian presentation, to a more appropriate basis of quasi-particle states that are close to the quasi-particles of the actual device. In this representation, the number of required basis functions is much less than in the original space, which allows to reduce the numerical costs significantly. In so far, this method is closely related to the before-mentioned mode space approach. However, the LRA method is a generalization to that, since it does not have any prerequisites to the device geometry. In addition, the LRA implementation of this work uses a third basis represen-

a) Electronic mail: langzeng@ime.pku.edu.cn
b) Electronic mail: tkubis@purdue.edu
tation to enable real space defined inelastic scattering mechanisms.

In Sec. III the method of this work is introduced, its numerical complexity is analyzed and differences of this method with existing approximations are discussed. In Sec. IIII transport in homogenous resistor and a resonant tunneling diode is calculated. The comparisons of exact NEGF calculations with the LRA approximated results show the accuracy of the presented method. Limitations that this method (as every approximation approach does) faces are also discussed in this section. To exemplify the computational strength of the LRA method, electronic transport in a 1000 nm resistor is calculated in the end of this section. Energy resolved density spectrum illustrates the transition from ballistic to drift diffusion transport in this resistor. The paper concludes with a summary in Sec. IV.

II. METHOD

A. Low Rank Approximation Method

NEGF calculations are time consuming since they involve the inversion and multiplication of matrices with the rank \( N \) of the system’s hamiltonian. The fundamental concept of the LRA method is to reduce the computational cost by transforming the NEGF equations into a space of lower rank \( n \) and solving the equations therein. It is expected that the closer the basis functions of the lower rank space are to the physically relevant quasi-particles of the device, the better the LRA approximation is and the smaller the ratio \( n/N \) can be chosen. The solution of the NEGF equations and all observables can be transformed back into the original space after self-consistent calculation is achieved. In this way, the matrices that represent the Green’s functions and self-energies still have the lower rank \( n \), but the dimensionality \( N \) which is required to maintain compatibility with other equations (such as the Poisson equation) that might still be given in the original space.

This method is exemplified on the stationary vertical transport in laterally homogeneous quantum well heterostructures that are in contact with two charge reservoirs. The electron structure is represented in terms of a single band effective mass hamiltonian \( H_0 \) that is represented in a basis of \( N \) position eigenfunctions

\[
H_0 = \frac{-\hbar^2}{2m^*} \frac{d}{dz} \frac{1}{m^*(z)} \frac{d}{dz} + \frac{\hbar^2 k_{||}^2}{2m^*} + V(z),
\]

where \( k_{||} \) is the in-plane electron momentum and \( V(z) \) represents a position dependent potential. In the NEGF formalism, stationary transport is determined by four coupled partial differential equations

\[
\begin{align*}
G^R &= \left( E - H_0 - \Sigma^R \right)^{-1}, \\
G^< &= G^R \Sigma^< G^R, \\
\Sigma^< &= G^< \Sigma^D, \\
\Sigma^R &= G^R D^R + G^R D^< + G^< D^R. 
\end{align*}
\]

Here, the electronic retarded and lesser Green’s functions are given by \( G^R, G^< \), respectively. \( D \) is the sum of all environmental Green’s functions that incorporate e.g. phonons, and \( \Sigma \) denotes the self-energies. The devices are in contact with two charge reservoirs, represented with contact self-energies. If not explicitly stated otherwise, all calculations in this work include inelastic scattering by longitudinal acoustic phonons given by the scattering self-energies.

\[
\Sigma_{ac}^< = \frac{1}{(2\pi)^3} \frac{k_B T D_{ac}^2}{2\rho v_s^2} \\
\times \int dq dq e^{i[q|z-z'|]} \left[ \tilde{G}_{<,R}^< \left( z, z', \left| \vec{k}_|| - \vec{q}_|| \right|, E + \hbar\omega_q \right) + \tilde{G}_{<,R}^< \left( z, z', \left| \vec{k}_|| - \vec{q}_|| \right|, E - \hbar\omega_q \right) \right],
\]

with the energy-averaged Green’s functions

\[
\tilde{G}^< \left( z, z', q_{||}, E \right) = \frac{1}{2\hbar\omega_{D_{ac}}} \int_{E-h\omega_{D_{ac}}}^{E+h\omega_{D_{ac}}} dE' G \left( z, z', q_{||}, E' \right).
\]

The acoustic deformation potential and the material density is denoted by \( D_{ac} \) and \( \rho \), respectively. The acoustic phonon frequency is \( \omega_q \) and \( v_s \) is the sound velocity. The Debye frequency \( \omega_{D_{ac}} \) limits the width of the average.

As the first step of this method, the \( n \) eigenfunctions of the free particle Hamiltonian \( H_0 \) with Neumann boundary conditions are solved that have smallest eigen energy \( E_i \)

\[
H_0 \phi_i = E_i \phi_i, \quad i = 1, 2, \ldots, n.
\]

Hereby, \( n \) is chosen such that the energy \( E_n \) is about several \( k_B T \) above the highest chemical potential of all leads (with the Boltzmann constant \( k_B \) and the temperature \( T \)). Thereby, all quasi-particles with energies below \( E_n \) are appropriately considered in the calculation. This is essential to capture all occupied electronic states and to predict the density accurately. It is worth to mention that if only the transmission around a given energy \( E_0 \) is required, it is sufficient to consider eigenstates of a few \( k_B T \) around \( E_0 \).

In the second step, the \( n \) orthonormal eigenstates \( \phi_i \) are set into the \( n \) columns of a \( N \times n \) dimensional matrix \( S \). This matrix \( S \) is unitary in the \( n \) dimensional space \( \Omega \) spanned by the wavefunctions \( \phi_i \), but note that it is not unitary in the \( N \) dimensional real space of step one

\[
S^\dagger S = I.
\]
To define the locality/non-locality of scattering self-energies, the position operator of the real space discretization $X$ is transformed into the reduced rank basis in the third step

$$X_S = S^T X S.$$  

The position operator $X$ is a diagonal matrix, whereas the reduced rank matrix $X_S$ is a dense matrix. Therefore, the operator $X_S$ is diagonalized to find the reduced rank position eigenfunction basis \{\psi_i\}

$$X_S \psi_i = x_i \psi_i, \ i = 1, 2, \ldots n.$$  

These orthonormal basis functions \{\psi_i\} define the columns of a squared, unitary $n \times n$ transformation matrix $P$. In the basis \{\psi_i\} the NEGF equations Eqs. \ref{eq:negf} read

$$G_P^R = (P^T T^T (E - H_0) T P - \Sigma_P^R)^{-1},$$

$$G_P^\Sigma = G_P^R \Sigma_P^\Sigma G_P^R,$$

$$\Sigma_P^\Sigma = \Sigma_P^R D_P^R,$$

$$\Sigma_P^R = G_P^R D_P^R + G_P^R D_P^\Sigma + G_P^\Sigma D_P^R.$$  

Since every basis function $\psi_i$ is associated with a position $x_i$ the equations above are discretized in a reduced rank real space representation. Position dependent scattering self-energies such as the acoustic phonon scattering self-energy in Eq. \ref{eq:acoustic} are then self-consistently solved with the non-equilibrium Green’s functions in the numerically efficient reduced rank real space. The introduction of the reduced real space helps to avoid the back-transformation of the Green’s functions into the original real space in the self-consistent calculation when position dependent scattering self-energy is calculated.

Once the NEGF equations Eqs. \ref{eq:negf} are converged, the diagonal and the first off-diagonal elements of $G^\Sigma$ are transformed back into the original rank $N$ real space representation. Observables such as the density or the current density can then be evaluated in the original, high resolution real space. However, the rank of the Green’s functions in the $N$ dimensional system equals the dimension of the space they are solved in, i.e. the rank equals $n$. The smaller $n$ is compared to $N$, the more reliable the $N$ dimensional spatial information is, i.e. the stronger deviations of the LRA results from the exact results are. It will be shown as one of the example results in the next section, that the LRA approximated current density oscillates in the original space, although the physical current of exact calculations is conserved. To predict current voltage characteristics in the LRA method, this inhomogenous current density is averaged over the device excluding areas within $\Delta N/n$ from the leads (where $\Delta$ is the average mesh point distance in the original real space representation).

### B. Comparison with existing efficient NEGF algorithms

It is important to highlight some differences of this method with other, well established efficient NEGF algorithms such as the CBR method\textsuperscript{26,27}, mode space approach\textsuperscript{45,46} and recursive Green’s function method\textsuperscript{24}.

In the CBR method, the NEGF equations are first transformed into an efficient representation to utilize the fact that ballistic calculations require only some sections of the retarded Green’s function $G^R$ to be solved. A rectangular transformation that reduces the rank of the NEGF equations is applied only after that first transformation. Although the CBR method is very efficient, it is fundamentally limited to ballistic calculations.

The mode space approach assumes a separation Ansatz for the wave functions of propagating quasi-particles. Typically, the Ansatz requires confined modes or plane waves perpendicular to the transport direction. The mode space approach allows a significant rank reduction of the NEGF equations. The computational burden is even further reduced if these modes are well separated in energy and the particle propagation does not couple different modes. However, if the device contains inhomogeneities (impurities, non conformal confinement, etc.) the number of the modes is no longer a conserved quantum number. Then, the modes are coupled and the rank of the mode space has to be large to predict transport without loss of accuracy.

The recursive Green’s function method allows to limit the calculation of the retarded Green’s function to selected parameter intervals of the propagation space (i.e. sub-matrices of $G^R$, when $G^R$ is represented in matrix form). This allows limiting ballistic NEGF calculations on the required elements of $G^R$ only, which results in much faster transport solutions than the case when the complete $G^R$ is solved.\textsuperscript{24} NEGF that includes incoherent scattering, however, requires the full $G^R$ which deteriorates the advantages of this recursive method.

In contrast to these three methods, the LRA method allows the inclusion of any incoherent scattering as well as arbitrary device geometries. The ”modes/sub-block matrix” of the LRA method are device dependent wave functions that automatically include non-conformal confinement - if such confinement appears.

### C. Numerical Complexity and Memory Usage Analysis

Coherent quantum transport calculations for realistically extended devices have been shown to efficiently consume the computational power of over 220,000 processing cores.\textsuperscript{45,46} Incoherent NEGF based calculations require about 100x more computational power, are limited to generally unrealistical small structures, and can only scale to about 100,000 cores.\textsuperscript{47,48} Involving incoherent scattering in realistically extended devices requires dramatically large computational resources.
The numerical complexity and memory usage of self-consistent NEGF calculations reduce when the LRA method is applied. To qualify that, this section compares the number of floating point operations and the memory usage of a "conventional" NEGF calculation with an approximated ballistic NEGF solution that employs the LRA method. In the following, the transport problem is assumed to be originally discretized with \( N \) orthogonal basis functions. Within the LRA method, the rank of the NEGF equations is reduced down to \( n \). The energy and other conserved quantum numbers of the NEGF equations are resolved with a mesh of \( N_E \) points. To get a conserved current density within the self-consistent Born approximation, \( N_i \) iterations of the Green’s functions and self-energies are required. The integral in Eq. (3) is solved with \( N_{ph} \) energy points.

**Exact NEGF:** The exact solution of one retarded Green’s function involves the inversion of a \( N \) dimensional matrix which requires \( O(N^3) \) floating point operations. The solution of each lesser Green’s function involves two matrix-matrix products with a numerical load of \( O(N^3) \) floating point operations. The solution of the local scattering self-energy of Eq. (3) is \( O(N_{ph} \times N) \) for each energy point in each iteration. In total, solving the NEGF equations exactly requires \( N_E \times N_i \times (O(N^3) + O(N_{ph} \times N)) \) floating point operations, while the memory needed to store the matrix representation of Green’s functions and self-energies is \( N_E \times O(N^2) \) floating point numbers.

**Approximate NEGF:** The LRA method can be decomposed into three steps: 1) the transformation of the NEGF equations into the reduced space, 2) the solution of the NEGF equations within the reduced space and 3) the back-transformation of some relevant results into the original space. Step 1) requires first to get the eigen states that construct the transformation matrix, i.e. \( O(N^2n) \) floating point operations. The memory used to store the transformation matrix is \( O(Nn) \) floating point numbers. The transformation of the device’s Hamiltonian into the reduced space requires then \( O(N^2n) \) floating point operations. The contact self-energies have to be transformed for every energy point in every iteration. Since the contact self-energy is zero except for the mesh points adjacent to the leads in the original space, each transformation requires only \( N_E \times N_i \times O(n^2) \) floating point operations and \( N_E \times O(n^2) \) floating point numbers to be stored. Solving the NEGF equations in the reduced space in step 2) requires \( N_E \times N_i \times O(n^3) \) floating point operations and memory usage of \( N_E \times O(n^2) \) floating point numbers. The calculation of the acoustic phonon self-energy costs \( O(N_{ph} \times n) \) operations in the reduced real space for each energy point in each iteration. To calculate the energy resolved densities and current densities in the original space, the step 3) requires to back-transform the diagonal and the two first off-diagonals of \( G^\langle \) of the original space. This transformation requires \( N_E \times O(Nn^2) \) floating point operations and memory usage of \( N_E \times O(N) \) floating point numbers.

In a typical effective mass NEGF calculation, the simulation setup reads \( N = 100, n = 10, N_E = 1000, N_i = 10 \) and \( N_{ph} = 10 \). According to the analysis above, the numerical complexity of standard NEGF calculation in the typical effective mass situation is \( O(10^{10}) \) floating point operations, and the memory usage is \( O(10^7) \) floating point numbers; the numerical complexity of LRA approximated NEGF calculation is \( O(10^7) \) floating point operations, and the memory usage is \( O(10^5) \) floating point numbers. This observation demonstrates clearly that LRA method can reduce both numerical cost and memory usage significantly.

The comparison of the amount of floating point operations and memory usage between the exact and the approximated LRA approach illustrate that the LRA method offers approximated solutions of the NEGF equations much faster and with a much smaller memory load than the exact solutions. In fact, one can easily find NEGF equations of state of the art devices that are only solvable when the LRA method is applied. To illustrate this, section III.C shows LRA approximated NEGF results of a 1000 nm homogeneous resistor with inelastic acoustic phonon scattering calculated on single CPU.

### III. RESULTS AND DISCUSSIONS

All devices in this section are laterally homogeneous layers grown in the \( z \)-direction. Stationary transport along the \( z \) direction is calculated for conduction band electrons in the effective mass approximation. In the original real space discretization (i.e. before LRA transformations are applied), the Green’s functions and self-energies are functions of two propagation coordinates \( z \) and \( z' \), the absolute in-plane momentum \( k \) and the electron energy \( E \). All devices of a given length \( L \) are considered to be in contact with two charge reservoirs at \( z = 0 \) and \( z = L \), respectively.

#### A. Homogeneous structure

Conduction band electrons of a 50 nm thick, homogeneous layer of GaAs with an effective mass of \( m^* = 0.067 \, m_e \) are considered in this section. The NEGF equations are discretized with a 0.5 nm mesh spacing. The Fermi energies in both leads are assumed to agree with the respective conduction band edge. The temperature is set to 300 K. The conduction band in the device is set to be constant in the first and last 5 nm of the device and to drop linearly by the amount of the applied bias voltage in the central 40 nm of the device.
are strongest close to the leads.

The electron density in the homogenous layer of GaAs in equilibrium and at finite applied bias voltage. In both cases, the deviations from the exact solution stronger, if the rank of the NEGF equations is reduced more: Figure 2 shows the electron density in the original real space indicate this kind of violation of particle conservation. Similar to previous figures, the deviation of the LRA approximated from the exact NEGF results is larger, the larger the rank reduction is. Nevertheless, a reduction of rank to 10\% is still able to well reproduce the I-V characteristics, since only a small fraction of electronic states in the low energy range contributes to the current density. In contrast, results of exact NEGF calculations with a ten times coarser grid deviate significantly from the full rank result: Such a coarser real space mesh yields a different effective electron dispersion\(^{29,31}\) that deviates from the parabolic dispersion within the relevant energies.

It is worth to mention that the boundary conditions for the electronic wave functions of Eq. (5) are relevant for the efficiency of the LRA method. In agreement to similar findings of Mamaluy et al.\(^{29–31}\) basis functions with Dirichlet boundary conditions turned out to be inferior to Neumann conditions.

The LRA method and standard NEGF calculations were implemented in Matlab with 8 cores parallelization. For this concrete homogeneous structure calculation, the

**Figure 1.** Spatially resolved current density in the homogenous structure described in the main text Sec. IIIA with a linear potential drop of 0.2 eV. The lines show result calculated with the NEGF method solved exactly (solid) and with the NEGF method solved approximately with a reduction of the matrix rank down to 20\% (dashed) and 10\% (dash-dotted).

Both of the above figures indicate that the LRA method can reproduce exact NEGF results in the device center up to close to the leads. This motivated the device average of the current density described in Sec. IIIA. All remaining current densities in this paper are such device averaged results.

**Figure 2.** Calculated electron density of the homogeneous device of Fig. 1 in equilibrium (a) and when a linear potential drop of 0.2 eV is assumed (b). Results of an exact NEGF calculation (solid) are compared with approximated NEGF calculations where the NEGF equations’ matrix rank is reduced down to 20\% (dashed) and 10\% (dash-dotted).
measured computational time for matrix rank reductions down to 10% and 20% is reduced by factories of 35X and 87X respectively compared to the full solutions, as listed in Table I. In our non-optimized LRA Matlab implementation, most of the time is spent to transform Green’s functions between different basis representations. If further optimization on matrix transformation is performed (as discussed in Sec. II C), the factor of speed up can be even larger.

B. Resonant tunneling diode

This section explores the compatibility of the LRA method in quantum confined systems. The NEGF equations are solved in a 80 nm GaAs/Al_{0.3}Ga_{0.7}As resonant tunneling diode (RTD) structure at 100 K. The RTD consists of two 3 nm wide Al_{0.3}Ga_{0.7}As barriers and a 5 nm quantum well in the center. In addition, a 40 nm flat band region is located at emitter region. The effective mass for GaAs is 0.067 m_0 and 0.0919 m_0 for Al_{0.3}Ga_{0.7}As. The band offset between these two materials is 230 meV. In the original real space representation, the device is discretized with a grid spacing of 0.5 nm. The Fermi energies in the leads are set 0.005 eV beneath the respective conduction band edges. The potential profile is assumed to be constant in the left most 40 nm and to drop linearly in the remaining RTD region. This is illustrated by the solid line in Fig. 3 (a) and (b) which show the same assumed conduction band profile of the RTD in an exact NEGF calculation (a) and a 10% LRA approximated NEGF calculation (b).

The effective mass for GaAs is 0.07 eV and positions z ∈ [65, 80]. Even the confined state in the triangular quantum well locating at left of the first RTD barrier (at energy of about 0.07 eV and position 50 nm) is well reproduced in the LRA calculation. This is remarkable, since electrons can enter this state effectively only via inelastic scattering. Therefore, inelastic scattering and tunneling are well reproduced with the LRA method. That can also be seen in Fig. 5, which shows the I-V characteristics of this RTD structure calculated in the exact NEGF method, as well as in the LRA method with 10% and 3.1% of the original matrix rank. Neither the current amplitude nor the resonance value get significantly altered when the NEGF equations are solved with only 10% of the original matrix rank. If the matrix rank is reduced too much, electronic states that are relevant for the transport are neglected. Consequently, the current density starts to deviate then. This is illustrated in Fig. 5 with the I-V characteristic results of a LRA approximated NEGF calculation of only 3.1% of the original matrix rank. As stated in Sec. II A, the ratio of the matrix rank reduction can be estimated from the energy interval in which the states are occupied.

For this RTD example, the measured computational time for matrix rank reductions down to 10% and 20% is reduced by factories of 39X and 150X respectively compared to the full solutions, as listed in Table II.
The new LRA method is not only more efficient than the standard NEGF approach, it also opens up a space of device configurations that previously could not be tackled. This section considers electronic transport in the presence of inelastic phonon scattering in a 1000 nm long homogeneous GaAs layer. In the range of 100 nm within the source and the drain contact/device interface, the conduction band is assumed to be constant. In the remaining device, the conduction band drops linearly according to the applied bias voltage. The temperature of the phonon bath and the electrons in the leads is 300 K according to the applied bias voltage. The temperature of the system is originally discretized with a mesh spacing of 1 nm. The resulting NEGF equations are approximated with a 20% matrix rank. This reduces the numerical complexity of the NEGF equations such that they have been solved on a single CPU without recursive approaches. The nature of the transport is tuned from purely ballistic to almost drift diffusion like by increasing the deformation potential $D$ of the phonon scattering self-energy of Eq. [3]. Hereby, three different scattering potentials have been considered: 27 eV, 60 eV and 135 eV, which corresponds to a scattering rate of $1 \times 10^{12}$ s$^{-1}$, $5 \times 10^{12}$ s$^{-1}$ and $2.5 \times 10^{13}$ s$^{-1}$ for electrons with kinetic energy of 0.3 eV. The impact of the scattering is illustrated in Fig. 6 as it shows the calculated I-V characteristics of the device with various scattering strengths. The I-V characteristic is almost ohmic in the case of a deformation potential of 135 eV. The nature of transport at this large deformation potential can be understood from Fig. 7. It shows the calculated I-V characteristics of the device at a scattering rate of 1$\times$ 10$^{12}$ s$^{-1}$, 5$\times$ 10$^{12}$ s$^{-1}$ and 2.5$\times$ 10$^{13}$ s$^{-1}$ for electrons with kinetic energy of 0.3 eV. The nature of transport at this large deformation potential can be understood from Fig. 7. It shows the calculated I-V characteristics of the device at a scattering rate of 1$\times$ 10$^{12}$ s$^{-1}$, 5$\times$ 10$^{12}$ s$^{-1}$ and 2.5$\times$ 10$^{13}$ s$^{-1}$ for electrons with kinetic energy of 0.3 eV.
increased to almost drift diffusion like transport. Out recursion and even incoherent scattering was calculated. An exact NEGF calculation of this long structure of Fig. 6 with a deformation potential of 135 eV and a potential drop of 0.1 V.

IV. CONCLUSION

In this work, the low rank approximation method is applied to efficiently and accurately solve the approximated NEGF equations in the effective mass approximation. It is shown that this method reliably solves the electronic transport in the ballistic and incoherently scattered transport regime. Quantum effects that are natively included in the NEGF equations (such as interferences, confinement and tunneling) are accurately reproduced by the LRA method, but with a fraction of the numerical load of the original NEGF equations. This method differs from existing NEGF approximations since it allows to include incoherent scattering (in contrast to the CBR method) and does not require specific device shapes (in contrast to the mode space approach and EM method).

In this paper, the LRA method has been applied to homogeneous resistors and resonant tunneling diodes, i.e. to classical resistors and quantum confined structures. In both systems, a very good agreement of the LRA-approximated I-V characteristics and energy and spatially resolved densities with exact NEGF solutions has been demonstrated. Significant deviations of the LRA method from exact results appear only for matrix rank reductions that are too strong and neglect states relevant for transport. To show the efficiency and power of the LRA method, transport in a 1000 nm long GaAs resistor has been calculated. An exact NEGF calculation of this long device is not feasible without recursive algorithms. The LRA method, however, allowed to solve this system without recursion and even when incoherent scattering was increased to almost drift diffusion like transport.

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