Session: Quantum Transport

Non-local scattering with a new recursive nonequilibrium green’s function method

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As modern nanodevice scales continue to shrink, sophis- ticated modeling methods that cover both coherent quantum mechanical effects and incoherent scattering on device imper- fections (i.e. roughness, impurities and lattice vibrations) are needed. The non-equilibrium Green’s function (NEGF) theory is widely accepted as one of the most consistent methods to model these phenomenon [1]. Solving the NEGF equations for atomistically resolved devices requires inverting large matrices that often do not fit into memory on modern computers. Efficient algorithms for solving only the relevant portions of the inversion have been developed [2]. In particular the so-called recursive Green’s function algorithm (RGF) limits the inversion to the diagonals only. This is sufficient for observables such as charge current and density only when all considered scattering mechanisms are local. However many scattering mechanisms have significant non-local contributions and the state-of-the-art RGF is not appropriate then. This is particularly true for all scattering mechanisms involving the Coulomb interaction, such as scattering on phonons in polar materials and scattering on charged impurities [3]. This work extends the local RGF algorithm to nonlocal RGF which allows the solution of the NEGF equations including incoherent scattering up to an arbitrary number of off-diagonal elements of the Green’s functions.

The nonlocal RGF (NL-RGF) method is presented for the first time in this work. It overcomes the constraint that is typically put on solving the NEGF equations in atomistic representations, i.e. the limitation of any scattering effect to the local range only. So far, the solution of the NEGF equations including incoherent scattering is numerically too expensive if solved without the RGF algorithm in local approximation. The so far very common truncation of scattering self-energy matrices to their local component only is typically justified with these numerical constrains only [4], [5]. The starting point for the NL-RGF derivation is the RGF method developed by Anantram and coworkers which is suitable for local scattering only [6]. The RGF method generally includes two main steps after decomposing the device into layers. The first step, the so-called "forward" step, is to solve the one-sided Dyson’s equation for *gR* recursively through the layers starting with the first layer connected to the first lead. Once the last layer is reached and connected to the other lead, the last diagonal block is now solved exactly for *GR*. The other layer’s diagonal block *GR* are solved in the second step, the "backward" step. To include effects of scattering on the particle occupancy functions, the lesser Green’s function, *G<*, is also solved recursively. The local RGF prescribed in Ref. [4] can be thought of as a special case of the *LDLT* decomposition method. The forward step for gR is equivalent to solving the decomposition *LDLT* [7]. *D* and *L* are constructed with recursive generator functions. In the block tri-diagonal case, *L* is the coupling Hamiltonian between adjacent layers and does not need to be solved explicitly. Note that *gR* is the inverse of *D*. Once the forward step is done and *gR* is solved, the decomposition is used to solve the backward step and it can be shown that:

$$G^R = D^{-1} L^{-1} + (I - L^T) G^R \tag{1}$$

Similar equations can be found for forward *g<* and *G<* using the *LDLT* decomposition. From these decompositions, recursive relations have been determined in this work that are compatible with RGF and allow arbitrary number of off- diagonal blocks for non-local scattering to be solved.

Figure 1 compares the anti-diagonal of the retarded Green’s function G^R for bulk silicon in $sp3d5s*$ tight-binding basis for the full inversion case and the non-local RGF when non- local RGF is used to solve for all off-diagonal blocks. The two methods agree exactly even for far-offdiagonal elements. Figure 2 shows the timing for NL-RGF as a function of the non-locality in the transport direction for a 2 nm Silicon nanowire with a length of 20 nm in a 10 band atomistic tight- binding representation. A best polynomial fit of the simulation time gives a complexity of $N^{2.4}$, with N being the number of nonlocal blocks. Figure 3 shows the memory analysis. The increase in memory as a function of the non-locality in the transport direction is linear as expected, since the number of off-diagonal blocks stored is scaling linearly. This is much less than in the full inversion case, where the memory needed to store the full matrix is about 150 GB (the memory needed to store a complex double matrix with rank 97280). To confirm the non-locality in polar optical phonon scattering is treated correctly, the anti-diagonal of the retarded scattering self- energy for a bulk GaAs system is shown in Fig. 4. Figure 4, also compares the scattering self-energies solved in the new

NL-RGF method with the full inversion results. The fact the results are identical confirms the correctness of the presented method.

The Recursive Green's Function method was augmented to support non-local scattering self-energies. The timing and memory performance was demonstrated on a silicon nanowire in tight-binding with non-local scattering that previously could not be solved due to memory constraints. The correctness of the method was illustrated on polar optical phonon scattering self-energies in bulk GaAs. This algorithm is implemented into the NEGF framework of the nanodevice simulation software NEMO5 (academic open source).

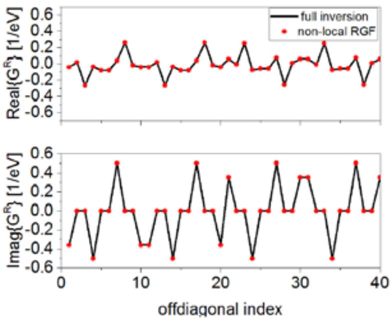

Fig. 1. Comparison of G^R for full inversion and non-local RGF for bulk silicon in *sp3d5s** tight-binding basis. Orbitals on the same atom are summed for clarity.

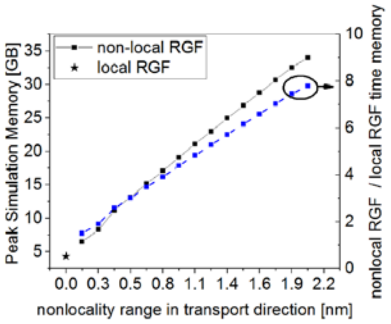

Fig. 3. Memory performance for non-local RGF as a function of non-locality in the transport direction.

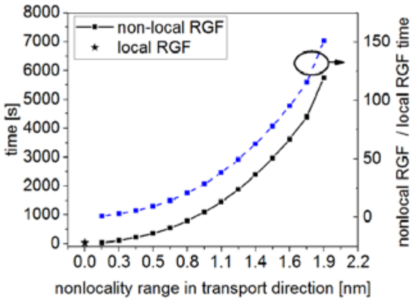

Fig. 2. Timing performance for non-local RGF as a function of non-locality in the transport direction.

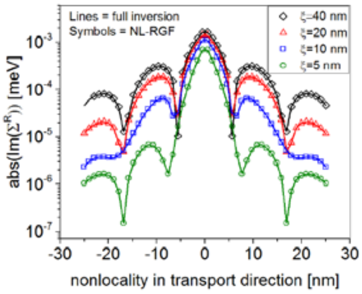

Fig. 4. Non-locality of the imaginary part of Σ^R at an energy k_BT above the bandedge for different screening lengths. For comparison, the non-locality solved using the NL-RGF method is also shown. Note that due to symmetries only the upper diagonal needs solved in the NL-RGF method.

[1] S. Datta, Superlattices and Microstructures, vol. 28, no. 4, pp. 253-278, 2000.

[2] R. Lake, G. Klimeck, R. C. Bowen, and D. Jovanovic, Journal of Applied Physics, vol. 81, no. 12, pp. 7845-7869, 1997.

[3] T. Kubis, PhD thesis, Verein zur Förderung des Walter Schottky Instituts der Technischen Universität München e.V., Garching, 2009.

[4] M. Luisier and G. Klimeck, Journal of Applied Physics, vol. 107, no.8, p. 084507, 2010.
[5] M. Luisier and G. Klimeck, Physical Review B, vol. 80, no. 15 155430, 2009.
[6] M. Anantram, M. S. Lundstrom, and D. E. Nikonov, Proceedings of the IEEE, vol. 96, no. 9, pp. 1511-1550, 2008.
[7] Krishnamoorthy, A., Menon, D., IEEE, pp. 70-72, 2013.

Plasmonic response of graphene nanoribbons

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Plasmonics, as a promising way for shrinking the size of photonic and electronic circuits, has attracted a great interest [1], [2]. Plasmons are collective excitations of surface electrons in a good conductor and can confine the electromagnetic energy beyond the diffraction limit. Conventionally, metals like gold have been used as plasmonic materials; however, because of high dissipation in these materials, plasmons cannot propagate long distances. Graphene [3], [4], a two dimensional semimetallic allotrope of carbon, has high electron mobility and has been of a great interest as a novel plasmonic material [5], [6], [7], [8].

Graphene has a gapless electron band structure with Dirac cones; so, its plasmon dispersion is different from the plasmon dispersion in quasi-two-dimensional (quasi-2D) electron systems with a parabolic band structure. The plasmon resonances in graphene typically fall into the terahertz and mid-infrared range. Unlike in metals, the carrier density in graphene can be controlled by applying a gate voltage, which provides plasmon-resonance tunability. However, it has been shown that gaining tunability by putting graphene on substrate reduces the plasmon propagation length [7]. However, by lowering the system dimension and moving from graphene to graphene nanoribbons, one can decrease the electron scattering rates. Thus, supported graphene nanoribbons (GNRs) have higher electron mobility and offer the tunability feature, as well.

Here, we calculate the plasmon dispersion and plasmon propagation length in armchair graphene nanoribbons (aGNRs) and zigzag graphene nanoribbons (zGNRs) via self-consistent field and Markovian Master equation (SCF-MMEF) [7]. Electrons in supported GNRs, as in every open system, interact with a dissipative environment. SCF-MMEF is able to capture all the concurrent dissipative mechanisms, such as phonons, ionized impurities, surface optical (SO) phonons, the line-edge roughness. We derive the interaction Hamiltonian for electrons and SO phonons in GNRs, and quasi-one-dimensional (quasi-1D) systems in general. The SO phonon and electron interaction only requires the momentum conservation along the length of the ribbon. This means that a single electron transition can be mediated by a number of SO-phonon modes, unlike in the quasi-2D systems. As a result, in narrow GNRs, SO-phonon scattering is as important as ionized impurity scattering for electron transport.

By calculating the dielectric function via the SCF-MMEF, we calculate the loss function for GNRs on the SiO_2 substrate. The loss function peaks at the plasmon resonances. The higher the peak, the farther the plasmons propagate. In zGNRs, because of heavy carriers (flat energy dispersions) and high scattering rates, plasmons are highly damped and the plasmon propagation length barely exceeds 100 nm. The same behavior happens in ($3N$)-aGNRs and ($3N+1$)-aGNRs, where N is an integer and $3N$ and $3N+1$ are the number of dimer lines. However, in ($3N+2$)-aGNRs, plasmons can propagate up to a micron. In Fig. 1, the loss function of three different ($3N+2$)-aGNRs on SiO_2 is shown. The sheet electron density is $ns = 7 \times 10^{12}$ cm^{-2}, and the impurity density is $N_i = 4 \times 10^{11}$ cm^{-2}. By increasing the width of the ($3N+2$)-