Inelastic scattering in nano-devices: One-shot current conserving approach

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In the last twenty years the non-equilibrium Green's functions (NEGF) formalism has demonstrated its efficiency to model quantum transport in nanoscale devices [1]. In particular, NEGF formalism has been extensively developed to treat inelastic scattering. The description of inelastic scattering by phonons and/or photons is based on the so-called selfconsistent Born approximation (SCBA), which is computationally very challenging when applied to realistic devices. In this work we present a one-shot current conserving approach to treat electron-phonon scattering and apply it to the modeling of n-type nano-transistors while avoiding the self-consistent SCBA procedure.

Let us start with the lowest order approximation (LOA), which within the SCBA is nothing but a perturbative expansion to first order in the interaction. We consider an ideal linear chain where electrons interact with one optical phonon mode [2]. Figure 1 shows the left (I_L) and right (I_R) currents calculated with the LOA for various arbitrary electron-phonon coupling M and applied voltages V. We note that LOA perfectly satisfies the current conservation law. Figure 2 compares the right spectral currents obtained with the ballistic regime, the SCBA and LOA. While SCBA spectrum depicts several well-resolved phonon emission peaks, the LOA only accounts for the emission of one phonon. For larger electron-phonon coupling M the LOA spectral current takes negative values signaling the failure of the LOA. Fortunately, given the ballistic current I_0 and a first-order correction ΔI, one can build the first Padé approximant, $I_0/(1 - \Delta I/I_0)$, to analytically-continue the perturbative Born series [3]. This is the simplest current-conserving one-shot approximation. We illustrate the application of the LOA and LOA analytically continued (LOA-AC), by considering electron-phonon scattering in Silicon double-gate and nanowire transistors (Fig. 3(a-b)).

For DG-transistor, current degradations as a function of the gate voltage obtained with the three approaches (SCBA, LOA, and LOA-AC) are shown in Fig. 4. We note that LOA overestimates the current degradation while its analytic continuation faithfully reproduces the SCBA results [4].

Nanowire transistor constitutes a relevant case since its transport properties are found to be strongly impacted by electron-phonon interactions. Indeed, $I_D - V_G$ current characteristics of Fig. 5 show that LOA fails in describing the phonon scattering influence. The breakdown of the LOA is mainly due to interactions with acoustic phonons which induce negative values of current spectrum (Fig. 6). Interestingly even in this case, the LOA-AC still provides current characteristics close to those of SCBA [5].

Therefore, we present a one-shot current conserving approach well suited to model inelastic transport in n-type nano-transistors with highly doped leads. This challenges the currently adopted view that heavy self-consistent calculations are required to preserve conservation laws.

This work is supported by the QUASANOVA and SIMPSSON contracts funded by the ANR.

References

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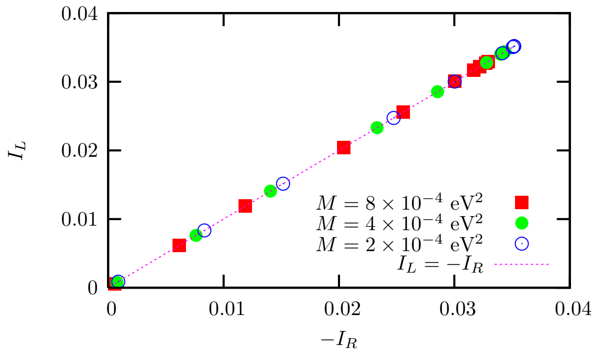

Fig. 1. Current conservation in the LOA calculated for an ideal linear chain. The model is numerically shown to exactly satisfy current conservation $I_L = -I_R$. The graph has been obtained for different electron-phonon couplings (M) and applied bias voltages (0< V <0.4 V). M represents the square of the matrix elements of the electron-phonon interaction.

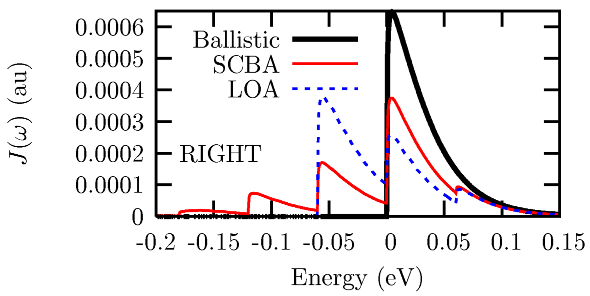

Fig. 2. Current spectrum of the linear chain at the right interface calculated in the ballistic regime (bold solid line), the SCBA (solid line) and the LOA (dashed line). $V = 0.2$ V and $M = 4.10^{-4}$ eV^2.

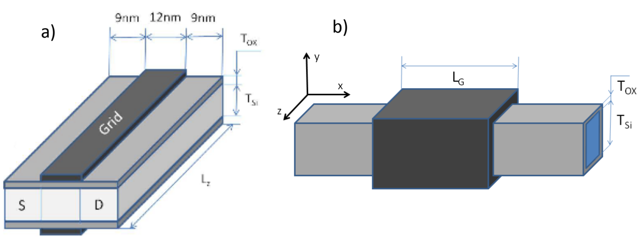

Fig. 3. Schematic representation of the devices considered in this work: a) the double-gate (DG) MOSFET and b) the nanowire (NW) MOSFET for which T_{OX}=1 nm, T_{Si}=2 nm and L_G=15 nm. Source/drain doping is N_D=10^{20}cm^{-3}.

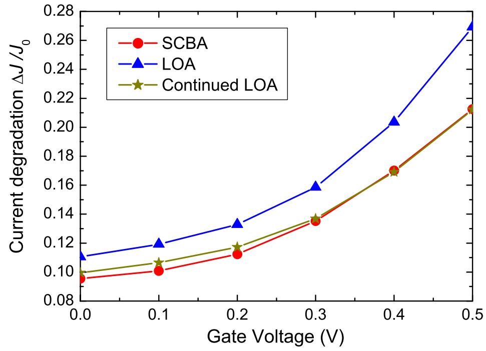

Fig. 4. Current degradation with respect to the ballistic result (J_0) when considering the SCBA (circles), the LOA (triangles) and the LOA-AC (stars) for the DG-MOSFET shown in Fig. 3a).

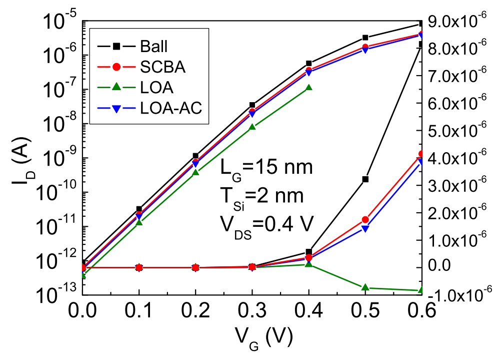

Fig. 5. $I_D - V_G$ current characteristics for Si NW transistor shown Fig. 3b), in the ballistic limit (squares), the SCBA (circles), the LOA (triangles), and the LOA-AC (reversed triangles).

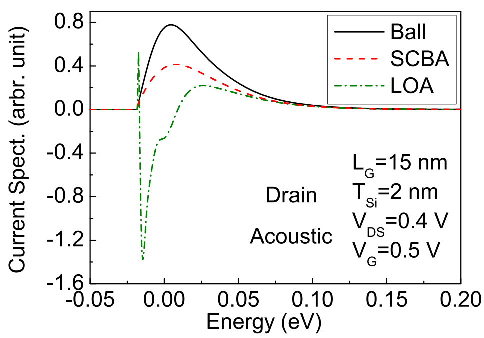

Fig. 6. Influence of acoustic phonon scattering on drain-edge current spectra in the NW transistor. Three models are shown: the ballistic regime (solid line), SCBA (dashed line) and LOA (dash-dot line).