One-shot Current Conserving Approach of Phonon Scattering Treatment in Nano-transistors

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***Abstract*—Phonon scattering can drastically influence transport properties of nanodevices. From a simulation point of view, the non-equilibrium Green's function formalism provides a natural way to include inelastic scattering in quantum transport codes, by means of self-energies. Phonon scattering is usually treated with the so-called self-consistent Born approximation which involves the evaluation of the SCBA self-energy together with the electrostatic potential; a computationally expensive self-consistent procedure. In this work we present an alternative one-shot current conserving method to treat phonon scattering and apply it to the modeling of silicon n-type nano-wire and p-type double-gate MOSFETs.**

I. Introduction

Electron-phonon scattering strongly impacts current characteristics in ultimately confined transistors [1]–[4]. Several theoretical approaches have been considered during the last decade to correctly predict their influence [5]–[7]. Among them, the non-equilibrium Green's function (NEGF) formalism [8] has been extensively developed to include inelastic scattering in quantum transport codes [9]–[15]. Unfortunately, the required computational burden to account for electron-phonon scattering in realistic devices within NEGF simulations is still very challenging. Indeed electron-phonon scattering is commonly implemented within the so-called self-consistent Born approximation (SCBA). The SCBA involves an additional loop with respect to the usual electrostatic self-consistent procedure between the charge density and the device potential through Poisson equation.

In this work we show that it is possible to treat electron-phonon scattering while avoiding the self-consistent SCBA procedure. Thus one-shot current-conserving estimates of SCBA results can, in principle, be obtained. Current-conserving lowest order approximation (LOA) described in ref. [16] and its simplest analytic continuation (LOA+AC) [17], [18] are then compared with SCBA calculations in silicon n-type nano-wire (NW) and p-type double-gate (DG) MOSFETs.

Section II details the methodology of LOA and LOA+AC starting from the usual SCBA. Section III shows their applications to the cases of n-type NW and p-type DG transistors, while Section IV summarizes the key findings.

II. One-shot approach: LOA+AC

Let's start from the SCBA scheme. Electron-phonon interactions are usually treated by solving the Dyson equation:

$$G = g + g\Sigma[G]G, \tag{1}$$

where G is the interacting Green's function, g is the non-interacting (*i.e.* ballistic) Green's function including only electrostatics and the self-energy of the reservoirs, and Σ is the electron-phonon interaction self-energy. Since G appears in both the left and right hand sides of Eq.(1), Dyson equation must be solved self-consistently. Therefore Eq.(1) is often written as $G = [g^{-1} - \Sigma[G]]^{-1}$ and it is solved within the SCBA iterative scheme:

$$G_N = [g^{-1} - \Sigma[G_{N-1}]]^{-1}, \tag{2}$$

where $G_0 = g$ and $G_\infty = G$ (if the sequence converges). In practice iteration of Eq.(2) is stopped when the criterion of convergence (*e.g.* current conservation) is reached. Self-consistency makes Σ Φ-derivable, satisfying $\Sigma[G] = \delta\Phi[G]/\delta G$, where Φ is the Luttinger-Ward functional [19]. From a computational point of view, the self-consistency associated to SCBA is numerically very expensive. It is often believed that a self-consistent approach is necessary to ensure conservation laws while it is just sufficient. What is necessary is to use a Φ-derivable approximation for Σ. Therefore non-selfconsistent conserving approximations, with well-established ranges of validity are much needed.

Our previous studies [16], [17] have shown that is possible to calculate conserving Green's functions in one shot based on the LOA Green's function, avoiding the self-consistent SCBA scheme. The main idea of the LOA is to approximate the Green's function G of Eq. (1) at the first order in the interaction. The resulting lowest order Green's function, G_{LOA} is then defined by:

$$G_{LOA} = g + \Delta g_1 = g + g\Sigma[g]g. \tag{3}$$

Since the current operator $\mathcal{I}$ is linear for g, it is possible to define an equivalent lowest order approximation for the current. Using the same notation, the current obtained from G_{LOA} is:

$$I_{LOA} = I_1 = I_0 + \Delta I_1, \tag{4}$$

where I_0 is the zero order ballistic current given by the non-interacting g, ΔI_1 is the component resulting from the first order of the Green's function of Eq.(3), $g\Sigma[g]g$. LOA is the simplest approximation able to include electron-phonon scattering. As already discussed in Ref. [16], LOA can only account for one phonon processes, making its direct application to the modeling of nano-transistors questionable. Indeed we showed that it provides accurate results only for weak interactions and that it could generate unphysical negative current spectra. We then introduce the LOA+AC, by combining LOA with a simple, physically motivated, analytic technique.

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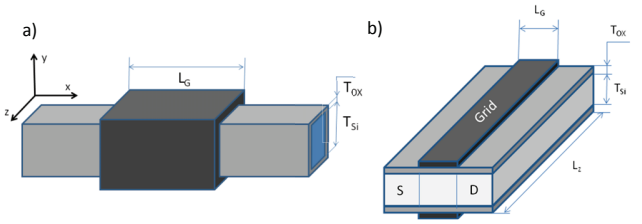

Fig. 1. Representation of the silicon devices considered in this work: a) n-type nano-wire (NW) and b) p-type double-gate (DG) MOSFETs. For both devices T_{OX}=1 nm, T_{Si}=2 nm and L_G=15 nm. Source/drain doping is N_{dop}=10^{20}cm^{-3} and source-drain bias $V_{DS} = 0.4$ V.

The two current values I_0 and I_1 of Eq.(4) can be interpreted as the two first terms of a current series from which the following analytic continuation (AC) can be performed [18], [20]:

$$I_{LOA+AC} = \frac{I_0}{1 - \frac{\Delta I_1}{I_0}} = \frac{I_0}{1 - \frac{I_{LOA} - I_0}{I_0}}. \quad (5)$$

As such, LOA+AC preserves the conserving laws in one-shot and as we will show in the next section greatly improves the accuracy of the LOA. From an implementation point of view the LOA+AC still requires the calculation of G_{LOA} which itself involves the matrix multiplications of the first order term, $g\Sigma[g]g$. We can however calculate G_{LOA} from the Green's function of the first SCBA iteration (G_1). Indeed, G_1 can be written as (for moderate interactions):

$$G_1 = [g^{-1} - \Sigma[g]]^{-1} \quad (6)$$
$$= g + g\Sigma[g]g + g\Sigma[g]g\Sigma[g]g + \cdots, \quad (7)$$

showing that G_{LOA} and G_1 are strictly equal at the first order of the interaction [20]. The higher order terms of G_1 in Eq.(7) do not obey the conservation laws. Using a rescaling strategy of the electron-phonon interactions and the linear dependence of the LOA current with with respect to the interactions, it is possible to deduce I_{LOA} from the current calculated with G_1 [18], [20].

To summarize, the LOA+AC current can be obtained as follows: (a) Calculate the current using the first SCBA iteration Green's function (G_1) with a rescaled electron-phonon interaction; (b) Deduce I_{LOA}, the lowest order current; (c) From I_{LOA} calculate the I_{LOA+AC} to analytically continue the current series (Eq.(5)).

LOA+AC is then a one-shot current conserving method capable of including electron-phonon scattering in NEGF codes. Its methodology is extremely simple and requires very few modifications from the usual SCBA algorithm.

III. Simulation Results

We first consider a n-type silicon gate-all-around (GAA) MOSFET (Fig.1-a). We use a 3D real-space hamiltonian expressed within the effective mass approximation. Hard wall boundary conditions are assumed and the temperature is fixed at 300 K. The hamiltonian is then projected on a 3D grid with a real-space mesh equals to 0.2 nm and an energy interval of 1 meV. Both acoustic and optical phonon couplings are considered and described within a local approximation. Acoustic phonons are treated in the elastic picture. The electron-phonon matrix elements are calculated using bulk deformation

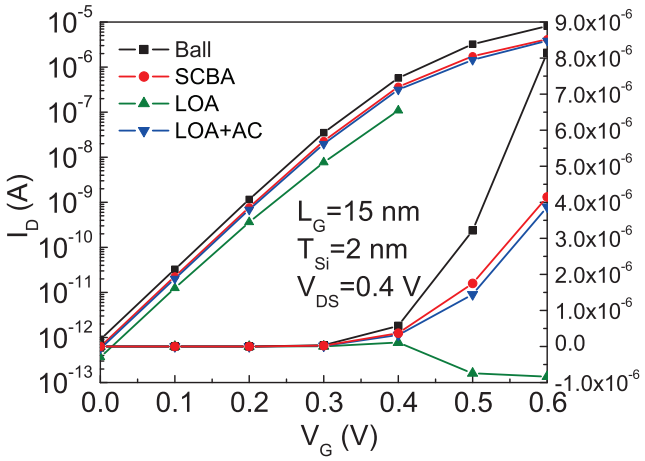

Fig. 2. $I_D - V_G$ characteristics resulting from ballistic approximation (squares), SCBA (circles), LOA (triangles) and LOA+AC (reversed triangles) for the n-type NW transistor of Fig. 1-a. The source-drain voltage is $V_{DS} = 0.4$ V.

potentials and phonon frequencies from Ref. [21]. Only the imaginary part of the self-energies is considered which stands for including the broadening of the energy levels and neglecting the shift in energy. For SCBA calculations a convergence criterion of 1% is applied on the current. Source, channel and drain regions are 15 nm long each. We take an ultra narrow cross-section of 2 $\times$ 2 nm^2 for which electron-phonon interactions are particularly strong. The channel is intrinsic and its crystallographic orientation along the <100> direction.

Figure 2 shows current characteristics obtained in the ballistic regime, SCBA, LOA, and LOA+AC. The current of each approach is calculated with the same self-consistent electrostatic potential obtained from ballistic simulations, *i.e.* when phonon scattering is not included in the electron density computation. The influence of phonon scattering on the electrostatic potential is assumed to be negligible. This assumption is particularly true when highly doped leads are considered, which is the usual configuration in nano-transistor architectures. As expected phonon-scattering reduces the current with respect to the ballistic results. From SCBA characteristics we note that phonon scattering is weaker in the off- than in the on-regime with a current reduction equals to 10% and 55% respectively. Figure 2 also shows that LOA fails to estimate SCBA current values. Indeed LOA induces a strong overestimation of the current reduction and even generates negative current values in the on-regime where phonon interactions are the most important. Interestingly, the LOA+AC still provides quite accurate current characteristics. N-type NW transistor is then a good example where the analytic continuation drastically improves the accuracy of a wrong first order estimate of the current.

We now investigate the origins of the LOA failure. Figure 3 represents the current spectra for V_G=0.5 V and V_{DS}=0.4 V at the drain-edge for the ballistic, SCBA and LOA approaches. The ballistic spectrum, which is constant along the transport direction, depicts a single peak that will be labelled as the ballistic one. The spectrum vanishes below the bottom of the

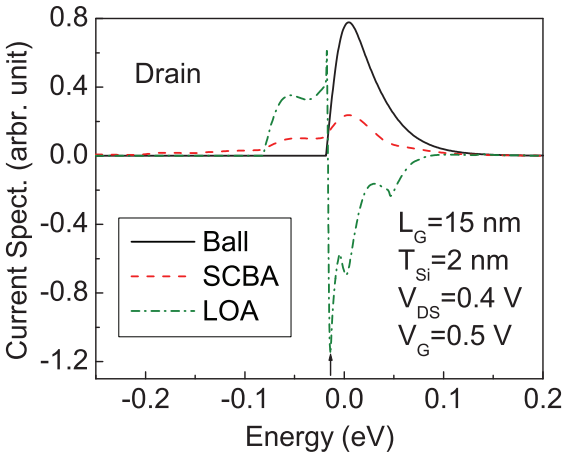

Fig. 3. NW transistor current spectra at the drain-edge in ballistic regime (solid line), SCBA (dash line) and LOA (dot-dash line). Both acoustic and optical phonons are considered. The arrow indicates the bottom of the first sub-band in the source region, E_{bot}. V_G=0.5 V and V_{DS}=0.4 V.

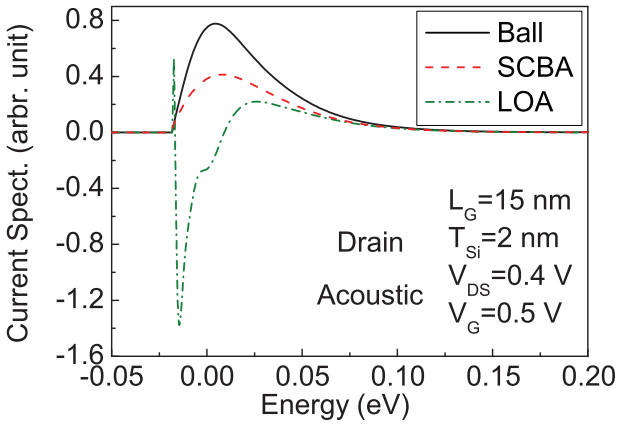

Fig. 4. NW transistor current spectra at the drain-edge when only acoustic-phonon scattering is included in SCBA (dash line) and LOA (dot-dash line). Ballistic result is in solid line. V_G=0.5 V.

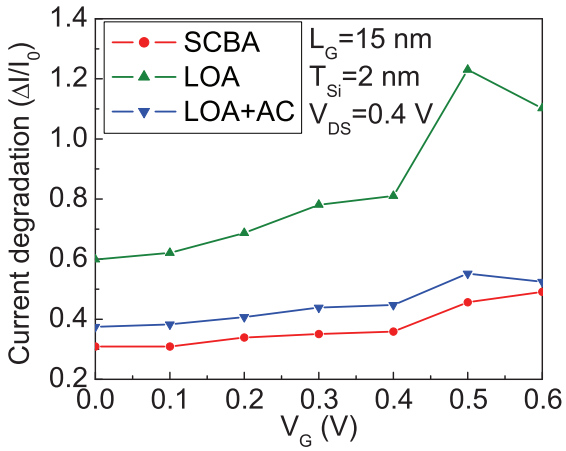

Fig. 5. NW current degradation with respect to the ballistic result (I_0) when considering SCBA (circles), LOA (triangles) and LOA+AC (reversed triangles).

first sub-band at the source edge (E_{bot}=-0.02 eV) since no electron relaxation or energy level broadening (in addition to those of the contacts) occur in that regime. SCBA spectrum presents a smaller ballistic peak due to i) back scattering of electrons and ii) electron relaxation via optical phonons. In that approach, optical phonon emissions generate a step-like shape spectrum below E_{bot} whose thickness roughly corresponds to the energy of the most impacting optical-phonon ($\hbar\omega$=64 meV). On the other hand, we note that LOA spectrum presents i) a strong negative divergence at E_{bot}, ii) only one positive peak below this same energy, illustrating that only one phonon-processes are described through this method.

To better analyze the negative divergence obtained at E_{bot} in the LOA spectrum, Figure 4 shows current spectra where only acoustic phonon interactions are considered (the optical-phonon self-energies are set to zero). We see that the negative divergence mainly results from interactions with acoustic phonons. The divergent character of the 1D electron density of states at the source edge significantly promotes interactions between electrons and acoustic phonons, which are described within the elastic picture. LOA spectrum with only optical phonons presents much less negative component (not shown). For the considered bias, ballistic current is equal to $3{,}22.10^{-6}$ A. When only optical-phonons are included, SCBA and LOA currents are equal to $2{,}61.10^{-6}$ A and $2{,}46.10^{-6}$ A respectively. On the other hand, acoustic phonons are much more impacting since SCBA and LOA currents are equal to $1{,}97.10^{-6}$ A and $-3{,}28.10^{-8}$ A respectively. This confirms i) the importance of acoustic phonons on the current degradation [22] and ii) the difficulty of the LOA to describe the interactions with acoustic phonons or with small frequency optical phonons.

Figure 5 compares the current degradations of SCBA, LOA and LOA+AC with respect to the ballistic values. It clearly illustrates the failure of the LOA to describe phonon scattering while LOA+AC quite faithfully reproduces the SCBA results. LOA+AC still generates a small current underestimation which can be however considered in the level of uncertainty of the simulations according to the various approximations commonly assumed in SCBA codes, by i) neglecting the real part of electron-phonon self-energies, ii) assuming local phonon interactions, iii) considering bulk deformation potentials, iv) keeping in mind that SCBA is only exact in one-phonon processes since the vertex corrections are not included [23].

LOA+AC is then expected to give reasonable results for n-type devices where band-structure can be defined with a single band approach. However we found that the method has some limitations to describe interactions at the band-edges. In order to evaluate this point, we now consider a p-type DG-MOSFET (Fig.1-b). Valence band-structure is more complicated than its conduction counterpart and presents various band edges/crossings (see inset of Fig. 6). Hole transport contains then a strong multi-band character. We conserve the previous theoretical framework but consider now a 2D

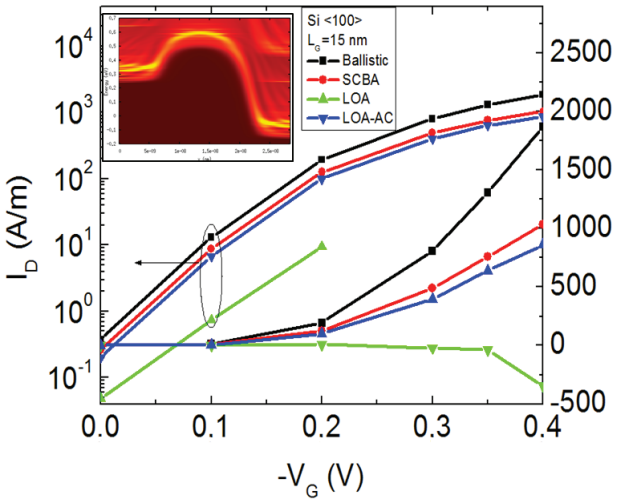

Fig. 6. $I_D - V_G$ characteristics of p-type DG-MOSFET shown Fig.1-b in ballistic regime (squares), SCBA (circles), LOA (reversed triangles) and LOA+AC (triangles). Inset: LDOS showing various band-edges and band-crossings (brighter lines) for V_G=0.2 V.

system described by a six-band k.p hamiltonian to correctly describe the top of the valence band [4]. Device dimensions and doping concentrations are indicated in Fig.1. Our previous study on n-type DG-MOSFETs showed the good accuracy of both LOA and LOA+AC to model electron-phonon coupling in these devices [17]. Here we find that the band-edges/-crossings degrade the accuracy of the one-shot methods (Fig. 6). Band-crossings can generate very large effective masses for holes and can also promote additional multi-phonon processes through band couplings. As a result, LOA induces negative current values for smaller gate voltages than in NW transistors. However LOA+AC still provides a fairly good estimate of the SCBA current. Deeper investigations will be conducted for different gate lengths and crystallographic orientations where band-structure is even less favorable (along the $< 110 >$ direction for instance).

IV. Conclusion

To conclude we presented a computationally-inexpensive approach to implement phonon scattering in device simulations. This challenges the currently adopted view that heavy self-consistent calculations are required to preserve conservation laws. LOA+AC is expected to capture the qualitative influence of phonon scattering in n-type nanowire transistors. This method is found to be limited when various band-crossings/edges are involved in the transport. The case of p-type DG MOSFET clearly illustrates this point. However LOA+AC only represents one analytic continuation method among many others and its relevancy is mainly related to its one-shot character. Solutions based on more sophisticated analytic continuation techniques, using higher order terms of the current series also exist. The method would then require an iterative scheme whose convergence should be still faster than in the SCBA approach [20]. This point will be the subject of forthcoming investigations.

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