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Efficient quantum approach of electron-phonon scattering for nanoscale device simulations

Y Lee[1], M Lannoo[1], N Cavassilas[1], M Luisier[2] and M Bescond[1]

[1]Aix-Marseille University, France, [2] ETH Zürich, Switzerland

In recent decades various transport approaches have been proposed to describe quantum effects occurring in nano-devices [1], [2]. Among them, Nonequilibrium Green's function formalism (NEGF) has been proved very suitable at treating inelastic interactions [3]. However, within this formalism the description of inelastic scattering is usually based on the computationally expensive self-consistent Born approximation (SCBA). As an alternative method to SCBA, we have proposed an efficient technique, the so-called Lowest Order Approximation (LOA) coupled with Padé approximants [4], [5]. In this work, we apply this approach to the treatment of phonon scattering in two 1D systems where phonon scattering is known to be important: the atomic linear chain and the nanowire transistor. In NEGF the interacting Green's function is calculated by combining an electron-phonon self-energy ($\Sigma[G]$) with the Dyson equation [3]:

$$G = g0 + g0\Sigma[G]G, \quad (1)$$

where $g0$ is the non-interacting Green's function. Since Dyson's equation (1) is non-linear, solving Eq. (1) is typically based on the iterative SCBA scheme. Alternatively, we define LOA Green's functions at a given order N in interaction as follows:

$$gN = gN - 1 + g0 \sum_{n=0}^{N-1} \Sigma [\Delta gN - n - 1] \Delta g_n, \quad (2)$$

where $\Delta g_n = gn - \Delta g_{n-1}$ and $\Delta g0 = g0$. By using Eq: (2), we can calculate current series $I_N = I(gN)$ and carrier density series ρN = ρ (gN) to Nth order in interaction. According to the strength of the electron-phonon scattering, the LOA series can diverge. We then use Padé approximant technique to operate a convergent resummation. Note that the LOA series can be also coupled to Hyper geometric resummation technique [6].

We first apply our technique to the ideal 1D linear atomic chain (Fig. 1) where one optical phonon mode ($\hbar\omega$ = 60 meV) is coupled with electrons de- scribed by a two-band *k·p* Hamiltonian (inset of Fig. 1). Figure 2 shows current-voltage characteristics in the ballistic regime, SCBA and with our LOA- Padé technique when electron-phonon coupling *M* is large. It is clearly shown that 3*rd* order LOA currents combined with Padé 1/2 successfully reproduce the SCBA values. Figure 3 shows that electron density along the device can also be reconstructed with the LOA-Padé approach even though it needs up to 5*th order* LOA (i.e. Padé 2/3). Moreover, the series of LOA physical quantities can be derived from the SCBA algorithm [7]. The approach can then be applied to the n-type 3D nanowire transistor (Fig. 4 (a)) where a full- band atomistic treatment for electrons (Fig. 4 (b)) and phonons (Fig. 4 (c)) is considered [8]. Figure 5 compares Id-Vg curves of

ballistic regime and SCBA with those obtained by Padé 1/2. We note that 3*rd order* LOA currents are enough to achieve high agreement with respect to SCBA (Fig. 6).

In conclusion, the results show the relevancy of our technique for efficient quantum transport modelling with high accuracy compared to SCBA.

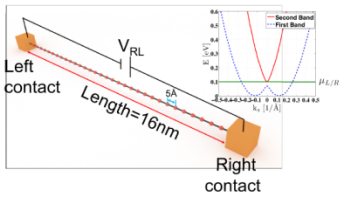


Fig. 1. Schematic view of a 1-D, 16 nm long atomic linear chain connected to left and right contacts at room temperature (T=300 K). The applied voltage between left and right contacts is V_{RL}. (Inset) The electronic bandstructure is described by the two band $k{\cdot}p$ method. The Fermi levels of left and right contacts ($\mu_{L/R}$) are located 0.1 eV above the bottom of the band.

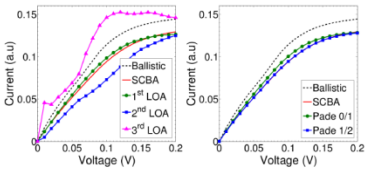


Fig. 2. I-V characteristics when electron-phonon coupling M is 1.5×10^{-3} eV^2 obtained (left) from ballistic, SCBA and first three LOA order and (right) from ballistic, SCBA, Padé 0/1 and Padé 1/2.

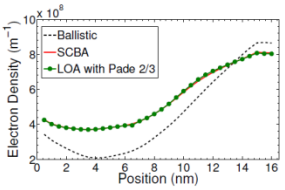


Fig. 3. Electron density profiles along the linear chain in ballistic regime and SCBA when electron-phonon coupling M is 1.5×10^{-3} eV^2. Electron density profile reconstructed by Padé 2/3 with first five order LOA electron densities is also shown and fits perfectly with SCBA values.

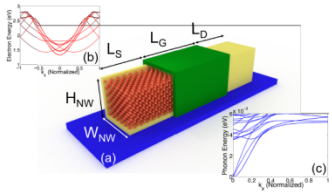


Fig. 4. (a) Schematic view of an n-type silicon 3D square cross-section nanowire transistor in ⟨100⟩ transport direction at room temperature (T=300 K) with $L_G = 13$ nm, $L_{S/D} = 9$ nm and $H_{NW} \times W_{NW} = 3 \times 3$ nm^2. The doping concentrations of donors in source and drain are 10^{20} cm^{-3}. (b) Electron band-structure as produced by the full-band tight-binding $sp^3d^5s^*$ model. (c) Phonon dispersion relation described by the valence-force-field method [8].

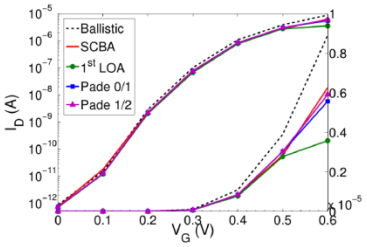
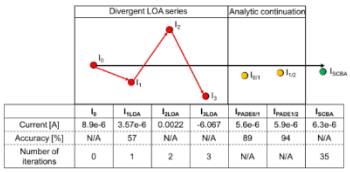


Fig. 5. I_D-V_G curves of the n-type 3D nanowire transistor for ballistic regime, SCBA, 1^{st} order LOA, Padé 0/1 and Padé 1/2.



	I_0	I_{1LOA}	I_{2LOA}	I_{3LOA}	I_{PADE01}	I_{PADE12}	I_{SCBA}
Current [A]	8.9e-6	3.57e-6	0.0022	-6.067	5.6e-6	5.9e-6	6.3e-6
Accuracy [%]	N/A	57	N/A	N/A	89	94	N/A
Number of iterations	0	1	2	3	N/A	N/A	35

Fig. 6. Comparison of the ballistic current, first three order LOA currents, Padé 0/1 and Padé 1/2 with the SCBA current for the n-type 3D nanowire transistor at $V_D = V_G = 0.6$ V. Accuracy with respect to the SCBA and number of iterations are reported in the table. Schematic diagram of the divergent LOA current series is also shown.

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