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► **To cite this version:**

H. Mera, M. Lannoo, C. Li, N. Cavassilas, M. Bescond. Inelastic scattering in nanoscale devices: One-shot current-conserving lowest-order approximation. *Physical Review B*, 2012, 86 (16), 10.1103/physrevb.86.161404 . hal-03477572

HAL Id: hal-03477572

<https://hal.science/hal-03477572>

Submitted on 24 Dec 2021

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Inelastic scattering in nanoscale devices: one-shot current-conserving lowest order approximation

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Abstract

We describe a lowest order approximation (LOA) to the nonequilibrium Green's function in the presence of interactions, and generally address how one can build Φ -derivable one-shot approximations that satisfy the continuity equation. These approximations produce conserved electronic currents in one-shot, requiring only one self-energy evaluation and, when applicable, are as accurate but much faster than the corresponding selfconsistent approximation. This challenges the currently adopted view that heavy self-consistent calculations are necessary to get a satisfactory prediction of transport in nanoscale structures. We illustrate this with the case of electron-phonon scattering expressed within the self-consistent Born approximation (SCBA). In the LOA the SCBA is further approximated by accounting only for one-phonon processes. LOA and SCBA are compared in one-dimensional wire where electrons interact with one optical phonon mode at room temperature. The LOA is found to provide considerable reduction in computational time. Its limitations and extensions to include two-phonon processes are discussed.

PACS numbers:

In the last twenty years we have witnessed great progress in the modelling of nanoscale devices and components using the theory of non-equilibrium Green's functions (NEGF)[1]. By combining NEGF with a mean-field-type of description for the electronic structure problem (Kohn-Sham density functional theory [2], tight-binding [3], extended Huckel [4] and effective-mass approaches [5]) the formalism has been applied to a great variety of systems such as nanowire devices, molecular junctions, quantum dots, graphene, etc.

Unfortunately the NEGF method itself and the typically large space of device parameters both impose severe computational demands thus restricting the applicability of the method. These constraints are particularly difficult to overcome when it comes to the perturbative treatment of inelastic scattering processes arising from the electron-electron, electron-phonon, or any other interactions. For instance the atomistic simulations including electron-phonon interactions at the level of the selfconsistent first Born approximation (SCBA) require a number of approximations in order to make the problem numerically tractable [6]. Self-consistency is often considered to be essential for an approximation to obey all conservation laws and to satisfy, say, the continuity equation [7]. When this is true complicated Dyson equations need to be iterated to selfconsistency in order to possibly obtain physically meaningful solutions.

However it has been noted that self-consistency typically renders spectral functions unphysical, and that there might be strong cancellations between the effects of self-consistency and those of frequently ignored vertex corrections[8]. Furthermore model calculations have shown violations of the current and particle number conservation laws to be possibly quite small[8, 9]. Finally nonselfconsistent *and* conserving approximations have been utilized on the electron-phonon problem before [10]. It is not clear at all then that demanding self-consistency is that essential as it is often implied: the (possibly small) gain in conservation laws might be lost to an unphysical spectral function as well as to a considerable increase on the computational demands of the method. One then wonders whether it is possible to generate systematically “current conserving” approximations in one shot.

The answer to these questions is given by Baym and Kadanoff[11], who provide a prescription to build conserving approximations using perturbation theory: in order to preserve conservation laws one can calculate the current from the one-electron GF G that solves the Dyson equation[16]

$$G = g_0 + g_0 \Sigma[G]G \tag{1}$$

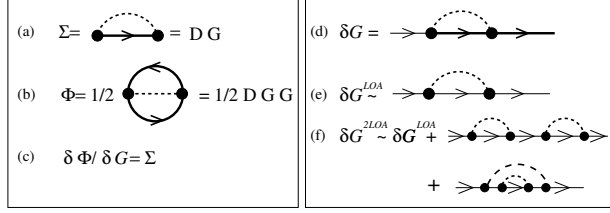


FIG. 1: In all the figures shown thick solid lines represent the selfconsistent electron GF G , thin solid lines represent the nonselfconsistent electron GF g_0 , while dashed lines represent the noninteracting phonon propagator, D . Left Panel: (a) the self-energy diagram in the SCBA; (b) To find Φ from Σ close Σ with a G and divide by the resulting number of G 's. By $\Phi = 1/2DGG$ we mean $\Phi = \frac{1}{2} \int d3d4G(4,3)G(3,4)D(3,4)$ (c) When Φ is built as in (b) then Σ can be obtained back from Φ as shown. Right Panel: Writing the Dyson equation as $G = G_0 + \delta G$ in (d) we show the diagrams for the exact δG ; in (e) we show δG in the LOA; in (f) we show an extension of the LOA that includes two-phonon processes (2LOA).

where g_0 is the nonequilibrium noninteracting/ballistic GF and Σ is the self-energy that takes into account interactions in the central region, which in this work is always a so-called Φ -derivable self-energy, satisfying $\Sigma = \delta\Phi[G]/\delta G$, where Φ is a functional of G built in the manner described by Luttinger and Ward[12, 13]. Examples of well-known Φ -derivable self-energy approximations are the selfconsistent first and second Born, GW and T-matrix approximations[11]; in all of these Σ can be found by plucking out one G from the diagrams that make up Φ . The procedure is illustrated for the electron-phonon scattering within the SCBA in Figs. 1(a)-(c). A self-consistent Φ -derivable approximation is, according to Baym and Kadanoff, conserving.

Therefore, to approximate inelastic-scattering corrections to the electronic current one can choose a suitable Φ -derivable approximation and solve Dyson's equations to self-consistency. The current flowing through interface α –typically the left ($\alpha = L$) or right ($\alpha = R$) interface between the central region and the L or R electrode– is obtained from the selfconsistent G as $I_\alpha[G] = e/\hbar \int d\omega J_\alpha(\omega)$ where $J_\alpha(\omega) = \text{Tr}(\Sigma_\alpha^>(\omega)G^<(\omega) - \Sigma_\alpha^<(\omega)G^>(\omega)) / 2\pi$ is the spectral resolution of the current, Σ_α is the self-energy describing the coupling to the α electrode and $G^{<,>}$ are the lesser/greater GF. The self-consistent evaluation of G using a Φ -derivable approximation for Σ , ensures the satisfaction of the continuity equation, which in turn

implies that in the steady-state $I_L = -I_R$ [1].

The purpose of this work is to show how current-conserving *one shot* approximations may be built, and to illustrate their properties and applicability for a simple example at the lowest order of approximation. To proceed we imagine a situation where one calculates a conserved noninteracting (or ballistic) steady-state current in a biased nanodevice from a g_0 [17]. We write $G = g_0 + \delta G$ in both sides of Eq. (1) and expand the right-hand side to first order in δG to get

$$\delta G \approx g_0 \Sigma[g_0] g_0 + g_0 \left(\frac{\delta \Sigma[G]}{\delta G} \delta G \right) g_0 + g_0 \Sigma[g_0] \delta G, \quad (2)$$

and thus the lowest order approximation (LOA) is,

$$\delta G \approx g_0 \Sigma[g_0] g_0 \quad (LOA), \quad (3)$$

while the second and third terms take into account the change in Σ due to changes in G and the effect of repeated scatterings by $\Sigma[g_0]$, respectively. These terms thus take into account higher orders in the interactions and are briefly discussed below. We emphasize that at this point we have not specified the interactions accounted for by Σ , nor the specific approximation to Σ , which could be in principle any self-energy for any interaction as long as it is Φ -derivable. For an example within the SCBA see Figs. 1(d-f).

It has been mentioned in earlier papers that the LOA is current-conserving. Here we note that the proof is the same as Baym's for the selfconsistent case. In the LOA one approximates $\Phi[G] \approx \Phi[g_0]$. Clearly $\Sigma[g_0] = \delta \Phi[g_0] / \delta g_0$, i.e., we find $\Sigma[g_0]$ by taking out a g_0 line from $\Phi[g_0]$. Now, by having the same g_0 everywhere in the skeleton diagrams that build up Φ one ensures its gauge invariance, which together with Φ -derivability implies the satisfaction of the continuity equation: in other words, the proof of the continuity equation given by Baym works also at the lowest order, when one replaces all the G 's by g_0 's. Thus currents calculated directly from g_0 can be conserving. Given a Φ -derivable approximation selfconsistency is a sufficient condition, not a necessary one. It also follows from these arguments that the GF obtained from first iteration of the Dyson equation, $G_1 = [g_0^{-1} - \Sigma[g_0]]^{-1}$, should *not* generally be a conserving GF since it does not take into account terms such as the one including $\delta \Sigma / \delta G$ in Eq. (2), accounting only for terms of the form $g_0 \Sigma \delta G$. Thus the current obtained from G_1 is not conserved in general to order δG^2 . The current obtained from the LOA GF $g_0 + g_0 \Sigma[g_0] g_0$ is, in contrast, always conserved: it is the lowest order of G_1 and its only conserving part.

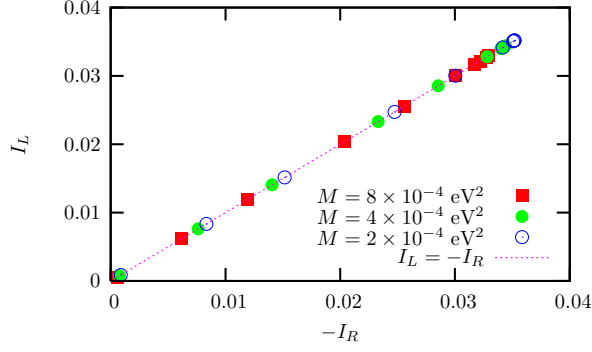


FIG. 2: (color online) Current conservation in the LOA. For the model described in the text the LOA is numerically shown to exactly satisfy current conservation $I_L = -I_R$. The graph has been obtained plotting I_L vs. $-I_R$ for different electron-phonon couplings $10^{-4} < M < 10^{-3}$ eV² and applied bias voltages $0 < V < 0.4$ V.

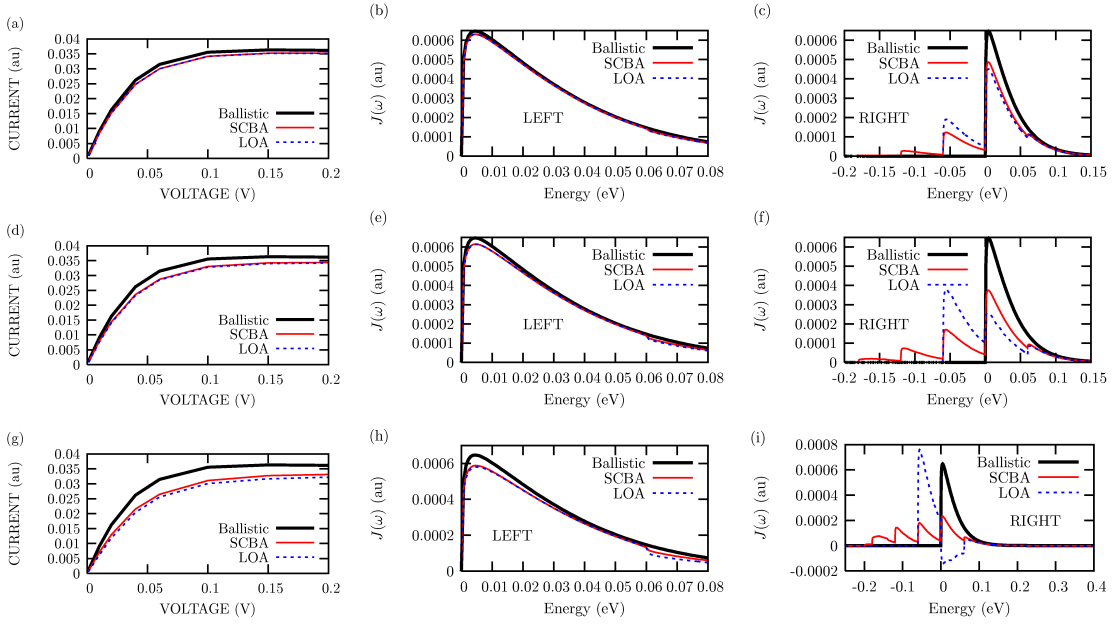


FIG. 3: (color online) Top Panel For $M = 2 \times 10^{-4}$ eV²: (a) the current-voltage characteristics; (b) Spectral resolution of the current density in the left interface, $J_L(\omega)$, calculated for $V = 0.2$ V; (c) The same as in (b) but for the right interface. Middle Panel (d), (e) and (f) are the same as (a), (b), (c) but calculated for $M = 4 \times 10^{-4}$ eV². Bottom Panel as above but for $M = 8 \times 10^{-4}$ eV². For one-phonon mode with $M = 8 \times 10^{-4}$ eV² and $V = 0.2$ Volts the phonon-induced on-current degradation is about 11% in the LOA compared to 8% in the SCBA.

Next we specialize to the electron-phonon interaction as described by the SCBA. We apply both the LOA and the SCBA to the interaction between optical phonons with frequency $\Omega \approx 60\text{meV}$ and otherwise noninteracting electrons moving in a one-dimensional ramp potential $v(x)$ at room temperature. The difference between chemical potentials of the L and R regions is $V = \mu_L - \mu_R$. The interacting central region has a length of $L = 30\text{ nm}$. The potential takes the values $v(x) = \mu_L = 0$, for $x < 0$, $v(x) = -Vx/L$ for $0 < x < L$, and $v(x) = -V$ for $x > L$. Our numerical implementation is based on Ref. 14 for a one-band hamiltonian and neglects the real part of the electron-phonon self-energy. The electron effective mass is $0.9m_0$, corresponding to the longitudinal effective mass of silicon. We find a 1000 energy points distributed over an energy interval of about 1 eV to be sufficient to illustrate the conserving nature of the LOA and to get insights into its validity. We take the electron-phonon coupling strength, M –representing the square of the matrix elements of the electron-phonon interaction–, and applied bias voltage, V , as free parameters varying them in the intervals $0 < V < 0.4(\text{V})$ and $10^{-5}\text{eV}^2 < M < 10^{-3}\text{eV}^2$.

In Fig. 2 we plot I_L versus $-I_R$ as given by the LOA. Our implementation of the LOA gives numerically perfect satisfaction of the current conservation law, $I_L = -I_R$, for all the values of M and V tried. Furthermore we have checked that the current density is constant along the device. Finally we mention that we have tried the LOA for a variety of other systems and interactions, reaching exactly the same conclusions. Thus the LOA is a conserving approximation, independently of M and V . Thus selfconsistency is not strictly needed for conservation laws to be obeyed: what is needed is to have order-by-order selfconsistency, where the same g_0 is used everywhere in Dyson’s equation. Note that an approximation can be “conserving” without being necessarily “good”: this criticism can certainly be applied to the LOA (see below) but also to selfconsistent approximations without vertex corrections, such as the *GW* approximation and the SCBA. Strictly speaking the SCBA can be exact only for the description of one phonon-processes since, although it includes two-phonon processes by being selfconsistent, it ignores the second order vertex diagram, with two crossed interaction lines, and thus ignores certain two-phonon processes. Seen as an approximation to the SCBA, the LOA ignores all two phonon processes (those coming from selfconsistency as well as those coming from the vertex) and can only be strictly valid for as long as only one-phonon processes are allowed, just as the SCBA. Nevertheless below we find out the limits of validity of the LOA for the model considered, using the

SCBA as benchmark but keeping in mind the intrinsic limitations of the SCBA: the SCBA is guaranteed to be accurate only for weak interactions [15].

In Fig. 3 we present a comparison between the transport properties of the model as given by the ballistic case, as well as in the interacting case, as described by both the LOA and the SCBA. Consider first the top panel where we show the I-V curves and spectral currents for $M = 2 \times 10^{-4} \text{ eV}^2$. For this value of M phonons have a very small effect on the I-V curves shown in Fig. (3a). The left spectral currents shown in Fig. (3b) are essentially ballistic. However the right spectral current in Fig. (3c) shows clearly the effect of the emission of two phonons in the SCBA and one phonon in the LOA, which misses the secondary emission peak. Consider now the middle panel, which is as the top panel but for $M = 4 \times 10^{-4} \text{ eV}^2$. The I-V curves in Fig. (3d) show excellent agreement between the LOA and the SCBA. The phonon-induced current degradation is appreciable and of a few percent. The left spectral currents in Fig. (3e) given by the LOA and the SCBA are also in good agreement, and clearly show a dip due to one-phonon absorption. The right spectral currents in Fig. (3f) are, however, markedly different. While the SCBA spectral current shows two well resolved phonon emission lines, the LOA spectral current only accounts for the emission of one phonon. The distribution of the spectral weight given by the LOA and the SCBA is very different at the right interface, yet both LOA and SCBA give nearly identical I-V curves. Finally in the bottom panel we show results calculated with $M = 8 \times 10^{-4} \text{ eV}^2$. Again we observe a good agreement between the LOA and SCBA I-V curves in Fig. (3g), which are however starting to diverge from one another. The phonon-induced on-current degradation is now significant of about 10 %, which seems large taking into account that we have considered only one mode; in more realistic model nanowires electrons interact with many modes of different frequency [6]. The left spectral current are again also in good agreement, with a clear dip due to one-phonon absorption. The right spectral currents however are now very different. While the SCBA shows a positive spectral current with three phonon-emission peaks, the LOA spectral current is negative and thus unphysical. Nevertheless the LOA and SCBA I-V curves are still in good agreement, as explained below.

Fig. 3 illustrates both the advantages and disadvantages of the LOA. The main advantage of the LOA is that it has built-in current conservation. Imagine cutting a conductor with an imaginary surface S and calculating the local spectral current in S ; if the LOA gives a good description of the local spectral current for some S then it will give a good approximation

to the total integrated current, for any S . This is shown in Fig. 3 where the LOA provides a good description of the total current and left spectral current, failing for the right spectral current. The main disadvantage is that for sufficiently large values of M the LOA will eventually give negative local spectral currents. These negative values signal the breakdown of the LOA. In a model with a single interacting site, negative local spectral densities are possible for model parameters such that $\text{Im}\Sigma^r(\omega)\text{Im}g_0^r(\omega) > 1$. In the model considered this condition is most easily satisfied for small ω and Ω . For these cases one can try to iterate Eq. (2) once, obtaining the second-to-lowest order expansion (2LOA) shown in Fig. (1f), which is also conserving and expected to provide spectral densities in better agreement with the SCBA for larger values of M .

To conclude, we have shown how, by keeping order-by-order Φ -derivability, one can preserve conservation laws in one-shot calculations, thus avoiding the need for iterating the Dyson equation to selfconsistency at large computational expense. We have obtained the LOA from an expansion of the Dyson equation about the nonequilibrium ballistic g_0 . We have shown the LOA to be a current-conserving one-shot approximation. In the second part of the paper we have applied both the LOA and the SCBA to the case of the electron-phonon interaction in a one-dimensional example, which exhibits both the advantages of using a conserving approximation and the disadvantages of a lowest order expansion. We outlined an extension of the LOA to account for two-phonon processes.

Acknowledgement

This work is supported by the QUASANOVA and SIMPSSON contracts funded by the ANR-French National Research Agency.

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- [17] If the starting GF is the G_0 that solves Dyson's equation $G_0 = g_0 + g_0\Sigma_{easy}G_0$ then replace $\Sigma[G]$ by $\Sigma[G] - \Sigma_{easy}[G_0]$ in the derivations given below.