Inelastic Scattering in Nanodevices: Conserving low-order approximation

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In order to properly model current-carrying nanoscale electronic devices it is paramount to account for inelastic scattering effects [1] arising from electron-phonon, electron-photon and electron-electron interactions. The non-equilibrium Green's function (NEGF) formalism can be used to describe quantum transport in the nanoscale. Within NEGF framework inelastic scattering is accounted for by approximated self-energies, $\sum[G]$, which are functionals of the Green's function (GF) G.

The calculation of inelastic-scattering corrections to the current is further complicated by the need to satisfy conservation laws, and thus of performing selfconsistent (SC) calculations, using a Φ-derivable [2] approximation to $\sum[G]$. However the nonselfconsistent (NSC), lowest order, conserving approximations one finds in the literature [3] pose an interesting question: Is there any systematic way of constructing nonselfconsistent, conserving, low-order corrections to the current within NEGF?

In this paper we answer this question in the affirmative and analyze the limitations of such an approach by means of simple examples. Given a noninteracting, nonequilibrium and conserving GF, G_0, the interacting GF is approximated by $G_0+\delta G$ where $\delta G= G_0\Sigma[G_0]G_0$. Then the first-order current ($\propto\delta G$) is conserved; violations of the continuity equation being of order δG^2. Hence such first-order approach is conserving to order δG and strictly valid only if $\delta G/G_0 << 1$.

Here we apply this approach to the electron-phonon, electron-photon and electron-electron interactions to model nanodevices. We test current conservation and compare NSC with fully SC solutions. Figs. 1-6 show results for the optical-phonon-limited current on a toy 1D effective mass model under source-drain (SD) bias, where the phonon is treated in the SC and NSC first Born approximations. The system is described in Fig. 1. The optical-phonon frequency is $\hbar\omega$=0.06 eV. In Fig. 2-4 we show that SC and NSC currents are conserved and in excellent agreement, for the parameters considered. The SC and NSC spectral currents can however be different for larger voltages ($V > 2\hbar\omega$) allowing for multiple phonon emission (Figs. 5 and 6). Electron-electron and electron-photon interactions, and the extension to higher orders are also addressed in our paper.

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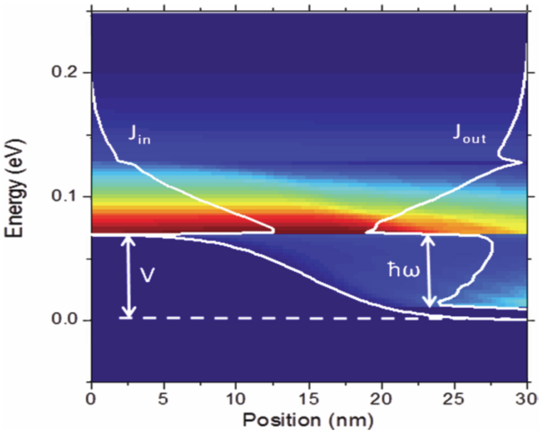

Fig. 1. (color map) Phonon-limited spectral current obtained with our non-selfconsistent method as a function of position and energy for V=0.07 eV, Mph^2=2x10^{-5} eV^2. In white we also represent the conduction band-edge (from the LDOS) *versus* position and current spectra at the source- and drain-edges (J_{in} and J_{out} , respectively).

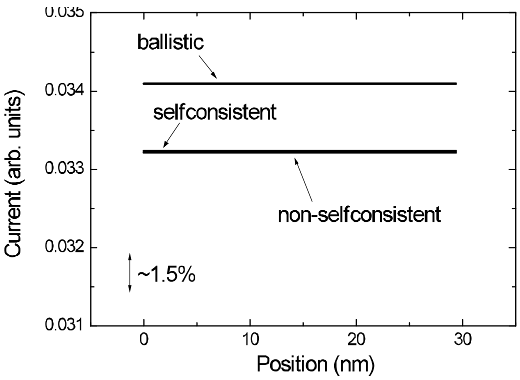

Fig. 3. The same as in Fig. 2 but for Mph^2=1x10^{-5} eV^2. By reducing the electron-photon coupling strength SC and NSC approaches are made to give identical results.

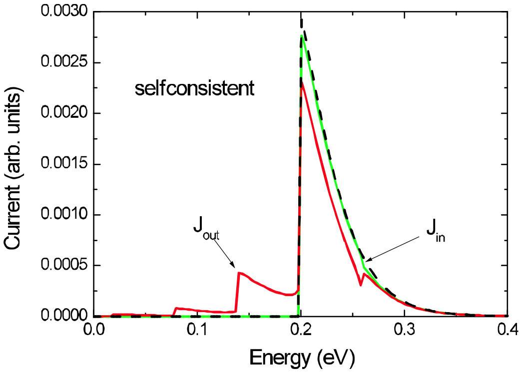

Fig. 5. For the parameters used in Fig. 4 we show the SC current-spectra (solid) at source- (J_{in}) and drain-edges (J_{out}) and ballistic case (dashed). Multiple phonon emission displaces spectral current from the multiple emission peaks at lower energies.

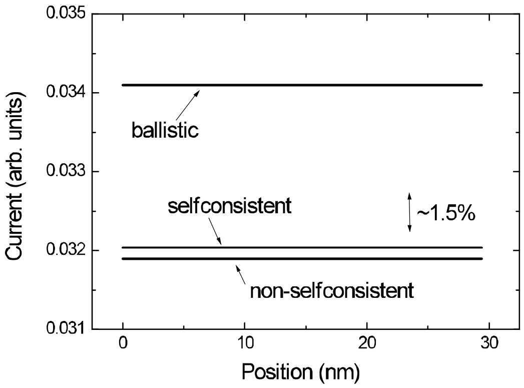

Fig. 2. Total-current *versus* position calculated in ballistic case, with the SC and NSC first Born approximation (V=0.07 eV, Mph^2=2x10^{-5} eV^2). Since $\hbar\omega\approx 0.06$ eV only one phonon can be emitted/absorbed and SC and NSC approaches agree well.

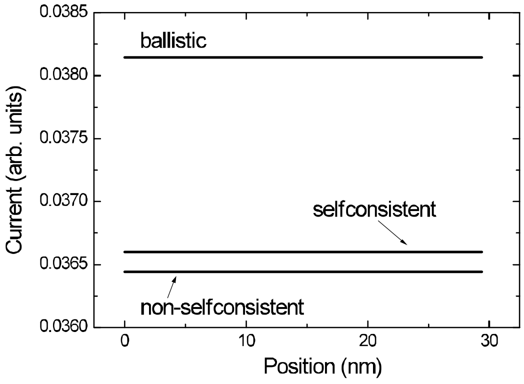

Fig. 4. The same as in Fig. 2 but for V=0.2 eV. Both SC and NSC currents are in good agreement and verify the continuity equation. Note that for such SD bias ($V\approx 3\hbar\omega$) multiple-phonon emission is possible.

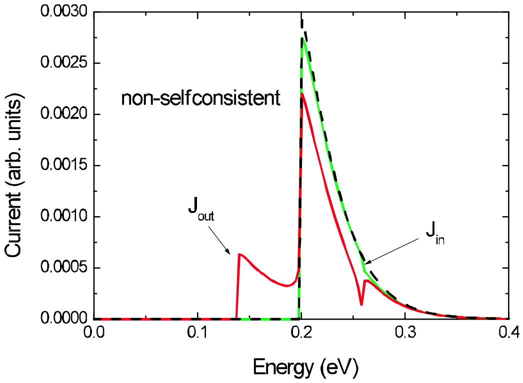

Fig. 6. The same as Fig. 5 but for the NSC case. The NSC only accounts for one-phonon processes and thus there is only one secondary emission peak in J_{out}. However, SC and NSC J_{in} agree well (see Fig. 4) and current conservation is maintained for these parameter values.