SCBA Made Simple

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Non-equilibrium Green's function (NEGF) techniques are commonly applied to the understanding and design of novel nanoelectronic devices. In many situations one needs to take into account interactions such as the electron-phonon/photon or electron-electron. Accounting for these within NEGF is theoretically and computationally challenging. Inexpensive approximations to treat interactions are thus very much in need. Selfconsistency is considered to be essential for conservation laws to be obeyed. According to this view it is necessary to iterate NEGF equations to selfconsistency, thus further complicating matters.

The purpose of this study is to provide a generalization and a full theoretical justification of our previous work at the lowest order [1-3]. We provide an infinite family of conserving but not fully selfconsistent approximations. We illustrate the performance of the newly developed approximations by considering the calculation of the photocurrent in a bias molecular-junction model.

In the NEGF method one accounts for interactions by means of a Dyson equation of the form

$$G=g+g\Sigma[G]G, \qquad (1)$$

where $\Sigma[G]$ is a Φ-derivable selfenergy that accounts for interactions and g is the noninteracting NEGF. Because the selfenergy is itself a functional of G, Eq. (1) needs to be solved selfconsistently. The standard way of iterating Eq. (1) is based on writing it as $G=[g^{-1}-\Sigma[G]]^{-1}$ leading to

$$G_n=[g^{-1}-\Sigma[G_{n-1}]]^{-1}. \qquad (2)$$

Unfortunately iterating Eq. (2) leads to a sequence of G_n's which are not conserving. Eq. (2) leads only to one conserving approximation, the fully self-consistent one. In strongly interacting systems many iterations might be needed for Eq. (2) to converge.

In this work we show how one can generate conserving approximations from the Born series for the NEGF. In the Born series the fully selfconsistent G is expanded as a partial power series in the interaction strength parameter, M^2, up to the desired order:

$$g_N = g+\sum_{n=1}^{N}\delta g_n M^{2n}, \qquad (3)$$

where the δg_n are M-independent coefficients. We will show that g_N is conserving. To estimate the SCBA current, $I[G]$, we evaluate instead $I[g_N]=I_{N/0}$, which is a Born series for the current. With $I_{N/0}$ we can calculate a Padé table of approximations, $I_{P/Q}$. Because g_N is conserving, observables calculated from it satisfy whatever conservation laws they ought to satisfy.

In Fig. 1 we show the photocurrent as a function of source-drain bias, calculated for a molecular junction model for various values of M. We compare the SCBA currents with those obtained from $I_{N/0}$ (top panel) and the diagonal Padé sequence $I_{P/P}$ (bottom panel). For small values of M, Fig. 1(a), the Born series works well, reproducing the full SCBA result. As M increases the Born series breaks down (see Fig 1(b) and (c)). In contrast the Padé approximations $I_{P/P}$, Fig. 1(d-f), work well or any value of M. The 1/1 Padé approximate is a two-shot conserving approximation.

We believe these techniques will lead to improved recipes for the nanodevice simulation accounting for inelastic scattering.

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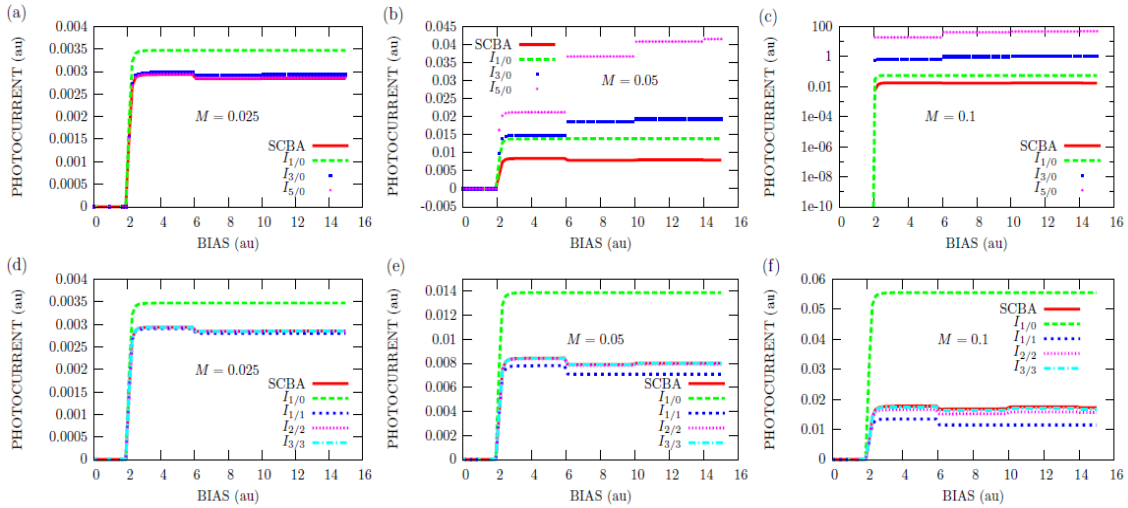

FIG. 2: Photocurrent as a function of source-drain bias. In (a)-(c) we show a comparison between currents calculated from the SCBA and the Born series, $I_{N/0}$ for n = 1, 3 and 5, for the values of M shown. (a) When interactions are weak the SCBA current is well approximated by currents calculated from the Born series for the NEGF. (b-c) The Born series is divergent. Outside its radius of convergence the estimates become worse and worse as M is increased. In (d)-(f) we compare SCBA currents with those obtained from the first three diagonal elements of the Padé table, $I_{P/P}$, P=1,2,3. For M small or large the Padé approximants give fairly good approximations for the SCBA current. In particular the two-shot approximate $I_{1/1}$ is both accurate and computationally inexpensive.