

The nonequilibrium Green's functions method and descendants: ways to avoid and to go

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Abstract— We present a novel quantum transport method that follows the non-equilibrium Green's function framework but sidesteps the iterative calculation of lesser self energies by replacing them by global relaxation parameters. This method generalizes the so-called Buttiker probe model but takes into account all relevant individual scattering mechanisms. It is orders of magnitude more efficient than a fully self-consistent non-equilibrium Green's function calculation for realistic devices, yet accurately reproduces the results of the later method.

quantum transport; NEGF

I. INTRODUCTION

Carrier dynamics in modern semiconductor nano-devices is virtually always controlled by a competition between incoherent relaxation processes and quantum interference effects. Consequently, they can neither be described (semi-) classically nor by a strictly coherent, ballistic quantum mechanical dynamics. A theory to capture all of these effects consistently has been developed almost 50 years ago by Keldysh and, independently, by Kadanoff and Baym, but a quantitative implementation of this so-called non-equilibrium Green's function (NEGF) formalism is still a highly challenging task [1-9].

II. METHOD

In fact, a full implementation of the non-equilibrium Green's function method even for stationary transport problems in open quantum systems requires the self-consistent solution of two Green's functions, G^R and $G^<$. The first one characterizes the width and energy of the scattering states, whereas the second quantity characterizes the state occupancy and determines the charge and current density. The self-consistent solution cycle involves the solution of 4 coupled integro-differential equations [10],

$$\begin{aligned} G^R &= (E - H_D - e\Phi - \Sigma^R)^{-1}, \\ \Sigma^R &= G^R D^R + G^R D^< + G^< D^R, \\ \Sigma^< &= G^< D^<, \\ G^< &= G^R \Sigma^< G^{R\dagger}. \end{aligned} \quad (1)$$

Here, H_D is the electronic device Hamiltonian, Φ is the electrostatic potential that needs to be solved by the Poisson equation self-consistently with the Green's functions, $\Sigma^R, \Sigma^<$

are the scattering self-energies including the coupling to the contacts, and $D^R, D^<$ represent the environmental Green's functions that contain the scattering vertices. All quantities are functions of space, momentum and energy. For a multi-quantum well structure along the z-axis, the lateral momentum conservation simplifies the arguments to the following functional form, $G = G(z, z', k_{||}, E)$.

While being the most rigorous and general framework for quantum transport, the non-equilibrium Green's function method has two weaknesses. First of all, it is difficult to develop approximations that maintain charge and current conservation. To achieve exact current conservation, for example, the scattering must be taken into account at least in terms of the self-consistent Born approximation, i.e. to infinite order in the coupling strengths. Another example is the approximation of decoupling the Green's functions G^R and $G^<$ that leads to a gross violation of Pauli's principle for highly doped structures. Secondly, the calculation of Eq. (1) requires integration over at least 4 variables $k_{||}, k'_{||}, E, E'$, in addition to the iteration over the 4 set of equations to achieve self-consistency. This renders such numerical calculations for realistic quantum devices extremely demanding and time consuming.

In this paper, we present a novel method that we termed multi-scattering Buttiker probe model (MSB). It generalizes the standard Buttiker model approach [11-12] by taking into account individual scatterings mechanisms, as illustrated in Fig. 1, ensures exact current conservation, and is orders of magnitude faster than the full NEGF method.

The key simplifications consist in (i) side-stepping the self-consistent solutions of $G^<$ and $\Sigma^<$ and (ii) by performing the $k_{||}$ integration analytically so that the Green's functions become functions of space and energy only, $G = G(z, z', E)$.

Within this method, the self-consistency cycle only involves 2 equations,

$$\begin{aligned} G^R &= (E - H_D - e\Phi - \Sigma^R)^{-1}, \\ \Sigma^R &= G^R D^R. \end{aligned}$$

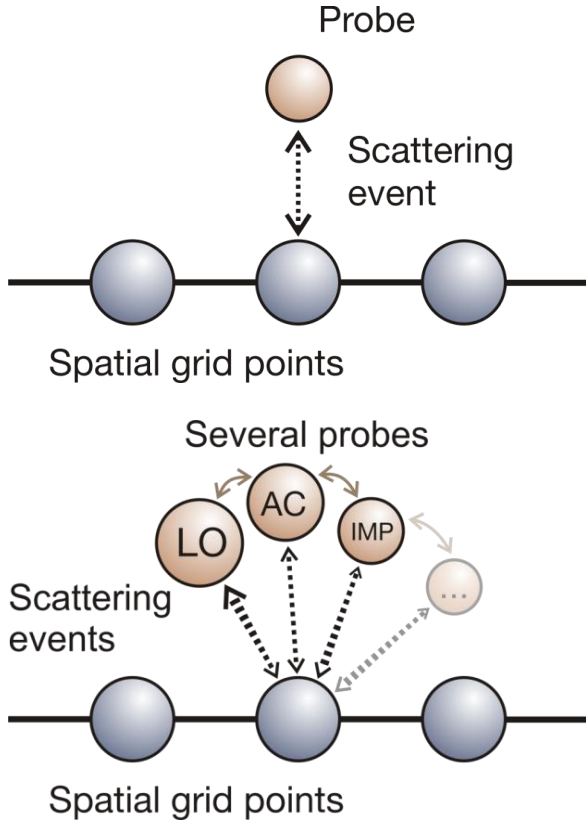


Figure 1: Top: The standard Buttiker probe model associates a single momentum and energy sink with each device node in position space. Bottom: The present multi-scattering Buttiker probe model accounts for individual scattering mechanisms by using multiple probes for each node

The self-energy Σ^R includes scattering by acoustic and optical phonons, impurity scattering and the coupling to the contacts. These various self-energies are adjusted to bulk scattering rates and depend on the material, temperature and carrier density.

The lesser Green's function is calculated by using the expression for an equilibrium system,

$$G^< = F_0(G^R - G^{R\dagger}),$$

albeit with Fermi integral $F_0(z, E)$ that contains a local Fermi level $\mu(z)$. The latter is determined in such a way as to guarantee current conservation, $\nabla \cdot j = 0$.

III. RESULTS

As an application, we consider the current-voltage characteristics of a GaAs/AlGaAs THz quantum cascade structure consisting of 4 quantum wells per period in the active region. In Fig. 2, we compare the results of fully self-consistent NEGF calculations for 2 different carrier concentrations with results obtained by the present MSB model. As one can see, one obtains very satisfactory agreement. The computer time required for the full NEGF calculation of the I-V characteristics amounts to roughly 1 week, whereas the MSB model took less than 1 hour.

The weakness of this method lies in the fact that each scattering mechanism dissipates both energy and momentum.

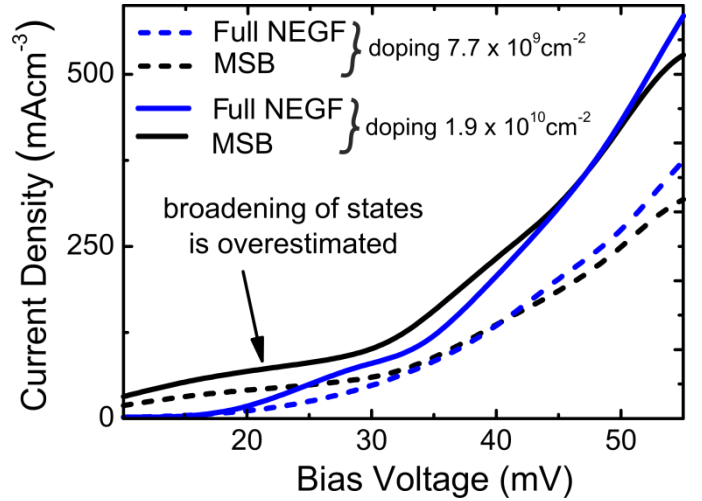


Figure 2. I-V characteristics of a GaAs/AlGaAs THz quantum cascade structure [3] for 2 different doping densities.

This approximation is obviously most critical for elastic impurity and interface roughness scattering. However, in all cases we have studied so far we find that the effects from this artificial inelasticity are small. The discrepancy between the NEGF and MSB results in Fig. 2 for voltages below 20 mV arises precisely from this approximation.

In summary, we have developed a quantum transport model that captures coherent as well as incoherent scattering processes, accurately mimics full non-equilibrium Green's function calculations, yet is orders of magnitude more efficient computationally.

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