EDISON 16 IOP Publishing
Journal of Physics: Conference Series **193** (2009) 012026 doi:10.1088/1742-6596/193/1/012026

Carrier transport in THz quantum cascade lasers: Are Green's functions necessary?

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Abstract. We have applied two different simulation models for the stationary carrier transport and optical gain analysis in resonant phonon depopulation THz Quantum Cascade Lasers (QCLs), based on the semiclassical ensemble Monte Carlo (EMC) and fully quantum mechanical non-equilibrium Green's functions (NEGF) method, respectively. We find in the incoherent regime near and above the threshold current a qualitative and quantitative agreement of both methods. Therefore, we show that THz-QCLs can be successfully optimized utilizing the numerically efficient EMC method.

1. Introduction

Accurate transport models are required to identify the detrimental effects [1, 2, 3, 4] that decrease the occupation inversion and the optical gain in state of the art THz quantum cascade lasers. Two of the most widely used models are the non-equilibrium Greens function method (NEGF) and the Ensemble Monte Carlo method (EMC). The NEGF method treats incoherent scattering such as energy dissipation and momentum relaxation as well as coherent effects such as multibarrier tunneling and correlation effects on an equal footing [5]. However exact inclusion of higher order many particle interactions such as the inelastic electron-electron scattering is typically unfeasible. In particular the numerical load of NEGF calculations usually prohibits a systematic optimization of QCL structure parameters. The EMC method is based on the semi-classical solution of the Boltzmann equation and provides a straightforward way of taking two-body processes such as electron-electron scattering into account. The most important advantage of EMC, however, is the comparably low numerical complexity which allows the systematic study of all QCL parameters. Nevertheless, EMC does not consider non-diagonal scattering [6] and misses an exact and consistent treatment of the broadening of the laser states. We show in this paper that the EMC method reproduces NEGF results in regimes where coherent transport plays a minor role. Since the threshold current of typical resonant phonon depopulation structures lies in the incoherent regime [7], the EMC method is a well suited method for modeling transport around the operation bias. In particular, the numerical efficiency of EMC allows for the systematic improvement of future THz-QCL designs.

2. Results

We apply the EMC and NEGF method on stationary transport in the THz-QCL structure of [8] at a lattice temperature of 40 K and a sheet doping density of 1.95×10^{10} cm^{-2}. A single period of this QCL consists of a sequence of GaAs and $Al_{0.15}Ga_{0.85}As$ layers of the widths (30) 92 (55) 80 (27) 66 (41) 155 Å, with the $Al_{0.15}Ga_{0.85}As$ barriers given in parenthesis. Please find details of our implementation of the EMC method in [1, 9] and the NEGF method in [5]. In both methods, we take all scattering mechanisms relevant for this QCL, i.e. electron-phonon, interface roughness [10] scattering and electron-electron interaction in the Hartree approximation into account. In addition, we also implement inelastic electron-electron scattering in the EMC method.

In order to illustrate the typical confinement energies and resonant laser states, figure 1 shows the magnitude squared of the wavefunctions used in the EMC method for the specified QCL at the peak gain bias of 54.16 mV per period. Upper and lower laser levels are marked by solid lines.

States of adjacent periods are separated by the energy of an LO-phonon (36 meV). Thus, electrons traverse between the states of adjacent periods by the resonant emission of an LO-phonon. Thereby, the lower laser level gets emptied [11, 12].

We want to emphasize that the EMC method models electronic transport with eigenfunctions of the Hermitian Hamiltonian of the QCL structure. Incoherent scattering mechanisms that limit the electronic lifetime are not included in the determination of the QCL states. Thus, the electronic states in figure 1 are given as discrete levels. In EMC, elastic and inelastic scattering is only included in the calculation of the state occupancy. In contrast, the resonant energies, the state linewidths and state occupancies are self-consistently determined in the NEGF method.

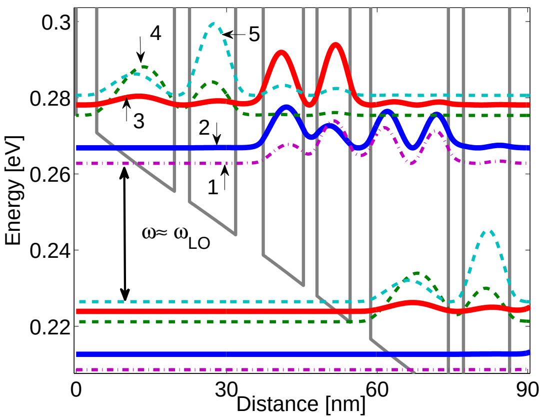

Figure 1. Energy levels and squared wavefunctions of the QCL at the peak-gain bias of 54.16 mV per period given by the EMC method.

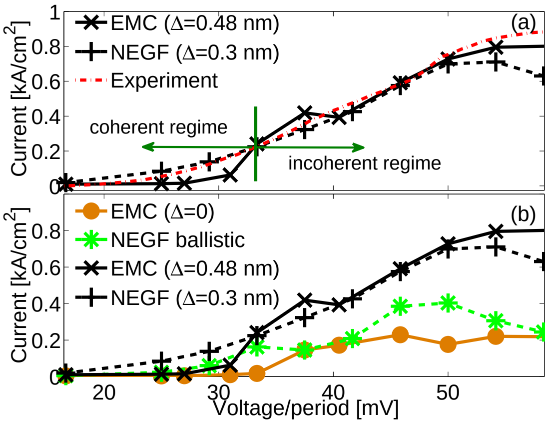

Figure 2. (a) Comparison of the simulated currents to experimental results. (b) Different cases of transport, which are shown to illustrate the contribution of the different scattering and transport mechanisms.

In spite of this discrepancy, both models reproduce the experimental current-voltage (IV) characteristics for bias voltages above 30 mV per period, as shown in figure 2 (a). For bias voltages below 30 mV per period, the EMC method yields a very small current density. In this voltage regime, the energy separation of the electronic states is too small to allow for the emission of LO-phonons. Here, the dominant transport mechanism is the coherent multi-barrier tunneling [5]. This is illustrated in more detail in figure 2 (b), as it shows the IV-characteristics resulting from a ballistic NEGF calculation when all incoherent scattering mechanisms are neglected (grey-dashed). At low bias voltages, results of the ballistic calculation agree with results of NEGF calculations including incoherent scattering (black-dashed). This shows that the transport is coherent in this regime. Since coherent transport is neglected in EMC (solid in figure 2(a)), the EMC method underestimates the current density in this regime. However, we want to point out that the current density of the EMC method remains very small in exactly that bias range which the NEGF formalism identifies as the coherent regime.

For voltages above 30 mV per period, the incoherent regime sets in. Here, incoherent scattering significantly enhances the current density in both methods. This is illustrated in figure 2 (b) for the example of interface roughness scattering. Calculations ignoring rough interfaces yield in the NEGF formalism (green dashed) and in the EMC method (orange solid) a significantly smaller current density than the respective calculations including this effect (black dashed for NEGF, black solid for EMC). Although the two methods require different interface roughness parameters (slightly larger interface roughness step height) to fit the experimental current, EMC can reproduce results of fully quantum mechanical calculations in the incoherent regime.

A well known issue comes about when the discrete sharp energy levels in the EMC method get aligned [13]. Any anticrossing of discrete states yield highly delocalized wavefunctions. Thus, the EMC method tends to overestimate the form factor and accordingly the scattering rate when discrete states are aligned. In this situation, the overestimation of scattering in the EMC method causes artificial current spikes [1] and often unreliable gain. For this reason, bias voltages that correspond to aligned discrete states are commonly avoided in EMC calculations [13].

In contrast to the IV-characteristics, the optical gain is sensitive to the linewidth of the resonant states for every bias voltage. Therefore, we have augmented in [9] the EMC method by a procedure that generates a spectrum of resonant QCL states with finite lifetime. In this procedure, the discrete energy spectrum in figure 1 is multiplied by Lorentzian functions of widths that correspond to the calculated out-scattering rates. In order to show that this procedure gives reasonable results, we compare in figure 3 the local density of states (LDOS) of the EMC (a) and the NEGF method (b).

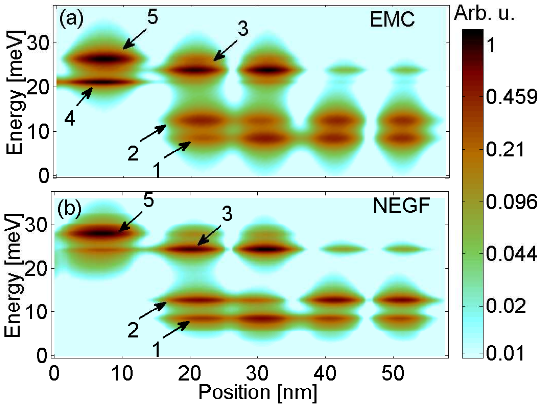

Figure 3. (a) EMC and (b) NEGF LDOS of the simulated QCL at the peak-gain bias of 54.16 mV per period. We observe similar linewidths and the missing level #4 in case of NEGF.

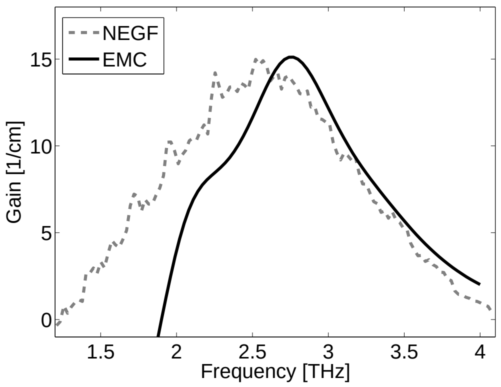

Figure 4. The optical gain in EMC (solid) and NEGF (dashed) at a bias of 54.16 mV per period. We get quantitative agreement. The slight assymetry in EMC is explained in the text.

We see a reasonable agreement between the resulting LDOS of both methods. The only significant difference is the missing resonance #4 in the NEGF calculation. The resonance #4 in the EMC method originates from an anticrossing of state #5 with a state of the preceding QCL period (see figure 1 and 3 (a)). We model in our NEGF implementation adjacent QCL periods with field free leads [14]. Therefore, the states of the preceding period lie at slightly different energies and this state anticrossing with state #5 is absent in the NEGF model (compare figure 3 (b) with (a)).

For the calculation of gain in the EMC method we use the same procedure as for the LDOS, but here the Lorentzians are weighted with the occupation inversion [9]. Optical gain in the NEGF method is calculated in linear response [5] taking into account the occupation inversion and the finite linewidths. The qualitative agreement in the LDOS of both models (see figure 3) explains the good agreement of the predicted gain spectra shown in figure 4. We find the small discrepancy for photon frequencies below approximately 2 THz to originate from the missing resonance #4 in the NEGF calculation, see figure 3 (a).

3. Conclusion

We have compared results of the semi-classical EMC and the quantum mechanical NEGF method for stationary charge transport in a recently fabricated THz-QCL. We find in the incoherent transport regime that the semi-classical transport model nicely agrees in the predicted current density and optical gain with results of the NEGF method. In particular, both models reproduce experimental results. For bias voltages significantly below threshold, coherent multi-barrier tunneling dominates the transport. Since EMC does not include this type of transport, it underestimates the current density in this regime. Nevertheless, the optimization of QCL designs requires reliable predictions close to and above threshold. Therefore, we have shown that for the purpose of design optimization, the numerical load of a detailed NEGF calculation can be avoided and the numerically efficient EMC method is appropriate.

4. Acknowledgments

C Jirauschek and A Mátyás acknowledge support the Emmy Noether program of the German Research Foundation (DFG, JI115/1-1), T Kubis acknowledges support from the Deutsche Forschungsgemeinschaft (SFB 631), the Österreichische Fonds zur Förderung der Wissenschaft (SFB IRON) and the Nano Initiative Munich.

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