Comparison between semiclassical and full quantum transport analysis of THz quantum cascade lasers[d]

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Abstract

We implement and compare two theoretical models for stationary electron transport in quantum cascade lasers and Stark ladders. The first one, the nonequilibrium Green's function method is a very general scheme to include coherent quantum mechanics and incoherent scattering with phonons and device imperfections self-consistently. However, it is numerically very demanding and cannot be used for systematic device parameter scans. For this reason, we also implement the approximate, numerically efficient ensemble Monte Carlo method and assess its applicability on the above mentioned transport problems. We identify a transport regime in which results of both methods quantitatively agree. In this regime, the ensemble Monte Carlo method is well suited to propose design improvements.

Keywords: Monte Carlo simulation, nonequilibrium Green's functions method, terahertz source, quantum cascade laser

1. Introduction

A detailed analysis of quantum transport is inevitable for the design improvement of modern nanodevices such as THz quantum cascade lasers (THz-QCLs) and Stark ladders. Among the most widely implemented transport models are the nonequilibrium Green's function method (NEGF) [1] and the ensemble Monte Carlo method (EMC) [2, 3]. The NEGF method is a very general scheme to treat quantum effects such as particle correlations, carrier confinement and interferences as well as energy and momentum relaxation and phase breaking scattering events self-consistently. Thus, the numerical load of an implementation of this method on realistic devices typically prohibits a systematic characterization of the transport with respect to all device parameters. In contrast, the EMC method is based on the solution of the semi-classical Boltzmann equation and treats several quantum mechanical effects such as coherent tunneling and lifetime broadening of device states in an approximate manner. However, the numerical load of the EMC method is much smaller than for NEGF calculations which makes it well suited for systematic variations of a large number of device parameters. The numerical efficiency of the EMC method is based on several approximations that may cause deviations of the EMC results from experimental data. First, the EMC method does not include non-diagonal scattering [4, 5] and misses an exact and consistent treatment of the broadening of the laser states [6]. This may lead to a significant overestimation of the current density in the presence of degenerate device states and an underestimation of coherent transport. Second, it is common for EMC based calculations to limit the number of explicitly considered quantum states per period. In devices with weak confinement and large applied bias fields, this limitation may underestimate the leakage of the charge carriers into the continuum of states.

We assess in this paper the applicability of the EMC method on charge transport in THz quantum cascade structures. EMC results for an experimental THz-QCL [2] are compared to NEGF calculations. Furthermore, comparisons are presented for Stark ladders, which were proposed as the most elementary THz quantum cascade structures [7]. These structures are favorable for our comparison, since an interpretation of the obtained simulation results is facilitated by the relatively small number of states per period. Additionally, the short period length of the Stark ladders is numerically advantageous for our NEGF simulations.

We apply both the EMC and the NEGF method to stationary electronic transport in recently fabricated THz-QCLs and in Stark ladders, and compare these approaches based on the obtained current-voltage (IV) characteristics and optical gain. All parameters of both methods are either well established material parameters or taken from literature. Overall, the results of both methods nicely agree with experiments. However, we identify several different transport regimes and find that the agreement of both methods depends on the respective regime. We show that the transport in bias ranges that are dominated by incoherent scattering can be very well described within the semi-classical EMC method. For low bias fields, the transport in THz-QCLs is typically dominated by coherent multi-barrier tunneling. In this case, a realistic model requires the self-consistent inclusion of the level broadening. Very high bias

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fields allow for the electrons to couple to the state continuum which cannot be described with the limited number of states typically used in the EMC method. Finally, we show that current carrying device states of the EMC method may not be lying too close in energy in order to avoid well known artificial peaks in the IV-characteristics.

The paper is organized as follows. We give a brief overview of both transport models and emphasize their differences in Section 2. We compare the theoretical results of both methods with experimental data in Section 3 and identify the transport regime in which the EMC method is appropriate. We also show that the gain spectra, self-consistently extracted from our EMC simulations based on lifetime broadening, agree well with results of the NEGF method. A summary of our results is given in Section 4.

2. Method

All quantum cascade structures in this paper are GaAs/AlGaAs quantum well heterostructures that are homogeneous in the lateral x,y directions. The electrons are described within a one-band model with a variable effective mass $m^*(z)$. Both transport models in this paper take into account the incoherent scattering of electrons with longitudinal polar optical (LO) phonons, acoustic phonons, charged impurities and rough interfaces, and the electron-electron interaction is considered in the Hartree approximation.

The NEGF method requires for the self-consistent solution of the Keldysh and the Dyson equation and the scattering self-energies of every implemented scattering mechanism. We have implemented these expressions in a real space. The choice of this basis increases the numerical load significantly but allows for the consideration of electrons confined in quantum wells as well as propagating electrons in the continuum. We have to solve a system of four coupled partial differential equations in order to determine the Green's function and self-energies. In this way, the scattering states, the transition probabilities between them and their occupations are calculated self-consistently. Once the Green's functions have been computed, observables such as the current and the electron density can be straightforwardly calculated [8, 9] and automatically include all coherent and incoherent effects that are represented by the system's Hamilton operator and the scattering self-energies. Further details of our NEGF model can be found in [8]. We emphasize, however, that the solution of four coupled differential equations is numerically very demanding. For this reason, approximate, numerically more efficient models are frequently implemented in literature. Such an approximate model is the EMC method which represents electrons in a subset of the eigenfunctions of the device Hamilton operator. This subset is restricted to low eigenenergies, thus excluding continuum states. The scattering rates between the basis states are given by Fermi's golden rule and enter the semi-classical Boltzmann equation. The latter equation is solved to determine the occupancies of the device states through distribution functions and scattering rates. Except for the Poisson equation, no further self-consistency enters the EMC method which gives a major

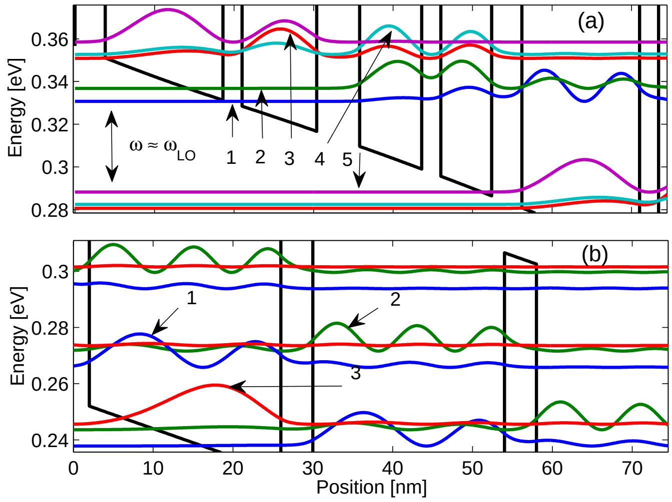

Figure 1: Conduction band profile and wavefunctions squared for the investigated structures.The wavefunctions serve as input for the semiclassical EMC simulation. (a) Modeled THz QCL (biased at 13.4 kV/cm) from Ref. [2]. It consists of $Al_{0.15}Ga_{0.85}As$ barriers and GaAs wells with layer thicknesses (given in Å): (38) 64 (24) 78 (54) 94 (24) 148, where the values in the brackets represent the barriers. The underlined well contains a uniform sheet doping of 2.8 $\times 10^{10}$ cm^{-2}. (b) Stark ladder of Ref. [7], biased at 10 kV/cm. It consists of 40 Å $Al_{0.1}Ga_{0.9}As$ barriers and 240 Å wells. The doping in the well is 10^{10} cm^{-2}.

numerical advantage. However, the device electrons in this method are represented in an incomplete basis which misses the states continuum. In addition, these basis functions have an infinite lifetime which is known to yield artificially sharp resonances in the charge transport. This is in particular problematic for the calculation of the optical gain. For this reason, we have previously extended the common EMC method and calculate the optical gain assuming a Lorentzian level broadening according to the intersubband outscattering rates [3]. Please refer to Refs. [3, 6, 10] for more details of our EMC method.

3. Results

We apply the EMC and the NEGF method on electronic transport in two THz quantum well structures, see Fig. 1. First, we investigate a resonant phonon THz-QCL from Ref. [2] at a lattice temperature of 25 K. The conduction band profile and the relevant resonant states in a single period of this QCL at a bias of 13.4 kV/cm are depicted in Fig. 1 (a). The upper laser level (labeled by 4 in Fig. 1 (a)) gets resonantly filled due to its alignment with states 4 and 5. Note that the energy separation of the lower laser level 2 and state 5 of the next period approximately equals the LO-phonon energy. Thus, the lower laser level is emptied by the resonant emission of polar optical phonons. Consequently, when the state alignment in this kind of QCL allows for the resonant emission of LO-phonons, a major fraction of the charge transport is controlled by incoherent scattering. This is illustrated in Fig. 2 which shows the calculated and experimental IV-characteristics of this THz-QCL. The ballistic NEGF calculation (dotted), which ignores any kind of incoherent scattering, strongly deviates from the

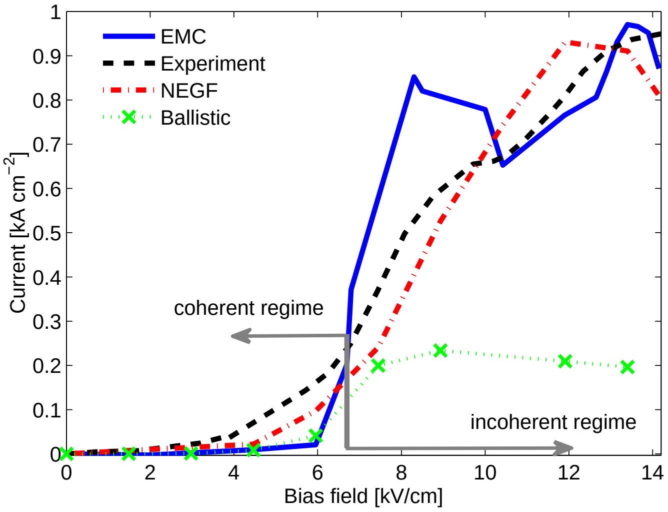

Figure 2: Calculated and experimental current-voltage characteristics of the THz-QCL in Ref. [2]. The ballistic NEGF calculation (dotted) ignores any incoherent scattering and yields much smaller current densities than results of NEGF calculations including all relevant scattering mechanisms (dash-dotted). Results of the EMC method (solid) agree quantitatively with NEGF calculations and experimental data (dashed) for bias fields above 10 kV/cm.

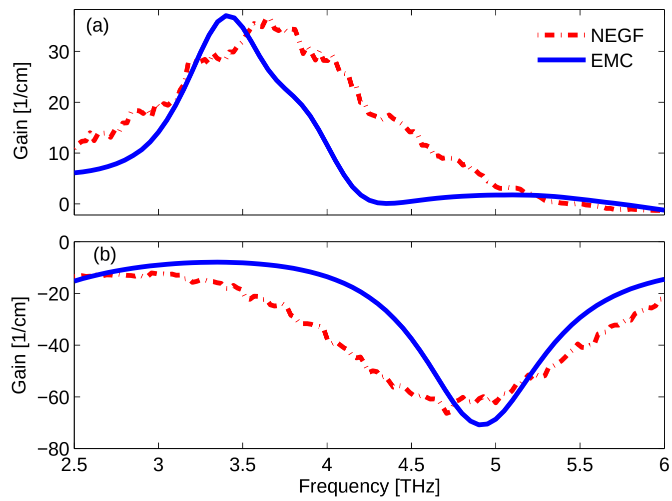

Figure 3: Theoretically predicted spectal gain for (a) the QCL around the lasing frequency of 3.4 THz and (b) the Stark ladder consisting of 40 Å, designed to operate at a frequency of 4.9 THz. Results of the EMC method (solid) nicely agree with results of the NEGF method (dash-dotted).

experimental data (dashed) for bias fields above 7 kV/cm. For applied fields below 7 kV/cm, the results of a NEGF calculation including all relevant incoherent scattering mechanisms (dash-dotted) agree with the ballistic NEGF results. Therefore, the bias of 7 kV/cm marks the borderline between the coherent and incoherent transport regimes. Since the EMC method does not include the finite linewidth of the resonant states, it notoriously underestimates the coherent tunneling at low bias fields. For this reason, the EMC method fails to predict transport in the coherent regime.

The current spike of the EMC method (solid in Fig. 2) at approximately 8.3 kV/cm originates from the alignment of the QCL states 1 and 3 (see Fig. 1 (a)). Due to the neglected state linewidth, the current density at fields around such an anticrossing is known to be overestimated in the EMC method. However, for fields above 10 kV/cm, all device states are well separated in energy and the EMC method agrees nicely with the NEGF results. Most notably, we also get a qualitative agreement for the calculated optical gain of both methods in the incoherent transport regime, as is illustrated in Fig. 3 (a).

Simulation results for Stark ladders are shown in Figs. 3 (b) and 4. Since the EMC method neglects the continuum states, it underestimates the tunneling processes into the continuum and thus the current for high biases gets lowered. This is illustrated in Fig. 4 (a) which shows the calculated IV-characteristics of the Stark ladder in Fig. 1 (b) for a barrier width of 20 Å. The lattice temperature and sheet doping density are 100 K and 10^{10} cm^{-2} (see Ref. [7] for details). The doping in this structure is reduced by a factor of 10 as compared to Ref. [7] for getting approximately the doping used in the QCL. The current in the Stark ladder in Fig. 1 (b) is then mainly carried by LO phonon scattering, and Coulombic scattering plays a secondary role. The calculated current densities agree very well for ap-

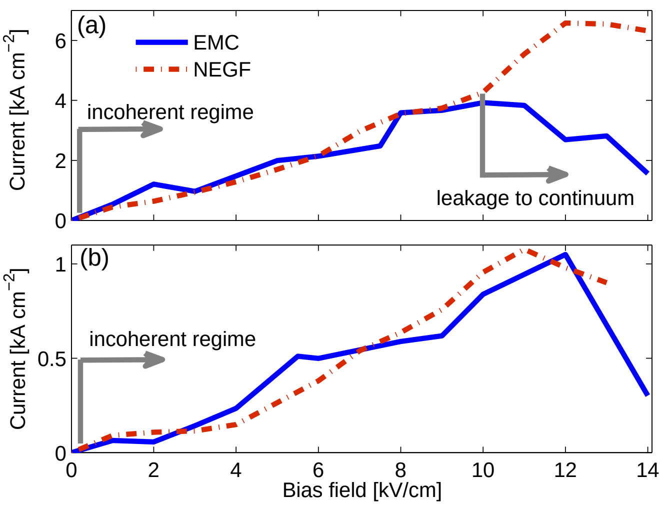

Figure 4: Calculated IV-characteristics of the GaAs/$Al_{0.1}Ga_{0.9}As$ Stark ladders operating in the THz regime. The wells are 240 Å. Barrier widths are 20 Å in (a) and 40 Å in (b) respectively. Results of the EMC method are depicted by the solid line and agree in a large bias range with NEGF calculations (dash-dotted).

plied electric fields below 10 kV/cm as shown in Figs. 4 (a) and (b) for Stark ladders with 20 Å and 40 Å barriers, respectively. At higher fields, the leakage into the state continuum sets in, and the EMC method underestimates the current density. This leakage is efficiently suppressed for increased barrier widths (see Fig. 4 (b)), where the onset of the leakage into the state continuum is shifted towards higher applied electric fields and the results of both methods agree in a larger bias range. It is worth mentioning that the coherent transport regime is not present for the Stark ladders, as shown in Fig. 4. We also emphasize that the obtained spectral loss of the Stark ladder agrees for both methods (see Fig. 3 (b)).

4. Conclusions

We have applied the ensemble Monte Carlo method (EMC) and the nonequilibrium Green's function method (NEGF) on stationary electron transport in resonant phonon THz-QCLs and Stark ladders. Our results show that the approximate treatment of coherent tunneling and leakage into continuum states limits the applicability of the EMC method on transport regimes that are dominated by incoherent scattering. When all device states that contribute to transport are clearly non-degenerate, results of the current density obtained by the EMC method quantitatively agree with NEGF results and experiment. Also the simulated spectral gain profile is in good agreement for both methods. This is in particular important because the numerical load of NEGF calculations exceeds the load of the EMC method tremendously and typically prohibits a systematic improvement of QCL designs.

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