Predictive Microscopic Approach to Transport in THz Quantum Cascade Lasers

T. Schmielau and M.F. Pereira
Materials and Engineering Research Institute, Sheffield Hallam University
S1 1WB, Sheffield, United Kingdom
mpereira@shu.ac.uk

Abstract. In this paper we present further details of a predictive Keldysh nonequilibrium many body Green’s functions theory for quantum transport including high order electron-electron, electron-phonon, electron-impurity and interface roughness scattering processes. Our approach is fully frequency and momentum dependent. Local current conservation is observed even if only few states are considered. The resulting algorithm has led to good agreement with experimental observations.

1. Introduction
The Quantum Cascade Laser (QCL) is the best candidate for efficient generation of terahertz (THz) radiation. QCL development is one of the current frontiers in semiconductor science from both the fundamental and applications points of view [1]. The systematic exploitation of THz waves has been hindered by the lack of a compact coherent source providing high output power. There is a huge potential for THz technology in a varied list of applications; detecting tumours and skin cancers, pharmaceutical applications, detecting and discriminating explosive threat materials, environmental sensing and gas monitoring, industrial process control, astronomy, semiconductor imaging, security and medical imaging and telecommunications [2]. A number of different materials and systems have been proposed to create compact sources [3] but so far QCLs remain the best candidates for this role.

It cannot be over emphasised what a tour de force a QCL is in both the design and the growth. For example, an average THz QCL contains about 1000 layers and takes about eight hours to grow, as compared to the two hours required for a moderately complex commercial device such as a GaAs high electron mobility transistor. Each design has to be optimised for the wavelength chosen, materials used, and growth technique employed, and trade-offs have to be made for pulsed or continuous use, and operating temperature. In fact, it is questionable how often this ideal is actually reached as design and growth are so difficult. The main difficulty so far is to achieve population inversion and it may well be that room temperature operation will only be reached through innovative concepts, like lasing without inversion [4-6]. A fully predictive and user-friendly QCL simulator is needed by manufacturers and research teams to design and simulate new devices easily and solve the current technical problems faster. In this paper we complement the material published recently [7-9] on our predictive transport simulator by presenting numerical results for the energetically and spatially resolved electronic density and density of states in a THz QCL. We further give more details of the performance of our algorithms.
2. Summary of the Main Equations and Numerical Method

Electronic states in the QCL are described by in-plane waves with wavevector \( \mathbf{k} = (k_x, k_y) \) and (Wannier or position) states \( \alpha, \beta \ldots \) in growth direction \( (z) \) and are denoted, e.g. \( \Psi_\alpha(z) \). We define \( \alpha = (\mu, m, s) \) and \( \beta = (\nu, n, s') \) and where \( m; n \) indicate the basic period where the state is located and the subband indices, \( \nu, \mu \) number the states inside that period. The spin indices \( s, s' = \pm 1/2 \) are dropped from now on as all occupations and interactions are spin independent. As translational invariance is broken in the growth direction, the usual Dyson equation for the retarded \( G \) becomes a matrix equation in the states

\[
G^{ret}_{\alpha\beta}(k, E) = (G^{ret}_{0}(k, E) - \Sigma^{ret}(k, E))^{-1},
\]

where the inverse unperturbed retarded Green's function \( G^{ret}_{0}(k, E)^{-1} = E\delta_{\alpha\beta} - H^{ret}_{0} + i\epsilon \) is determined by the single-particle Hamiltonian \( H^{0} = H_{kin} + V_{SL} + V_{H} + V_{field} \) containing kinetic energy, superlattice potential, mean field, and electric potential \( V_{field} = eez \) due to the applied electric field \( e \), respectively. In order to reduce the matrix equation to finite size, the periodicity of the superlattice is exploited (period length \( d \))

\[
G_{\mu m + \nu n + s, \mu m' + \nu n' + s'}(E + eezd) = G_{\mu m, \mu m'}(E).
\]

Furthermore, Greens Functions spanning more than two basic periods are assumed to vanish. The greater \((\rangle)\) and lesser \((\langle)\) components of the GF, which determine the actual occupation of the electronic states, are then obtained from the Keldysh relation

\[
G^{\langle\rangle}_{\alpha\beta}(k, E) = \sum_{\mu\nu} G^{ret}_{\alpha\mu}(k, E) \cdot \Sigma^{\langle\rangle}_{\mu\nu}(k, E) \cdot \left(G^{ret}_{\beta\mu}(k, E)\right)^{\ast},
\]

and similarly exchanging \((\langle)\) by \((\rangle)\). The additional initial condition term has been omitted from Eq. 3 as it vanishes due to dissipation. As a numerical cross-check it has been verified that the Kubo-Martin-Schwinger (KMS) [10] condition between \( G^{>\rangle} \) and \( G^{<\langle} \) is fulfilled at zero applied voltage, indicating relaxation to thermal equilibrium. The spatially and energetically resolved electron density reads (see also Ref. [11])

\[
n_e(z, E) = \sum_{\mathbf{k}} n_e(z, \mathbf{k}, E) = \frac{1}{imA} \sum_{\alpha\beta\mathbf{k}} \Psi_{\alpha}^{\ast}(z) \Psi_{\beta}(z) G_{\beta\alpha}^{<\langle}(k, E),
\]

where \( A \) denotes the sample area.

3. Numerical Results

Wavenumber resolved quantities can be defined by leaving out the \( k \) summation as shown in Eq. (4). Figures 1 and 2 depict the electronic density resolved both spatially and energetically at \( k=0 \) for the QCL of Ref. [12]. Equilibrium conditions are shown in Fig. 1 while in Fig. 2 the system is out of equilibrium and polarized with a voltage drop of 62 mV per period. The development of gain requires a combination of allowed transitions, upper laser states more populated than the lower sates (population inversion) and a relatively small dephasing so that the resulting gain can overcome waveguiding losses. Local gain is achieved when certain regions of \( k \)-space (normally for small \( k \)) are inverted and compensate the losses in other \( k \)-space regions when all contributions are summed up. The active region is typically designed so that electronic overlap between the relevant states lead to large transition dipole moments. Figure 1 shows only lower laser levels occupied at equilibrium while Fig. 2 under nonequilibrium conditions clearly shows more occupation in the upper levels in the active region \( 5.5nm < z < 22.4nm \). This indicates local population inversion in \( k \)-space that can potentially lead to gain and thus lasing.
Those plots allow further insight into the nonequilibrium charge distribution in the structure and use it to analyse potential design failures and re-design the lasers based on those studies. Similar studies already led to deeper insight into the characteristics of mid infrared and THz QCLs [11, 13]. The self energies included in the calculations include high order electron-electron, electron-phonon, electron-impurity and interface roughness scattering processes. To the best of our knowledge this is the first time that those plots are presented with a consistent inclusion of electron-electron scattering within a dynamic single-plasmon pole approximation. The numerical results presented here were obtained with our optimized simulator, which is fully parallelized and optimized for vector units (SSE2 / AltiVec). The self energy calculation, which is the main numerical task, achieves ~ 60% of the CPU's theoretical peak performance (~ 43 GFLOP/s on a 2.2 GHz quad core CPU).

![Figure 1. Equilibrium energetically and spatially resolved electronic density at \( k=0 \), \( n_e(z,k=0,E) \) in Eq. 4, for the QCL of Ref. [12].](image)

A compensation between coherent and scattering processes leads to local current conservation even if only a small number of states is considered. Our algorithm is fully frequency and momentum dependent The numerical results presented here assume the plasmons to be in thermal equilibrium with the lattice phonons. This approximation should be more accurate when the plasma frequency characterizing a given subband [14] is close to the optical phonon frequency, thus leading to stronger coupling between those modes [15, 16]. However, the plasmons are still part of the electron gas and in future work we plan to develop a more complete theory that also consider details of the energy transfer from plasmons to phonons, leading to a nonequilibrium plasmon distribution function.

In summary, our efficient numerical scheme can be used to predict transport of electrons as they cascade down a polarized quantum cascade laser and yields microscopic insight that can help understand the current bottlenecks in the development of new THz designs. It can help create structures that will operate at higher temperature more efficiently.
Figure 2. Nonequilibrium energetically and spatially resolved electronic density at $k=0$, $n_e(z,k=0,E)$ in Eq. 4 for the QCL of Ref. [12] polarized with a voltage drop of 62 mV per period. Note the local population inversion in the active region $5.5 \text{ nm} < z < 22.4 \text{ nm}$.

References
[1] R. Köhler, A. Tredicucci, F. Beltram, H. E. Beere, E. H. Linfield, G. A. Davies and D. A. Ritchie, Advances in Solid State Physics 43, 327 (2003).
[2] M.F. Pereira, Journal of Telecommunications and Information Technology 4, 118 (2009).
[3] M.E. Portnoi, O.V. Kibis, M. Rosenau da Costa, Superlattices and Microstructures 43, 399 (2008).
[4] A. Wacker, Nat. Phys. 3, 298 (2007).
[5] R. Terazzi, T. Gresch, M. Giovannini, N. Hoyler, F. Faist, and N. Sekine, Nat. Phys. 3, 329 (2007).
[6] M. F. Pereira Jr., Phys. Rev. B, vol. 78, 245305-1 (2008).
[7] T. Schmielau and M.F. Pereira, Appl. Phys. Lett. 95, 231111 (2009).
[8] T. Schmielau and M.F. Pereira, Microelectronics Journal 40, 869 (2009).
[9] T. Schmielau and M.F. Pereira, physica status solidi b 246, 329 (2009).
[10] R. Zimmermann, Many-Particle Theory of Highly Excited Semiconductors, Teubner, Leipzig (1987).
[11] A. Wacker, phys. stat. sol. (c) 5, No. 1, 215–220 (2008).
[12] S. Kumar, B. S. Williams, S. Kohen, Q. Hu and J. Reno, Appl. Phys. Lett. 84, 2494 (2004).
[13] R. Nelander, A. Wacker, M.F. Pereira Jr., D.G. Revin, M.R. Soulby, L.R. Wilson, J.W. Cockburn, A.B. Krysa, J.S. Roberts, and R.J. Airey, Journal of Applied Physics 102, 113104 (2007).
[14] M. F. Pereira, Jr., W. Chow, and S. W. Koch, J. Opt. Soc. Am. B 10, 765 (1993).
[15] C. Peschke, J. Appl. Phys. 74, 327 (1993).
[16] P. Borowik, J. Appl. Phys. 82, 4350 (1997).