Quantum transport calculations for quantum cascade laser structures

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Abstract

We apply a quantum transport theory based on nonequilibrium Green’s functions to quantum cascade laser (QCL) structures, treating simultaneously the transmission through the injector regions and the relaxation due to scattering in the active region. The quantum kinetic equations are solved self-consistently using self-energies for interface roughness and phonon scattering processes within the self-consistent Born approximation. In this way, we obtain the current density $J$, and the average electronic distribution $f(E)$ at a given energy $E$, as a function of applied bias. As a test case, we apply the theory to a GaAs/Al$_x$Ga$_{1-x}$As QCL structure reported in the literature. The theoretical results reproduce well reported voltage-current (V-I) measurements, and also demonstrate a population inversion at a bias that agrees well with the range of currents and fields at which lasing is observed.

Key words: quantum cascade laser, quantum transport

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Quantum cascade laser (QCL) heterostructures[1] are unipolar devices which operate on the basis of light-emitting intersubband (intraband) transitions. They are designed with a complicated sequence of semiconductor layers with varying widths. This sequence of layers is repeated up to, for example, 30 periods. Part of the semiconductor layer sequence in each period operates as the active region within which the lasing transition occurs. The remaining layers in the period play the role of an injector for the active region, as well as a collector of carriers from the preceding period. Fig. 1 shows an example of the conduction band line-up of a QCL structure taken from Ref. [2].

The transport of carriers through QCL structures is governed by a complex interplay between transmission through the injector region, and relaxation in the active region through scattering processes and light emission ([3], [4]). To investigate the carrier transport in QCL structures, we apply a quantum transport theory based on nonequilibrium Green’s functions [5], which incorporates both transmission in the injector region and scattering-induced relaxation processes. The quantum transport equations for the nonequilibrium Green’s function $G^{\text{ret}}(k, E)$, and the correlation function $G^{\text{<}}(k, E)$, are solved self-consistently with self-energies for phonon and interface roughness scattering processes, within the self-consistent Born approximation. From $G^{\text{ret}}(k, E)$ and $G^{\text{<}}(k, E)$, we can determine the current density $J$, and the average electronic distribution $f(E)$, which gives the average occupation of the levels at a given energy $E$.

To model a QCL structure we treat the system as a periodic superlattice structure where each period consists of $N$ barriers and wells with varying widths. The Hamiltonian for this structure may be separated into two parts, $\hat{H} = \hat{H}_o + \hat{H}_{\text{scatt}}$. The Hamiltonian $\hat{H}_o$ contains the superlattice potential and, if present, a static electric field $E$ applied in the growth direction, i.e., $\hat{H}_o = \hat{H}_{\text{SL}} + \hat{H}_E$. A plane-wave basis is used in the plane of the semiconductor layers. In the growth direction, we use a localised, Wannier state basis [6]. Hence, we write

$$\hat{H}_{\text{SL}} = \sum_{n,\nu} \left[ \int d^2k \ E^\nu(k) \ a_n^{\nu\dagger}(k) \ a_n^\nu(k) \right. $$

$$ + \left. \int d^2k \ T_1^\nu \left( a_{n+1}^{\nu\dagger}(k) \ a_n^\nu(k) + a_{n-1}^{\nu\dagger}(k) \ a_n^\nu(k) \right) \right],$$

(1)

where the index $n$ labels a period in the superlattice, and the index $\nu$ labels a Wannier level $\psi^\nu(z)$ within a period. $a_n^{\nu\dagger}(k)$ and $a_n^\nu(k)$ are creation and annihilation operators for an electron with the two-dimensional in-plane wavevector $k$, in the $\nu$th Wannier level, in period $n$. The Wannier states are not eigenstates of $\hat{H}_{\text{SL}}$, and therefore $T_1^\nu$ represents the off-diagonal coupling between Wannier levels in different periods, and $E^\nu$ represents the diagonal elements of $\hat{H}_{\text{SL}}$ in this basis. We only take into account couplings between adjacent
periods. The Hamiltonian $\hat{H}_{E}$, due to the electric field, is written as

$$\hat{H}_{E} = \sum_{n,\nu,\mu} \int d^2k \left[ -eE R_0^{\mu\nu} a_n^{\mu\dagger}(k) a_{n+1}^{\nu}(k) -eE R_1^{\mu\nu} \left( a_{n+1}^{\mu\dagger}(k) a_n^{\nu}(k) + a_n^{\mu\dagger}(k) a_{n+1}^{\nu}(k) \right) \right], \quad (2)$$

where $R_0^{\mu\nu} = \int dz \psi^\mu(z - ld) z \psi^\nu(z)$. $d$ is the length of one period. The interface roughness and phonon scattering processes expressed by $\hat{H}_{scatt}$ are treated in the form of self-energies which are described below. We have neglected electron-electron scattering processes in this present work because of the increased complexity in the theory when they are included. These processes should, however, be treated in a more comprehensive study at a later stage.

The quantum transport equations derived from the Hamiltonian $\hat{H}$ have the following form ([5],[6]). The retarded Green’s function $G_{\alpha_1\alpha_2}^{\text{ret}}(k, E)$ is given by the Dyson equation

$$EG_{\alpha_1\alpha_2}^{\text{ret}}(k, E) - \sum_{\beta} \left[ (\hat{H}_o)_{\alpha_1\beta} + \Sigma_{\alpha_1\beta}^{\text{ret}}(k, E) \right] G_{\beta\alpha_2}^{\text{ret}}(k, E) = \delta_{\alpha_1\alpha_2}, \quad (3)$$

where $\alpha_1$ and $\alpha_2$ are general indices that include both the period and Wannier level indices, e.g. $\alpha_1 \equiv (m, \mu)$. The correlation function $G_{\alpha_1\alpha_2}^{<}(k, E)$ is obtained from the Keldysh relation:

$$G_{\alpha_1\alpha_2}^{<}(k, E) = \sum_{\beta\beta'} G_{\alpha_1\beta}^{\text{ret}}(k, E) \Sigma_{\beta\beta'}^{<}(k, E) G_{\beta'\alpha_2}^{\text{adv}}(k, E), \quad (4)$$

where $G_{\alpha_1\alpha_2}^{\text{adv}}(k, E) = [G_{\alpha_1\alpha_2}^{\text{ret}}(k, E)]^\dagger$. The self-energies $\Sigma_{\alpha_1\alpha_2}^{\text{ret}}(k, E)$ and $\Sigma_{\alpha_1\alpha_2}^{<}(k, E)$ describe the scattering processes arising from $\hat{H}_{scatt}$, and are evaluated within the self-consistent Born approximation. Assuming that the diagonal parts of $G(k, E)$ and $\Sigma(k, E)$ dominate, the self-energy for interface roughness scattering has the form:

$$\Sigma_{m\mu,m\mu}^{<,\text{rough}}(k, E) = \sum_{n\nu,k'} \langle |V_{m\mu,n\nu}^{\text{rough}}(k - k')|^2 \rangle G_{n\nu,n\nu}^{<}(k', E). \quad (5)$$

$V_{m\mu,n\nu}^{\text{rough}}(k' - k)$ is the matrix element for interface roughness scattering. The equation for $\Sigma_{m\mu,m\mu}^{<,\text{rough}}$ is obtained by the replacements: $\Sigma_{m\mu,m\mu}^{<,\text{rough}} \rightarrow \Sigma_{m\mu,m\mu}^{\text{ret},\text{rough}}$, and $G_{n\nu,n\nu}^{<} \rightarrow G_{n\nu,n\nu}^{\text{ret}}$. For optical or acoustic phonon scattering, the self-energies are:

$$\Sigma_{m\mu,m\mu}^{\text{ret},\text{phon}}(k, E) = \sum_{n\nu,k'} |V_{m\mu,n\nu}^{\text{phon}}(k, k')|^2$$
\[ x \left\{ f_B(E_{\text{phon}}) + 1 \right\} G_{n\nu,n\nu}^{\text{ret}}(k', E - E_{\text{phon}}) + f_B(E_{\text{phon}}) G_{n\nu,n\nu}^{\text{ret}}(k', E + E_{\text{phon}}) + \frac{1}{2} \left[ G_{n\nu,n\nu}^{<}(k', E - E_{\text{phon}}) - G_{n\nu,n\nu}^{<}(k', E + E_{\text{phon}}) \right] \right\} (6) \]

and

\[ \Sigma_{m\mu,m\mu}^{<,\text{phon}}(k, E) = \sum_{n\nu,k'} |V_{m\mu,n\nu}^{\text{phon}}(k, k')|^2 \left\{ f_B(E_{\text{phon}}) G_{n\nu,n\nu}^{<}(k', E - E_{\text{phon}}) + \left[ f_B(E_{\text{phon}}) + 1 \right] G_{n\nu,n\nu}^{\text{ret}}(k', E + E_{\text{phon}}) \right\}, \tag{7} \]

where \( V_{\text{phon}}^{\text{phon}} \) represents the interaction with optical or acoustic phonons, and \( E_{\text{phon}} \) represents the energy of the optical or acoustic phonon. \( f_B(E) = 1/[\exp(E/k_B T) - 1] \) is the equilibrium phonon distribution at a temperature \( T \). For practical purposes, we use momentum independent scattering matrix elements \( V_{\text{phon}}^{\text{rough}}(k, k') \), employing a representative momentum \( k_{\text{typ}} \). We find the Green’s functions \( G_{\text{ret}} \) and \( G^{<} \) by solving the quantum transport equations, Eqs. (3) and (4), self-consistently with the equations for the self-energies, Eqs. (5) – (7). Periodic boundary conditions are used, i.e., \( G_{m\mu,n\nu}(k, E) = G_{(m+l)\mu,(n+l)\nu}(k, E - l\varepsilon d) \).

Once \( G_{\text{ret}} \) and \( G^{<} \) have been determined, we can evaluate experimentally-related quantities such as the current density \( J = J_{\text{coh}}^{0 \rightarrow 1} + J_{\text{scatt}}^{0 \rightarrow 1} \) between periods 0 and 1 with

\[ J_{\text{coh}}^{0 \rightarrow 1} = \frac{2e\rho_o}{h} \int_0^\infty dE_k \int \frac{dE}{2\pi} \Re \{ \sum_{\mu,\nu} \hat{\Sigma}_{\mu,\nu}^{(0)}(k, E) g_{1\nu,0\mu}^{<}(k, E) \} \tag{8} \]

and

\[ J_{\text{scatt}}^{0 \rightarrow 1} = \frac{2e\rho_o}{h} \int_0^\infty dE_k \int \frac{dE}{2\pi} \Re \left\{ \sum_{\mu} \Sigma_{0\mu,0\mu}^{\text{ret},(1)}(k, E) g_{0\mu,0\mu}^{<}(k, E) + \sum_{0\mu,0\mu}^{<,(1)}(k, E) g_{0\mu,0\mu}^{\text{adv}}(k, E) \right\} \tag{9} \]

where \( \rho_o = m_e/\pi h^2 \). \( \Sigma^{(1)} \) is given by Eqs. (5) – (7) where the sum over \( n \) is restricted to \( n = 1 \). \( J_{\text{coh}} \) is the coherent contribution to the current density arising from the off-diagonal couplings in \( \hat{H}_o \), i.e., \( T_{1\nu}^{\mu} \) in \( \hat{H}_\text{SL} \) and \( -e\varepsilon R_{1\mu}^{\mu\nu} \) in \( \hat{H}_E \). \( J_{\text{scatt}} \) represents the current contribution due to the scattering processes described by \( \hat{H}_\text{scatt} \). We note here that the division between coherent and
scattering contributions to the current is artificial since it depends on the basis set used in the calculation. If, for instance, the eigenstates of $\hat{H}_o$ were chosen as the basis, there would be no coherent contribution to the current.

We apply the theory to the GaAs/Al$_x$Ga$_{1-x}$As QCL structure (Fig. 1) described by Sirtori et al. in Ref. [2]. To calculate the voltage-current (V-I) characteristic, we evaluate the current density $J$. Fig. 2 shows a plot of voltage vs. current calculated for a lattice temperature of 77 K. A comparison with experimental measurements (Fig. 3(a) in Ref. [2]) shows good agreement between the theoretical and experimental results. For instance, at a current of 4 A, the measured voltage is around 11 V, while the theoretical curve in Fig. 2 shows a voltage of $\sim$ 7 V which agrees very well with the experimental results when a residual series resistance of $\sim$ 1 $\Omega$ (see Ref. [2]), probably originating from the cladding layers, is taken into account. We comment here on the finding of Iotti et al. [7], of a strong influence of electron-electron scattering on the I-V curve. Our calculations include interface roughness scattering, but not electron-electron scattering. The converse is true in the calculations of Iotti et al. where electron-electron scattering is included, but interface roughness scattering neglected. In both cases, I-V curves in fairly good agreement with experimental measurements are obtained. We therefore conclude that interface roughness and electron-electron scattering play similar roles in determining the I-V curve, and that the I-V characteristic is not sensitive to which type of scattering is present in the calculation.

In Fig. 3, we show the density of states $\rho_{\text{DOS}} = -2 \sum_{\nu, \mathbf{k}} \Im \left[ G_{0\nu,0\nu}^{\text{ret}}(\mathbf{k}, E) \right]$ and the electron distribution function $f(E) = \sum_{\nu, \mathbf{k}} \Im \left[ G_{0\nu,0\nu}^{<}(\mathbf{k}, E) \right] / \rho_{\text{DOS}}$. Curves at three different applied voltages are shown: 0, 3, and 7 V. At 0 V, we see, as expected, a thermal Fermi distribution corresponding to a lattice temperature of 77 K. As the applied voltage increases, the occupation probability at higher energies increases. In addition, phonon replicas become visible in $f(E)$. At 7 V, the occupation probability is higher at an energy of 0.2 eV than at lower energies between 0 to 0.1 eV. This demonstrates the onset of a population inversion. At this voltage, the current is 4.5 A, corresponding to a current density of 7.5 kAcm$^{-2}$. This is in good agreement with the threshold current density of 7.2 kAcm$^{-2}$ for laser emission which is reported in Ref. [2].

In summary, we have applied a quantum transport theory based on nonequilibrium Green’s functions to QCL structures. The initial results for transport properties such as current densities are in good agreement with experimental data reported in the literature. The calculated electron energy distribution also demonstrates a population inversion at a current density which agrees well with the range of fields and currents at which lasing is observed.

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FIGURE CAPTIONS

Fig. 1 Example of the conduction band line-up in a QCL structure taken from Ref. [2]. Each period contains 16 semiconductor layers giving a period length \( d = 45.3 \) nm. There are 30 periods in this structure. The in-plane area is \( 6 \times 10^{-4} \) cm\(^2\). The Wannier functions used as the basis set for the calculations are also shown.

Fig. 2 Calculated V-I characteristic for the GaAs/Al\(_x\)Ga\(_{1-x}\)As QCL structure described in Ref. [2]. Sample area \( 6 \times 10^{-4} \) cm\(^2\).

Fig. 3 The lower row shows the distribution function of electrons for different applied bias. The current and applied bias are shown with each curve. The corresponding electric fields are 0, 22, and 53 kV/cm, and the current densities are 0, 85, and 7500 A/cm\(^2\). The upper row shows the corresponding density of states \( \rho_{\text{DOS}} \) (scaled with \( \rho_o \)) for each bias.
Fig. 1

\[ \varepsilon = 55 \text{ kV/cm} \]

GaAs/Al\textsubscript{0.33}Ga\textsubscript{0.67}As

active region

injector
Fig. 2

![Graph showing current density vs. voltage at 77 K](image-url)
Fig. 3

![Graphs showing density of states and electron distribution for different voltages and currents.](image-url)