Density Matrix Superoperator for Terahertz Quantum Cascade Lasers

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1. Introduction

Terahertz-frequency quantum cascade lasers (THz QCLs) require very small energy difference between the lasing states (~10 meV), and modelling of these devices can be challenging. Various models for transport in QCLs exist [1]; most commonly employing semi-classical approaches such as self-consistent rate-equation (RE) modelling, which provide nonphysical results for sequential tunnelling. Density matrix (DM) model includes quantum transport effects and is able to overcome known shortcomings of RE models. In this work [2], we present a DM approach applicable for arbitrary number of states per module and we formulate a superoperator for partitioned Hamiltonians that are usually employed in periodic quantum systems.

2. Theoretical consideration

The time evolution of the density matrix is described by the Liouville equation. We consider periodic QCL structure with infinite number of periods, which implies infinite-sized matrices, but due to the nearest neighbour approximation and the symmetry of QCL structure, Hamiltonian and the corresponding density matrix can be represented on three periods as:

$$H=\begin{bmatrix}H_1 & H_2 & 0\\ H_3 & H_1 & H_2\\ 0 & H_3 & H_1\end{bmatrix}+eKL_P\begin{bmatrix}I & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & -I\end{bmatrix}=H_0+\Upsilon,\quad \rho=\begin{bmatrix}\rho_1 & \rho_2 & 0\\ \rho_3 & \rho_1 & \rho_2\\ 0 & \rho_3 & \rho_1\end{bmatrix},$$

$$D=\begin{bmatrix}D_1 & D_2 & 0\\ D_3 & D_1 & D_2\\ 0 & D_3 & D_1\end{bmatrix}=-\begin{bmatrix}\tau_{||}^{-1}+\tau^{-1} & \tau_{||}^{-1} & 0\\ \tau_{||}^{-1} & \tau_{||}^{-1}+\tau^{-1} & 0\\ 0 & \tau_{||}^{-1} & \tau_{||}^{-1}+\tau^{-1}\end{bmatrix}\circ\rho$$

Where K is the applied external bias, L_p the period length and $H_{1,2,3}$ and $\rho_{1,2,3}$ are Hamiltonian and density matrix submatrices describing how central period interacts with neighbouring upstream and downstream period. D is a tensor that represents the dissipater of the system, and we are using Fermi golden rule for intrasubband transitions (τ^{-1}) and an approximation for the pure dephasing ($\tau_{||}^{-1}$) [2].

3. Lioville equation and linearization

In general Liouville equation of the form $\dot{\rho}=-\frac{i}{\hbar}[H,\rho]+D$ linearizes the commutator part of the system as $L=H\otimes I-I\otimes H^T$ and the system can be linearized as $\dot{\rho'}=-\frac{i}{\hbar}L\rho'+D'\rho'$ where ρ' is vectorised form of the density matrix (unpacked row-wise), however such formulation is inconvenient for infinite-sized Hamiltonians and the density matrices. We show that for QCL, Liouville equation folds into the system of 3N × 3N block equations (where N is the number of states in the single module):

$$\frac{d\rho_2}{dt}=-\frac{i}{\hbar}\left([H_2,\rho_1]+[H_1,\rho_2]+eKL_p\rho_2\right)-\frac{\rho_2}{\tau_{||}}$$
$$\frac{d\rho_1}{dt}=-\frac{i}{\hbar}\left([H_3,\rho_2]+[H_1,\rho_1]+[H_2,\rho_3]\right)-\frac{\rho_1}{\tau_{||}}-\frac{\rho_1}{\tau}$$
$$\frac{d\rho_3}{dt}=-\frac{i}{\hbar}\left([H_3,\rho_1]+[H_1,\rho_3]-eKL_p\rho_3\right)-\frac{\rho_3}{\tau_{||}}$$

We can linearize each commutator in the system by introducing a submatrix - Liovillians $L_i=H_i\otimes I-I\otimes H_i^T$ and newly obtained linear system can be neatly represented by using Khatri-Rao type of product:

$$\frac{d\rho''}{dt}=-\frac{i}{\hbar}(H\boxtimes I_U-I_U\boxtimes H^{.T})\rho''-\frac{i}{\hbar}\Upsilon'\rho''+D'\rho''$$

Where ρ'' is column vector that stacks vectorised forms of ρ_2,ρ_1,ρ_3 respectivally, while Υ' and D' are derived in different manner, but in essence are block diagonal matrices [2].

4. Modelling 2 THz QCL

We apply our model on 2THz bound to continuum (BTC) QCL [2] and compare our results with RE model. The fitting procedure allows us to achieve very good agreement with the experimental data at cold finger temperature of 20K.

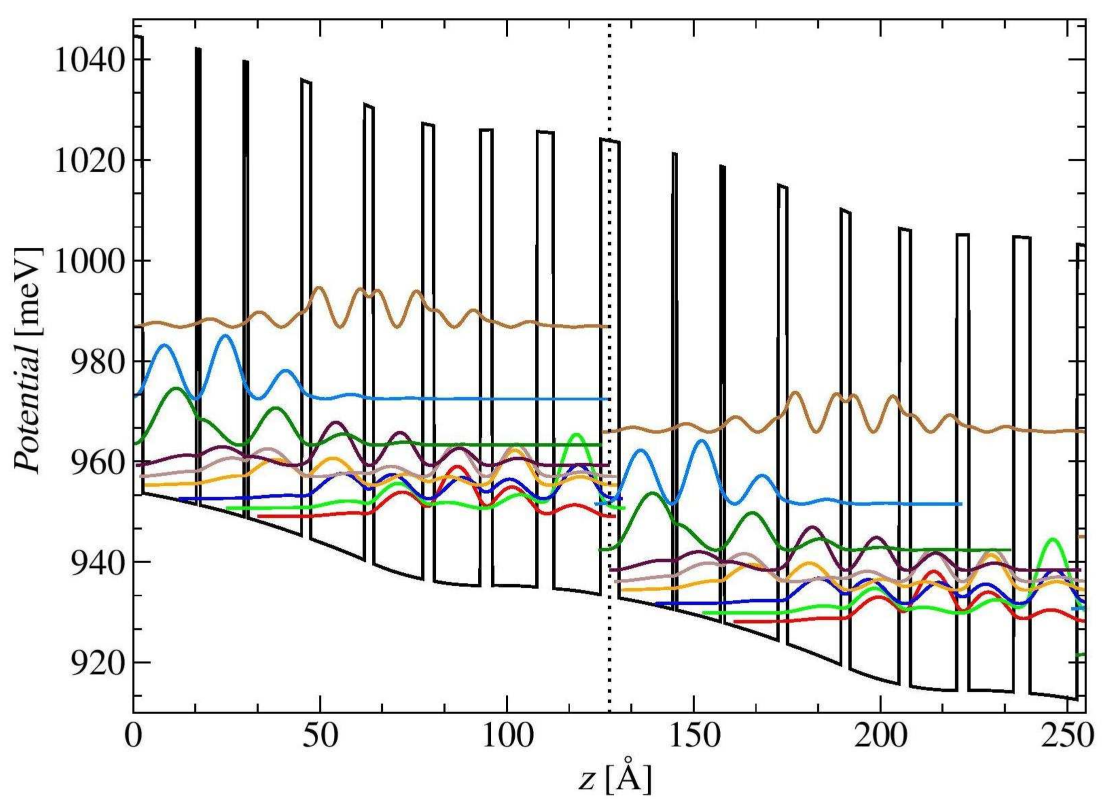

Figure 1: . Band diagram and wavefunction plot for the exemplar BTC QCL [2]. The layer thicknesses, starting with the injection barrier (until dotted horizontal line), are **5.0**/14.4/**1.0**/11.8/**1.0**/14.4/**2.4**/14.4/**2.4**/13.2/**3.0**/12.4/**3.2**/12.0/**4.4**/12.6 nm, $Al_{0.1}Ga_{0.9}As$ barriers are shown in bold and wells doped to 1.3 10^{16} cm^{-3} are underlined

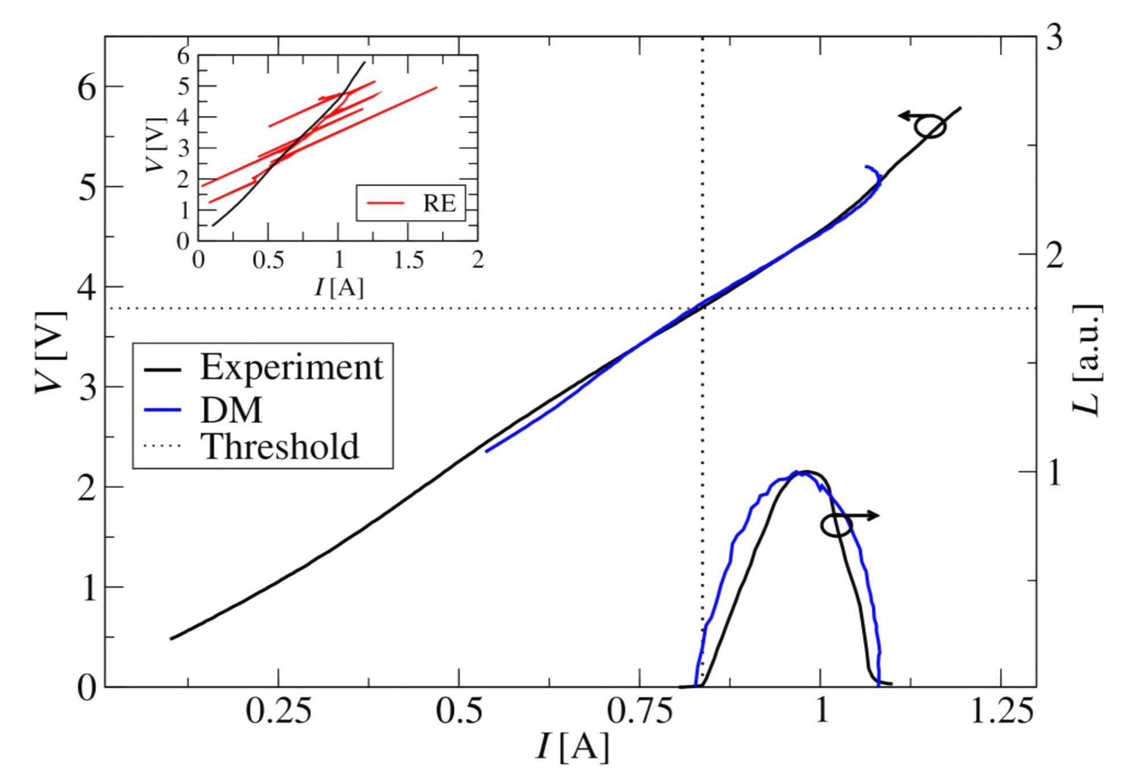

Figure 2: . *L–I–V* characteristics of the BTC device at 20K for pulsed operation. Contact resistance is 2.15 . Experimental *L-I* data is presented along DM *L-I* data and normalized in arbitrary units. RE model result is presented in the inset.

5. Temperature issues

Our model assumes that lattice temperature is equal to the cold finger temperature, which is only valid for pulsed operation at low temperatures, therefore, the results for higher temperatures do not agree with the experiment, however, relative change is similar which shows promise for the thermal modelling similar to [3].

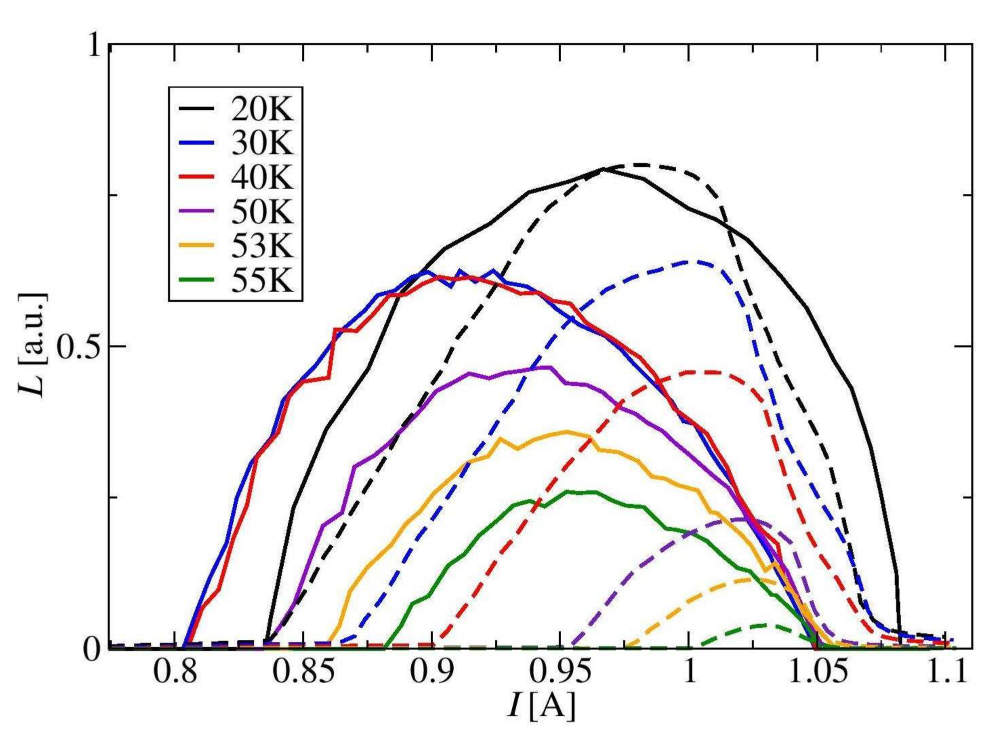

Figure 3: *L-I* characteristics for different cold finger temperatures. Full lines represent simulation result, while dashed lines represent the experimental measurement.
Scaling was performed so peak ratio is consistent in both results.

6. Conclusion

We formulated density matrix superoperator for periodic systems described by partitioned Hamiltonian. In general, our superoperator, describes the same system as the Liovillian, however the order in which the equations are written is different. Our formulation is convenient for partitioned Hamiltonians and it results in system of equations that can be written in dependence of partitions of the Hamiltonian and the density matrix which can have the intuitive physical interpretation. We presented the application of our model on 2 THz BTC QCL and demonstrated very good agreement with the experimental data at 20K.

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