Conference or Workshop Item:

Demic, A, Grier, A, Ikonic, Z et al. (6 more authors) Density Matrix Superoperator for Terahertz Quantum Cascade Lasers. In: Photonica 2017, 28 Aug - 01 Sep 2017, Belgrade, Serbia.

Density Matrix Superoperator for Terahertz Quantum Cascade Lasers

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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 considers non-radiative transitions of carriers due to various scattering mechanisms. Although these models provide insight into the scattering behaviour, they are unable to correctly describe transport between adjacent periods of a QCL structure [2] because they do not take injection barrier thickness into account in transport calculations. This leads to the prediction of instantaneous transport between the periods, whereas the actual transport that occurs is based on resonant tunnelling. Alternative approaches, based on density matrix (DM) modelling include quantum transport effects and are able to overcome known shortcomings of RE models. In this work, we present a DM approach that extends the model presented in [3], applicable for arbitrary number of states per module. This model has proved successful for a variety of QCL simulations [4-8].

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 symmetry of QCL structure Liouville equation folds into the system of $mN \times mN$ block equations (where N is the number of states in the single module and m is the number of considered periods (in general $m = 2x + 1$, $x -$ number of neighbours, in our case (the nearest neighbour approximation) $m = 3$). We show that commonly known form of the Lindblad superoperator $L = H \otimes I - I \otimes H^T + i\hbar D$ where H is the Hamiltonian of the entire system, I is the identity matrix, D is the dissipater of the system and $\otimes$ is the Kronecker tensor product, can be formulated for periodic system as $L_{per} = H_{per} \boxtimes I_{per} - I_{per} \boxtimes H_{per}^T + i\hbar D_{per}$ where H_{per} is block-partitioned Hamiltonian of $mN \times mN$ size (in our case three-diagonal block matrix), I_{per} is a matrix filled with m^2 identity matrices (each of size $N \times N$), D_{per} is the corresponding dissipater form for periodic system and $\boxtimes$ is Khatri-Rao product. This formulation of Lindblad superoperator enables simple numerical implementation and provides a system of equations that can be intuitively interpreted. The dissipater in our model has similar form as in RE and we can formulate the density matrix formalism in similar intuitive manner as in RE.

We apply our model to 2 THz bound-to-continuum structure and compare our results with RE model [8]. We obtained smooth results (contrary to RE) and managed to reconstruct the entire $L - I - V$ characteristic of the experimental result in pulsed operation at 20K.

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