Monte Carlo Simulation of Electron Transport in Quantum Cascade Lasers

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We describe a numerical simulator for the electron transport in quantum cascade lasers (QCLs). A semi-classical transport model based on the Pauli master equation (PME) is used as it is considered a good trade-off between physical accuracy and computational efficiency [1]. The basis states for the PME are determined using a multi-band k*p Hamiltonian in order to account for the effects of band non-parabolicity. The incoherent scattering processes included are due to acoustic and optical deformation potential interaction, polar optical phonons, alloy disorder and interface roughness. The master equation is solved using a Monte Carlo method [2]. To optimize the simulator for efficiency several unique features have been introduced: A new algorithm to automatically distinguish the field-periodic wave functions from the spurious states due to the artificial boundaries has been developed; we use quasi-bound states as basis functions, the life times of which allow us to estimate the coherent tunneling current; the computation time for the polar-optical scattering rate has been reduced by more than three orders by a reformulation of the multiple integrations involved; for the stationary transport problem considered a single-particle MC algorithm is applied which takes less resources than the ensemble MC method. Output quantities of a transport simulation are current-voltage characteristics, the coherent current component, optical gain, incoherent lifetimes, and subband populations. A mid infrared QCL [3] has been analyzed, where good agreement between measurement and simulation was found.

References:

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[3] H. Detz et al., Journal of Modern Optics (2011), in print