Simulation of Quantum Cascade Lasers using Robin Boundary Conditions

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***Abstract*—We present a study on tunneling current density and an investigation of the optical gain of GaAs/Al$_x$Ga$_{1-x}$As quantum cascade lasers. Current carrying states are obtained by taking into account Robin boundary conditions. Our simulation results show that this approach gives a very good agreement with other calculations using the Tsu-Esaki model and with simulations based on nonequilibrium Green's functions. Furthermore, by incorporating this method into optical gain calculations we establish good agreement with experimental results.**

I. Introduction

In 1970, Esaki and Tsu [1] proposed using heterostructures for applications in optoelectronics. The first suggestion to use intersubband transitions in order to create a laser was made by Kazarinov and Suris [2]. Over the past several years, quantum cascade lasers (QCL's) have proved to be very promising candidates for practical sources of radiation, particularly in the midinfrared region [3].

Transport modelling of charge carriers in semiconductor devices is done by means of boundary value problems. In order to model situations with net current flows and obtain current-voltage characteristics of a quantum device, one has to devise boundary conditions which allow current carrying states instead of using unappropriate ones like the homogeneous Neumann or Dirichlet boundary conditions which yield a self-adjoint Hamiltonian matrix. The system described by such a Hamiltonian is closed. Hence, there is no interaction with the environment and the current density is identical zero [4]. This leads to the necessity to consider open quantum systems with non-selfadjoint boundary conditions.

The focus of this work is on boundary conditions which yield current carrying states as solutions of the Schrödinger equation. The theoretical development is based on a Robin boundary condition approach when a solution with the Dirichlet boundary condition is available [5]. Within this scheme, the main focus of our work is to calculate the current density and the optical gain from the wave functions satisfying these boundary conditions. Comparing the results obtained with the proposed approach to other simulations and experimental measurements, we find that the concept of non-selfadjoint boundary conditions for the Schrödinger equation is satisfactory to QCL simulations. Our results indicate the importance of considering adequate boundary conditions in determining fundamental properties of QCL's.

II. Theoretical Model

Let $\Omega = [0, L]$ be the domain of the QCL perpendicular to quantum well layers. We regard Schrödinger's equation

$$\left[-\frac{\hbar^2}{2}\frac{\partial}{\partial z}\frac{1}{\mathrm{m}^\star(z)}\frac{\partial}{\partial z} + \mathrm{V}(z) - eFz\right]\Phi_i(z) = E_i\Phi_i(z) \quad (1)$$

where E_i is the energy of the ith state and F is the applied electric field. Assuming an incoming wave from $-\infty$ and no wave incident from $+\infty$, we can deduce a boundary condition at $\partial\Omega = 0$ and $\partial\Omega = L$ that does not involve reflection and transmission coefficients [6]

$$\hbar\Phi_i'(0) + i\sqrt{2\mathrm{m}^\star E_i}\Phi_i(0) = 2i\sqrt{2\mathrm{m}^\star E_i} \quad (2)$$

$$\hbar\Phi_i'(L) - i\sqrt{2\mathrm{m}^\star(E_i - V)}\Phi_i(L) = 0 \quad (3)$$

The transport of charge through the structure arises as a property of the quantum mechanical wave function satisfying the boundary conditions above. The current density is expressed as [7]

$$\mathrm{J}_{(z)} = -\frac{2e}{A}\sum_{i,k_\parallel}\mathrm{f}(E_i, k_\parallel)\mathrm{Re}\left[\Phi_i^\star(z)\frac{i\hbar}{\mathrm{m}^\star(z)}\frac{\partial}{\partial z}\Phi_i(z)\right] \quad (4)$$

where A is the cross-sectional area of the quantum well structure. The distribution functions are determined according to the Fermi-Dirac distribution for electrons

$$\mathrm{f}(E_i, k_\parallel) = \frac{1}{1 + \exp\left(\frac{E_i(k_\parallel) - E_F}{k_B T}\right)} \quad (5)$$

where E_F is the Fermi energy and $E_i(k_\parallel) = E_i + \hbar^2 k_\parallel^2/2\mathrm{m}^\star$. The E_i are quantized energies obtained by solving the Schrödinger equation with Dirichlet boundary conditions (1). The optical gain in semiconductor lasers can be estimated as [8]

$$\mathrm{g}(\hbar\omega) = \frac{e^2|z_{12}|^2\mathrm{m}_r\omega}{\hbar^2 c n_r \epsilon_0 L}\int_0^\infty dE\,\frac{\hbar\gamma(E)[\mathrm{f}(E_2) - \mathrm{f}(E_1)]}{\pi[\hbar\omega - E]^2 + [\hbar\gamma(E)]^2} \quad (6)$$

where z_{12} is the dipole matrix element, n_r is the refractive index, ϵ_0 is the vacuum permittivity and c is the speed of light. The homogeneous broadening γ is given by

$$\gamma(E) = \gamma_0 \times \begin{cases} N_{ph}, \\ (N_{ph}+1)\Theta(E - \hbar\omega_{ph}), \end{cases}$$

where the top line describes phonon absorption and the bottom line phonon emission.

III. Results and Discussion

Figure 1 compares the simulated current density using the Robin boundary condition approach with the current density calculated by the Tsu-Esaki model for a GaAs/$Al_{0.3}Ga_{0.7}As$ Fibonacci superlattice (FSL) [9] which is a quasi-periodic multibarrier system. The FSL type considered has the sequence BBABBABBBABBABBBA, where A and B are the elementary blocks corresponding to the GaAs quantum well and the $Al_{0.3}Ga_{0.7}As$ barrier, respectively. The width of the well block is taken to be 5 unit cells, whereas the number of the unit cells for the barrier block equals to 3. The appearance of resonance-type peaks in the current density curves is typical for quasi-periodic systems, and the results obtained are in good agreement with the Tsu-Esaki model.

The ability of the chosen boundary conditions to produce satisfactory current carrying states is also verified by comparing our results for the tunneling current density with calculations based on nonequilibrium Green's functions [7]. For this purpose a typical example of a midinfrared quantum cascade laser is considered [10]. The comparison of the obtained current-voltage results with the simulation employing the nonequilibrium Green's functions method is illustrated in Figure 2. The layer sequence of one period belonging to the GaAs/$Al_{0.33}Ga_{0.67}As$ structure, in nanometers, starting from the injection barrier is: **5.8**, 1.5, **2.0**, 4.9, **1.7**, 4.0, **3.4**, 3.2, **2.0**, 2.8, **2.3**, 2.3, **2.5**, 2.3, **2.5**, and 2.1, where normal scripts represent the wells, bold the barriers. The simulation is performed with the number of periods to be 30 and the temperature is taken to be 77 K. As in the case of quasi-periodic superlattices, the application of our method to calculate current carrying states proves to be very promising for periodic QCL structures as well.

Finally, we focus on the calculation of optical gain under consideration of the proposed boundary conditions. Figure 3 shows our simulation results to be in good agreement with measurements that are performed on a GaAs/$Al_{0.15}Ga_{0.85}As$ QCL [11].

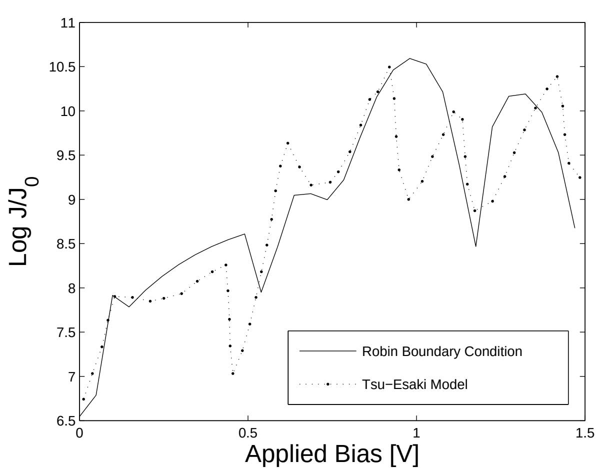

Fig. 1. Current-density voltage characteristics of a GaAs/$Al_{0.3}Ga_{0.7}As$ Fibonacci superlattice at $T = 200$K. The current density is scaled by $J_0 =$ A m^{-2}.

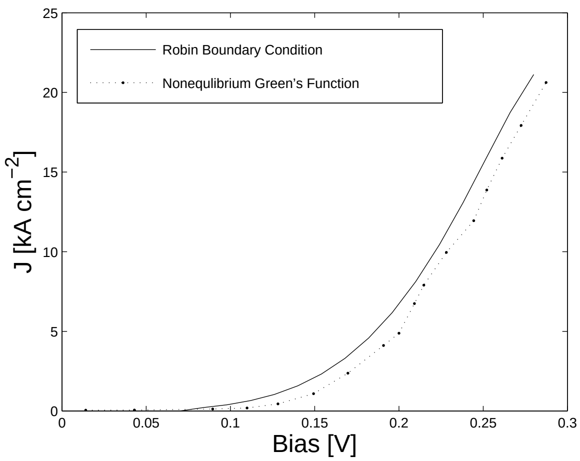

Fig. 2. Comparison of the current-voltage characteristic of a GaAs/ $Al_{0.33}Ga_{0.67}As$ QCL calculated using the Robin boundary condition approach with a nonequlibrium Green's functions simulation.

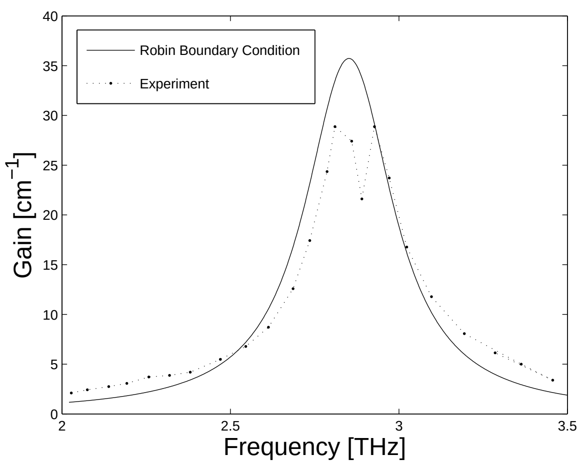

Fig. 3. Optical gain of a THz GaAs/$Al_{0.15}Ga_{0.85}As$ QCL driven at 160 A cm^{-2}. The solid line represents the result calculated by using the Robin boundary condition approach and the dashed line corresponds to measured values.

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