Influence of Eigenstate Basis Sets on Self-Starting Harmonic Comb Simulations in THz QCLs

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***Abstract*—Quantum cascade lasers (QCLs) in self-starting harmonic comb operation are highly attractive for applications in optical and quantum communication. Recently, harmonic mode-locking in QCLs has been reported in several experimental studies, which demands for a robust theoretical description. Here, we provide an extensive numerical study of a terahertz QCL active gain medium capable of self-starting harmonic mode-locking. Our theoretical characterization is divided into stationary carrier transport simulations based on the ensemble Monte Carlo method and dynamical simulations of the light-matter interaction based on multi-level Maxwell-Bloch equations. We investigate the influence of the chosen eigenstates basis on the gain spectrum and present self-consistent simulation results of stable harmonic comb operation with a mode spacing of four times the free spectral range.**

***Index Terms*—quantum cascade laser, terahertz frequency combs, harmonic combs, Monte Carlo, Maxwell-Bloch.**

I. INTRODUCTION

Quantum cascade lasers (QCLs) are a special type of semiconductor laser, where the active gain medium consists of a multiple quantum well heterostructure. Due to the one-dimensional confinement quantized energy states are formed and act as laser levels, where the optical transition frequency is selected by quantum engineering. QCLs serve as a compact and powerful on-chip source for coherent terahertz (THz) and mid-infrared (mid-IR) frequency comb (FC) emission [1], [2]. Efficient phase locking of the cavity modes is obtained by four-wave-mixing processes arising from the huge third order nonlinearity present in QCL gain media. Provided that the group velocity dispersion is sufficiently small, FC emission with a broad bandwidth can be accomplished [3]. Even more intriguing is the effective coherent emission of harmonic combs (HCs) featuring mode spacings of multiples of the free spectral range (FSR). In both the mid-IR and THz spectrum, harmonic comb states with varying orders were obtained for different bias points and waveguide geometries [1], [2].

Towards a full understanding of the physical mechanisms behind the harmonic comb generation and the selection of the harmonic ordering, a detailed theoretical characterization of the QCL gain media is necessary. In this paper, we provide an extensive numerical study of a THz QCL design featuring robust self-starting harmonic mode-locking [1]. For the characterization of the active gain medium we use our in-house *monaco* framework, featuring a versatile wavefunction solver and a stationary carrier transport model, which is based on the ensemble Monte Carlo (EMC) method [4]. Subsequently, we present dynamical simulation results of the unsaturated gain profile and long-term simulations of the four quantum well QCL design in harmonic comb operation. As it was pointed out in a recent theoretical analysis of THz QCL gain media, the chosen wavefunction basis has a significant impact on the gain characteristics [5]. In order to analyze the influence of the eigenstate basis set on the laser output state, we simulate the THz QCL design in two basis state configurations. The eigenstates of the tight-binding (TB) potential are depicted in Fig. 1(a) at a bias of $50\,\mathrm{mV/period}$. In Fig. 1(b), the EZ transformation has additionally been used for calculating the eigenstates. As dynamic model of the THz QCL, we use the open-source solver tool *mbsolve* for the full-wave generalized Maxwell-Bloch equation system [6].

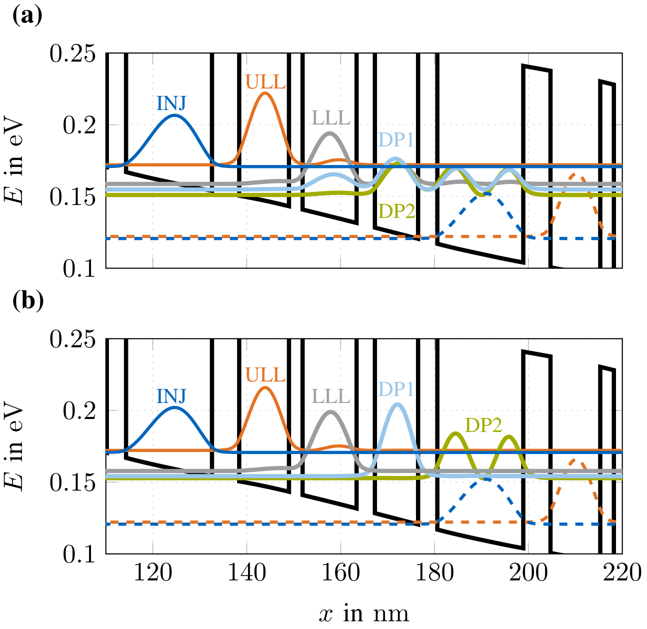

Fig. 1. Calculated conduction band profile and probability densities of the investigated THz QCL structure [1] with an optical transition frequency around $3\,\mathrm{THz}$ and at a bias of $50\,\mathrm{mV/period}$. A comparison of two Schrödinger-Poisson solutions (a) based on a tight-binding potential [4] and (b) additionally using the EZ-transformation [5].

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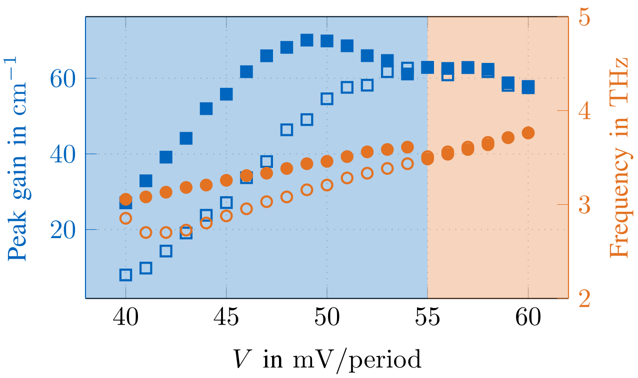

Fig. 2. Monte Carlo simulation results of the THz QCL gain medium using tight-binding (open marks) and EZ-states (filled marks). Simulated unsaturated peak gain values (squares) and frequencies (dots) are shown as a function of the applied bias V.

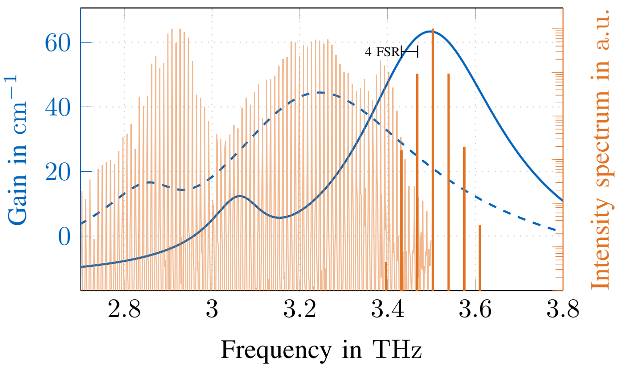

Fig. 3. Maxwell-Bloch simulation results for $V = 50\,\mathrm{mV/period}$. Unsaturated gain curves (blue line) for the TB-configuration (dashed) and the EZ-configuration (solid) are depicted. The intensity spectra of the THz QCL in both configurations are illustrated (orange lines). Here, the intensity spectra for the TB-configuration are drawn slightly shaded.

II. SIMULATION

In order to specify the important coherent regimes of the THz QCL, we simulate the carrier transport in the full lasing regime. In Fig. 2, the peak gain and center frequency for the bias range $40\,\mathrm{mV/period}$ to $60\,\mathrm{mV/period}$ is illustrated. We can identify two regimes: In the lower bias range $< 55\,\mathrm{mV/period}$, a significant difference between EZ-states and TB-states is present. Using the EZ-configuration, eigenstates separated by an energy of less than $5\,\mathrm{meV}$ are summarized within a multiplet. These subsets of eigenstates are diagonalized with respect to the dipole moment operator [5]. Both the peak gain and center frequency tend towards higher values for the EZ-configuration. Above $54\,\mathrm{mV/period}$, the two configurations converge to similar values, as the energy gap between the lower laser level LLL and the depopulation level DP1 exceeds $5\,\mathrm{meV}$.

From the stationary carrier transport simulation results, we extract the quantum mechanical description of the QCL active gain medium used as input for the dynamical Maxwell-Bloch solver. To specify the influence of the tunneling transition INJ → ULL on the spectral gain profile, we have to perform a dynamical gain analysis within the Maxwell-Bloch framework. Therefore, we seed a weak Gaussian pulse on the left facet and record the electric field at the middle of the $4\,\mathrm{mm}$ waveguide. A linear loss term $\alpha = 6.5\,\mathrm{cm}^{-1}$ is additionally considered. The resulting unsaturated gain spectrum is depicted in Fig. 3. The weak side gain lobe slightly above $3\,\mathrm{THz}$ results from the inclusion of the tunneling transition INJ → ULL in the system Hamiltonian. For the TB-states, a smaller peak gain is obtained, while the second lobe arising from the tunneling transition is more pronounced and the gap between the two lobes is narrower.

For the long-term simulations, we obtain harmonic comb emission with 4 FSR mode spacing for the EZ-states. From the dynamical field evolution we observe that the QCL initially operates as a fundamental comb and from there evolves to a harmonic comb state. During this transition, a strong center mode only changes weakly, whereas the energy of the extinguishing modes is transferred to the harmonic sidemodes. For the TB-states we see a broadband unlocked multimode emission. The modes with the highest intensities are located at the second gain lobe, which is related to the tunneling transition. Here, the strong influence of the tunneling transition on the main gain lobe hinders the locking of fundamental cavity modes into a FC and in consequence prevents harmonic comb operation.

III. CONCLUSION

In summary, we provide a substantial theoretical analysis of self-starting THz HC emission in QCLs. The investigation of different basis states reveals its influence on the gain characteristics and the formation of HC states in THz QCLs. By comparing TB-states with EZ-states, we identify an overestimation of the tunneling transition from the injector state to the upper laser level in the TB-configuration, which hinders the formation of a pure FC. In contrast, the more pronounced gain spectrum in the EZ-basis with a dominant optical transition ULL → LLL helps to form a dense FC comb, which subsequently evolves to a harmonic comb with a mode spacing of 4 FSR.

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