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Dynamic modeling of mode-locked pulses and frequency combs in strongly microwave-modulated semiconductor lasers ^F

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ABSTRACT

Strong microwave injection into semiconductor laser waveguides has recently gained enormous attention due to the demonstration of novel frequency comb states. The progress in this field demands new theoretical models that are able to accurately describe microwave-optical co-propagation effects along the waveguide. We address this issue by presenting a self-consistent approach based on the Maxwell-density matrix equations. The injected microwave field is included through analytical solutions of the transmission line equations for the specific laser waveguide geometry, which may either be of Fabry-Pérot-type or a ring-like cavity. Based on our model, we show numerical results of real-world devices, which are in excellent agreement with experimental data. This validates the ability of our model to accurately capture the laser dynamics governed by the injection of a strong microwave field.

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1. INTRODUCTION

Mode-locking refers to the generation of a periodic optical waveform,^{1–3} which in the Fourier domain corresponds to a set of discrete, longitudinal cavity modes with equidistant frequency spacing and fixed phase relation, constituting a frequency comb.^{4,5} Depending on the concrete phase relation of the comb lines, the time domain profile of this waveform can be frequency-modulated (FM) and/or amplitude-modulated (AM). The unabated interest in this operating regime is well deserved because of its intriguing properties and increasingly important use in applications^{6,7} and fundamental scientific interest.^{8,9} Mode-locking of a laser can be achieved in a passive manner using, e.g., saturable absorbers, or actively by inserting a loss modulator into its cavity.^{1,10,11} In addition, self-mode-locking in free-running semiconductor lasers induced by nonlinear four-wave mixing has been observed.^{9,12}

Recently, strong radio frequency (RF) injection, where the microwave frequency is in the order of the cavity repetition rate, has caused a paradigm shift in active mode-locking of semiconductor lasers by facilitating the engineering of short-pulse trains and broadband frequency combs.^{13–18} Here, specially engineered waveguides^{14,19,20} are employed to enable co-propagation between the optical waveform and the externally injected microwave signal (see Fig. 1), greatly increasing the effective modulation depth. This combination of quantum optoelectronics with microwave engineering offers new unique possibilities in the field of microwave photonics.^{21–23} Important advances comprise the generation of a vast selection of optical waveforms, including both AM and FM combs,^{20,24} which are associated with, e.g., quantum walks,^{24,25} Bloch oscillations,²⁶ or active mode-locking with a tunable repetition frequency.²⁷ As expected, these developments lead to new challenges in the numerical modeling of such devices.

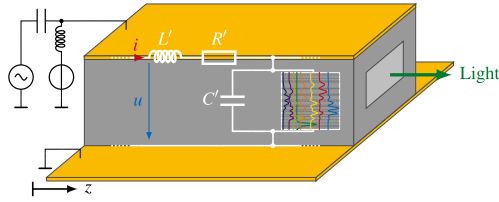


FIG. 1. Schematic illustration of a double-metal laser waveguide under RF modulation. The equivalent circuit of a transmission line segment used to describe the propagation of the bias voltage $u(z, t)$ and the current $i(z, t)$ along the electrical contacts is indicated in white. In our model, the RF behavior of the device is determined by the distributed elements R' , L' , and C' and the current density through the active region, represented by an exemplary QCL bandstructure.

Up to now, co-propagation effects have not been taken into account in theoretical works on actively mode-locked semiconductor lasers,^{28–32} even though they are crucial if the modulation is not restricted to a short waveguide section. The recently published Maxwell–Lindblad transmission line (MLT) model addresses this issue and constitutes a general theory of the co-propagation mechanism, where the microwave field can either be externally injected or self-generated.³³ Here, the Maxwell-density matrix equations in the rotating wave and slowly varying envelope approximations (RWA/SVEAs) describe the underlying laser dynamics, offering a good compromise between accuracy and numerical efficiency. Besides the current focus on microwave-optical co-propagation, their inherent flexibility also enables the treatment of numerous other physical effects, such as spatial hole burning (SHB),^{34,35} distributed saturable absorption for passive mode-locking,^{29,36,37} noise,^{38,39} linewidth enhancement,^{40,41} and Bloch gain for intersubband transitions, which can be treated by suitable electron wave vector averaging^{41,42} or based on quantum thermodynamical principles.⁴³ We note that this model is especially well suited for quantum cascade lasers (QCLs),⁴⁴ but can also be adapted to other semiconductor laser types, such as interband quantum well⁴⁵ and quantum dot⁴⁶ lasers. Furthermore, this approach forms the basis for simplified models, which provide insights into the underlying physical mechanisms.^{24,42,47–50}

In this paper, we adapt the MLT equations for the case of strong injection and present a hybrid approach, combining numerical and configuration-dependent analytical solutions. Here, we treat the two most important cases, namely ring and Fabry–Pérot cavities. This strategy has the following benefits: First, it achieves a substantial reduction of complexity, not requiring a full frequency characterization of the transmission line properties while still capturing the relevant physical effects correctly for strong microwave injection. Second, its implementation is much easier compared to the full MLT equations. Finally, it provides a straightforward viewpoint that is helpful for the understanding of microwave-optical co-propagation effects. Therefore, the resulting model is of great use for the interpretation and explanation of experimental findings and future device optimizations.

This paper is structured as follows: In Sec. II, we introduce an efficient model for the coupled optical, microwave, and carrier dynamics. This enables the practical simulation over thousands of optical round trips, as needed for the study of frequency comb proliferation. Subsequently, we discuss the accuracy and limitations

of the proposed model in Sec. III. Section IV contains the comparison between our simulation results and experimental findings, demonstrating that our model is able to reproduce a wide range of AM and FM frequency comb states. The conclusion and outlook are presented in Sec. V.

II. THEORETICAL MODEL

Our model for the laser dynamics is based on the Maxwell-density matrix formalism, a multilevel generalization of the well-known two-level Maxwell–Bloch equations. Both models are frequently applied for investigating the interaction between a quantum system and a classical electromagnetic wave.^{51,52} It is advantageous to treat the RF wave separately within the transmission line (TL) formalism, rather than describing both fields using one set of Maxwell’s equations, for the following reasons: The propagation parameters in the two distinct regions of the electromagnetic spectrum differ drastically, and the optical field is typically treated in the SVEA, while for the RF field, the full wave dynamics is needed.³³ In addition, it is beneficial for the subsequent interpretation if both fields can be traced individually.

A. Maxwell-density matrix equations

To reduce the numerical load of the simulations, the propagation of the optical field is described by an effective 1D model, which can be derived by separating the longitudinal from the transversal field components in the laser waveguide.⁵¹ Furthermore, the SVEA is invoked by making the ansatz

$$E(z, t) = \Re \left\{ E_+(z, t) e^{i(k_c z - \omega_c t)} + E_-(z, t) e^{i(-k_c z - \omega_c t)} \right\} \quad (1)$$

for the electric field. Here, k_c and ω_c denote the wave number and frequency of the optical carrier, which are linked via the dispersion relation, $k_c = n\omega_c/c_0$, involving the effective waveguide refractive index n and the vacuum speed of light c_0 . Moreover, $E_{\pm}$ are the complex, slowly varying envelopes of the forward and backward traveling waves. In the SVEA, the optical field dynamics is described by the propagation equation,⁵¹

$$v_g^{-1} \partial_t E_{\pm} \pm \partial_z E_{\pm} = i p_{\pm} - \frac{a_w}{2} E_{\pm} - \frac{i}{2} \beta_2 \partial_t^2 E_{\pm}, \quad (2)$$

where v_g denotes the group velocity, a_w is the waveguide power loss coefficient, β_2 is the background group velocity dispersion (GVD), and $p_{\pm}$ is the polarization caused by the quantum system. To guarantee a unique solution, Eq. (2) must be supplemented with initial and boundary conditions, where the latter depend on the cavity geometry. A ring cavity fulfills periodic boundary conditions, i.e., $E_+(0, t) = E_+(L, t)$ and $E_-(0, t) = E_-(L, t)$, while a Fabry–Pérot cavity requires the boundary conditions $E_+(0, t) = r_L E_-(0, t)$ and $E_-(L, t) = r_R E_+(L, t)$, with the field reflection coefficients at the two waveguide facets r_L and r_R , respectively. Here, L denotes the Fabry–Pérot cavity length or ring circumference.

The temporal evolution of the density operator $\hat{\rho}(z, t)$, describing the quantum system, is governed by the Lindblad equation,^{51,53,54}

$$\partial_t \hat{\rho} = (i\hbar)^{-1} [\hat{H}_0 - \hat{\mu} E, \hat{\rho}] + \mathcal{D}(\hat{\rho}), \quad (3)$$

where $\hbar$ is the reduced Planck's constant, $\hat{\mu}$ is the dipole moment operator, and $\hat{H}_0$ is the unperturbed system Hamiltonian. In addition, the superoperator $\mathcal{D}(\hat{\rho})$ accounts for dissipation effects, such as incoherent scattering or dephasing. Within the Lindblad formalism, these effects are modeled by rate-type equations. For the populations, we have $\partial_t \rho_{nn}|_{\mathcal{D}} = \sum_{m \neq n} r_{mn} \rho_{mm} - r_n \rho_{nn}$, where r_{mn} denotes the scattering rate from level $|m\rangle$ to level $|n\rangle$ and $r_n = \sum_{m \neq n} r_{nm}$ is the total outscattering rate from level $|n\rangle$. The coherences obey $\partial_t \rho_{nm}|_{\mathcal{D}} = -\gamma_{nm} \rho_{nm}$, where the dephasing rate $\gamma_{nm} = (r_n + r_m)/2 + \gamma_{p,nm}$ also depends on the pure dephasing $\gamma_{p,nm}$. To reduce the numerical load, an RWA ansatz similar to Eq. (1) is chosen for the matrix elements $\rho_{mn} = \langle m|\hat{\rho}|n\rangle$ associated with the near-resonant optical transitions.^{33,51} A detailed derivation of the resulting time evolution equations for ρ_{mn} , including diffusion and SHB, can be found in the Appendix.

We note that in the dipole approximation, the optical field enters the Lindblad equation directly via the interaction Hamiltonian $-\hat{\mu}E$. On the other hand, the quantum system couples to the optical field via the polarization $p_{\pm}$, which can be directly calculated from the density operator $\hat{\rho}$ [see Eq. (A9)]. Together, the resulting Maxwell-density matrix equations constitute a closed system of equations.

B. Transmission line equations

To adapt the standard TL equations for the case of a laser waveguide, the leakage current through the device is represented by the current density J through the active region. Hence, the TL equations for voltage $u(z, t)$ and current $i(z, t)$ read

$$\begin{aligned}\partial_z u &= -L' \partial_t i - R' i, \\ \partial_z i &= -C' \partial_t u - Jw,\end{aligned}\quad (4)$$

where w denotes the width of the waveguide ridge, and R' , C' , and L' are the distributed resistance, capacitance, and inductance of the transmission line, respectively. Here, it is important to note that $R'(\omega)$ commonly exhibits a strong frequency dependence (see Ref. 14 for the QCL case). Generally, this can be included into the model by a frequency dependent R' , which is represented in the time domain by an operator function $R'(i\partial_t)$.

In Eq. (4), the back-action from the optical field onto the microwave is mediated by the photon-driven current through the active region included in the term Jw . For strong microwave injection, the modulation signal imprints the waveform into the device, and the back-action becomes negligible for the microwave dynamics.³³ This effect becomes even more pronounced if the laser operates close to threshold, resulting in small optical intensities. Consequently, the photon-driven current can be disregarded (for more details see Sec. III), allowing for an analytical solution of the TL equations. To this end, we approximate the transversal current density through the active region via the equation $Jw \approx \Delta Jw + J_0 w$, where $\Delta Jw \propto \Delta u$ is assumed to depend linearly on the RF field and J_0 denotes the current density at a specified voltage u_0 . Furthermore, we split the voltage $u(z, t) = u_0 + \Delta u(z, t)$ and the current $i(z, t) = i_0(z) + \Delta i(z, t)$ into their AC and DC components. Here, u_0 and i_0 represent the DC components at the operating point of the device, while $\Delta u(z, t)$ and $\Delta i(z, t)$ denote the zero time-average modulation signals. In contrast to the voltage operating point u_0 ,

which can be assumed to be spatially constant for a DC bias supply along the waveguide,^{24,27} the DC component of the current $i_0(z)$ must exhibit a z -dependence to satisfy boundary conditions dictated by current conservation in the respective cavity geometry. We assume a sinusoidal modulation signal injected at $z = 0$, giving rise to the boundary condition $\Delta u(0, t) = U_m \cos(\omega_m t)$. Hence, the frequency dependent TL parameters are evaluated at the modulation frequency $\omega_m = 2\pi f_m$, and the voltage, current, and transversal current density through the active region can be described by plane waves,

$$\begin{aligned}\Delta u(z, t) &= \Re \left\{ U_+ e^{i(\beta_m z - \omega_m t)} + U_- e^{i(-\beta_m z - \omega_m t)} \right\}, \\ \Delta i(z, t) &= \Re \left\{ \frac{U_+}{Z_m} e^{i(\beta_m z - \omega_m t)} - \frac{U_-}{Z_m} e^{i(-\beta_m z - \omega_m t)} \right\}, \\ \Delta J(z, t)w &= \Re \left\{ Y'_{AR} U_+ e^{i(\beta_m z - \omega_m t)} + Y'_{AR} U_- e^{i(-\beta_m z - \omega_m t)} \right\},\end{aligned}\quad (5)$$

where $\beta_m = n_m \omega_m / c_0 + ia_m$ denotes the complex microwave propagation constant, with the loss coefficient a_m and the refractive index n_m . Moreover, Z_m represents the characteristic impedance and $U_{\pm}$ represents the complex amplitudes of the forward and backward traveling waves, respectively. In Eq. (5), the RF behavior of the active region is described via a complex admittance Y'_{AR} , whose real part corresponds to a distributed conductance G' while its imaginary part accounts for quantum inductance effects.⁵⁵ By inserting Eq. (5) together with the above expressions for Δu , Δi , and Jw into Eq. (4), we obtain the formulas $\beta_m = i\sqrt{Z'Y'}$ and $Z_m = \sqrt{Z'/Y'}$, with $Z' = R'(\omega_m) - i\omega_m L'$ and $Y' = Y'_{AR} - i\omega_m C'$. In order to determine a closed expression for the RF field $\Delta u(z, t)$, further boundary conditions are needed depending on the geometry of the device in question. In the following, this derivation is carried out for the two

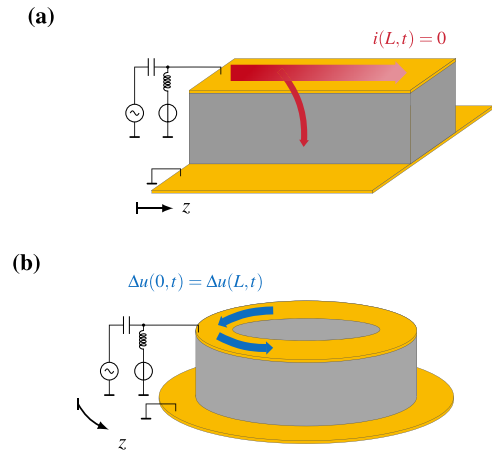


FIG. 2. Schematic visualization of the two cavity geometries under consideration with a bias tee for the injection of an RF wave. (a) Red arrows represent the current density through a Fabry-Pérot cavity that splits into a transversal contribution through the active region and a longitudinal current flowing along the device contacts. Here, the decay of the longitudinal current in propagation direction, needed to fulfill the open circuit boundary condition $i(L) = 0$, is indicated by a fading of the color. (b) Propagation of the RF bias field in a ring cavity is illustrated via blue arrows. The periodicity of the ring imposes periodic boundary conditions onto the RF field, i.e., $\Delta u(0, t) = \Delta u(L, t)$.

most important cases, namely a Fabry–Pérot cavity and a ring cavity (see Fig. 2).

1. Fabry–Pérot cavity

First, a Fabry–Pérot cavity, forming a lossy half-wavelength resonator with a repetition rate $f_{\text{RT}} = c_0/(2nL)$, is considered.³³ Figure 2(a) shows a sketch of such a cavity with length L and an applied modulation signal at $z = 0$. The longitudinal and transversal contributions of the resulting current are marked with red arrows. This current decays to zero at the right facet, i.e., $i(L) = 0$, due to open circuit boundary conditions. By setting the temporal derivatives to zero and using $i_0(L) = 0$, the DC component of the current becomes $i_0(z) = J_0 w(L - z)$. Likewise, the boundary condition $\Delta i(L, t) = 0$ together with $\Delta u(0, t) = U_m \cos(\omega_m t)$ yields the result

$$\Delta u(z, t) = U_m \Re \left\{ \frac{\cos[\beta_m(z - L)]}{\cos(\beta_m L)} \cdot e^{-i\omega_m t} \right\} \quad (6)$$

for the bias field modulation. For the lossless case, i.e., $a_m = 0$, the term $\cos(\beta_m L)$ in the equation above can approach zero, leading to huge values for the modulation $\Delta u(z, t)$ and stability issues in numerical simulations. However, this is not an issue for realistic devices, since the microwave damping is usually significant.⁵⁶ We note that the case where only a subsection of the waveguide $0 \leq z \leq L_m$ (with $L_m < L$) is modulated^{28,57} can also be treated by replacing L with L_m in the formula derived above.

2. Ring cavity

Second, we look at a ring cavity that constitutes a resonator with a repetition rate $f_{\text{RT}} = c_0/(nL)$. This cavity with a bias tee at $z = 0$ is schematically depicted in Fig. 2(b). A ring of circumference L imposes the periodic boundary condition $\Delta u(0, t) = \Delta u(L, t)$ for the bias field, visualized via blue arrows. The current in the device obeys the condition $i_0(L/2) = 0$, resulting in the expression for the DC component of the current, $i_0(z) = J_0 w(L/2 - z)$. In analogy to above, we obtain with the periodic boundary conditions and $\Delta u(0, t) = U_m \cos(\omega_m t)$ the expression,

$$\Delta u(z, t) = U_m \Re \left\{ \frac{\cos[\beta_m(z - L/2)]}{\cos(\beta_m L/2)} \cdot e^{-i\omega_m t} \right\}. \quad (7)$$

Again, if the denominator in Eq. (7) approaches zero, the modulation $\Delta u(z, t)$ assumes huge values, causing numerical instabilities. As mentioned above, this problem does not arise for real lossy transmission lines.

C. Simulation model

Since the back-action from the photon-driven current is omitted in our model, only the coupling from the microwave to the optical field must be considered. We note that some simulation parameters, such as the Hamiltonian and dipole matrix elements, i.e., $H_{0,ij} = \langle i | \hat{H}_0 | j \rangle$ and $\mu_{ij} = \langle i | \hat{\mu} | j \rangle$, generally depend on the bias field applied to the device.^{58,59}

We include this effect by approximating the voltage dependence in terms of a first order Taylor expansion around the operating point u_0 ,³³ i.e.,

$$\begin{aligned} H_{0,ij}(u) &\approx H_{0,ij}(u_0) + H'_{0,ij} \cdot (u - u_0), \\ \mu_{ij}(u) &\approx \mu_{ij}(u_0) + \mu'_{ij} \cdot (u - u_0), \\ r_{ij}(u) &\approx r_{ij}(u_0) + r'_{ij} \cdot (u - u_0), \\ \gamma_{ij}(u) &\approx \gamma_{ij}(u_0) + \gamma'_{ij} \cdot (u - u_0). \end{aligned} \quad (8)$$

Each primed value represents the slope of the corresponding simulation parameter. In Eq. (8), we made the assumption that the scattering and dephasing rates r_{ij} and γ_{ij} follow the bias field modulation instantaneously.

Altogether, we obtain a closed model for the microwave-optical co-propagation in semiconductor laser waveguides. In order to conduct numerical simulations, the optical propagation Eq. (2) is discretized using the Risken–Nummedal finite difference scheme,^{51,60} where the GVD is treated separately using a split-operator approach.⁶¹ For solving the density matrix equation, the explicit third order Adams–Bashforth method is well suited.⁵¹ During a simulation run, the current value of the voltage dependent parameters can be evaluated from Eq. (8), where the bias field modulation is computed from Eq. (6) or Eq. (7).

This results in a simplified model for strong RF injection with a considerably reduced numerical complexity compared to solving the full MLT equations. In particular, the MLT equations require tedious fitting of the (often experimentally not fully characterized) transmission line frequency characteristics to the Debye rational functions,³³ while for strong modulation, only the parameter values at the modulation frequency matter. Moreover, the numerical implementation of the full model is far more complicated. A general restriction is that the MLT equations require an exact quantitative model for the current density. Thus, they cannot be used together with reduced (e.g., two-level) descriptions of quantum-engineered active regions, as widely employed for simulations. Consequently, the simplified treatment presented here also forms the basis for compact, (semi-)analytical laser models, which are widely used since they provide an intuitive understanding of the device dynamics.

III. MODEL VALIDATION

In the following, we investigate the regimes where the central assumption of Sec. II is valid, i.e., the back-action of the optical waveform onto the microwave field can be disregarded. For this purpose, we directly compare our simulation results with those obtained from the full MLT equations.

A. Reference device setup

All simulations presented in this section are based on an actively mode-locked semiconductor laser design, experimentally demonstrated in Ref. 13. The laser constitutes a THz QCL emitting around 2.6 THz, which features a three quantum-well active region, integrated into a metal–metal waveguide of length $L = 3.1$ mm. Dynamical simulations of microwave-optical co-propagation within this device using the full MLT equations, including the optical back-action onto the microwave, have been reported in Ref. 33. For comparison with our simplified model, we replicate these results.

In the published setup, a microwave with modulation frequency $f_m = 12.866$ GHz and a modulation amplitude of $U_m = 0.8$ V is injected at the left end ($z = 0$) of the waveguide. At this modulation frequency, the waveguide can be described as a transmission line with distributed elements $R' = 4.33$ k Ω m $^{-1}$, $L' = 164.93$ nH m $^{-1}$, and $C' = 1.11$ nF m $^{-1}$. In the full model, the microwave dynamics is treated numerically by using a finite-difference time-domain^{62,63} solver, where the frequency dependence of the waveguide parameters R' and L' is approximated using the Debye rational functions⁶⁴ to reflect the behavior $R' \propto \sqrt{f/\text{Hz}} \Omega \text{ m}^{-1}$ caused by the skin effect.

To conduct numerical simulations with the simplified model, we first have to compute the propagation constant β_m for this device (see Sec. II B). For this reason, we need to find the value of the complex admittance Y'_{AR} , which encodes the current response to a voltage applied at frequency f_m across the QCL active region. Hence, this quantity can be determined by seeding a modulation $\Delta u(0, t) = U_m \cos(\omega_m t)$ and tracing the resulting current density J through the active region over time at the position $z = 0$. Here, J is computed with the help of Eq. (A10) in the Appendix, where the rates are extracted from carrier transport simulations of the QCL. To prevent the influence of a photon-driven current on J , the optical intensity I is here set to zero. This method yields the value $Y'_{AR}|_{I=0} = 75.76 \text{ S m}^{-1} + i4.96 \text{ S m}^{-1}$ at f_m , resulting in $\beta_m = 10.96 \text{ cm}^{-1} + i6.29 \text{ cm}^{-1}$ for the simplified model. Since the Y'_{AR} is clearly dominated by the real part, quantum inductance effects play only a subordinate role. In this case, the transversal current density can be written as $\Delta J_w \approx G' \Delta u$.

As a first order correction, we reintroduce the back-action of the photon-driven current in Secs. III B and III C by running a simulation with optical field ($I > 0$) using $Y'_{AR}|_{I=0}$ and extracting a corrected $Y'_{AR}|_{I>0}(z)$. To obtain a position independent $Y'_{AR}|_{I>0}$ as needed for the simplified model, we determine its value at the position of maximum intensity. The simulations in Sec. III B indicate that this correction mainly affects the peak intensity, but has little influence on the temporal waveform.

B. Comparison of outcoupled fields

First, we investigate the accuracy of our approximation with respect to the intracavity intensity, by comparing the simplified model to full MLT simulations. To this end, we sweep the DC pumping strength $p = g_0/g_{th}$, where g_0 and g_{th} denote the unsaturated and threshold gain of the laser, respectively. Here, $g_{th} = (a_w + a_{mr})/\Gamma$ depends on the overlap factor Γ , the waveguide loss a_w , and the mirror loss a_{mr} . We vary p by changing a_w , while keeping g_0 fixed. Figure 3 displays the RF wave at the right facet of the device ($z = L$), where the deviations between both models are strongest, for the case of weak vs strong pumping in steady state. The corresponding intensities outcoupled from the right facet are shown in Fig. 4. While good agreement is obtained close to threshold [Figs. 3(a) and 4(a)], the non-negligible difference in Figs. 3(b) and 4(b) can be attributed to a strong back-action onto the modulation wave, mediated by the photon-driven current.

Next, we assess the performance of our model regarding the modulation strength U_m . Figure 5 shows the optical intensity I outcoupled from the right facet ($z = L$) of the waveguide for U_m between

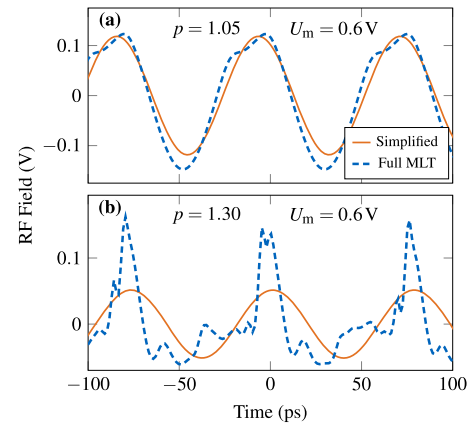


FIG. 3. Time trace of the modulation field at the right facet $\Delta u(L, t)$, obtained from simulations using the full MLT equations (dashed blue lines) and the simplified model (orange lines): (a) results for near-threshold DC pumping of $p = 1.05$, where the low intensity inside the cavity has only little impact on the modulation field. (b) Higher DC pumping of $p = 1.30$, where the increased intracavity intensity induces a stronger photon-driven current, clearly modifying the modulation waveform.

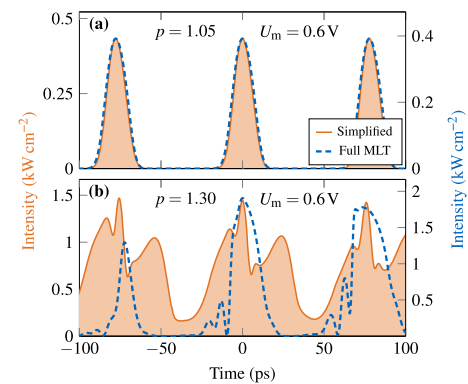


FIG. 4. Optical intensity at the right facet ($z = L$) corresponding to the data shown in Fig. 3. Results for (a) a near-threshold DC pumping of $p = 1.05$ and (b) a higher DC pumping of $p = 1.30$.

0.1 and 1.0 V, at a constant DC pumping $p = 1.10$. Both models predict predominantly FM behavior for the weakest injection case. Upon increasing the modulation depth, we find periodic pulse trains with increasingly shorter pulse durations, as has also been observed in experiment.²⁰ Moreover, for stronger modulation, we obtain improved quantitative agreement between the simplified and the full model. For $U_m = 1.0$ V [see Fig. 5(c)], the comparison yields two almost identical symmetric pulses with a full-width half maximum (FWHM) of ~ 12 ps. The explanation for the good agreement has already been discussed in Sec. II B: The back-action of the light on the bias modulation can be disregarded, as it is relatively weak in comparison to the strong modulation waveform imprinted into the device. Still, it should be noted that the overall peak pulse intensity might vary between both models, as can be seen from the two y-axes in Figs. 4 and 5. The parameters for the device simulations presented

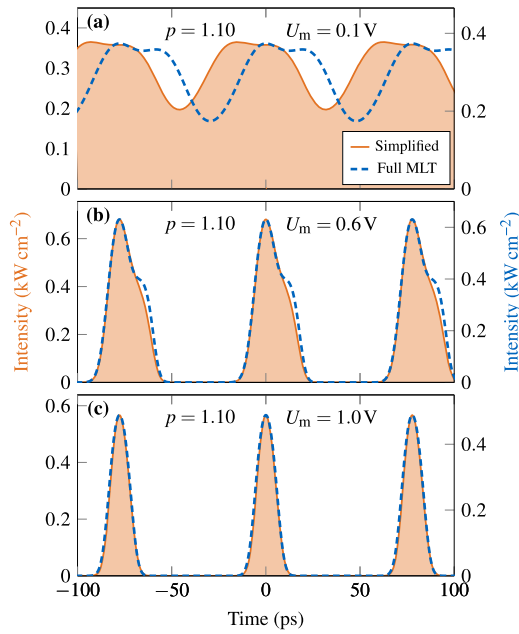


FIG. 5. Time trace of the optical intensity outcoupled from the right facet, obtained from simulations using the full MLT equations (dashed blue lines) and the simplified model (orange lines): (a) results for a weak modulation ($U_m = 0.1$ V), where both models predict predominantly FM behavior. (b) and (c) Stronger modulations ($U_m = 0.6$ V and $U_m = 1.0$ V, respectively), where the laser emits a periodic waveform with shorter pulse duration for increased modulation depth. It becomes apparent that for higher modulation, the injection imprints its waveform into the device, dominating the microwave dynamics in comparison with the relatively weaker back-action. This results in a better fit between both models.

in Sec. IV lie in the regime where our model is valid, as will also be evidenced by the excellent agreement with experimental findings.

C. Comparison of intracavity fields

After discussing the validity of the assumptions made during the development of our model, we now compare the intracavity dynamics resulting from both approaches. For this purpose, we present the intensities of the forward and backward traveling pulses alongside the RF bias field in Fig. 6 for the full MLT equations, and in Fig. 7 for the simplified model. The data shown here correspond to the outcoupled pulses from Fig. 5(b). Overall, both models predict very similar results.

In order to develop an intuitive understanding of the physical behavior within the cavity, we also compute the gain experienced by the optical fields, using the expression³⁷

$$g_{\pm} = \pm \text{Re} \left\{ \frac{2p_{\pm}}{v_g E_{\pm}} \right\}. \quad (9)$$

For ease of interpretation, $g_{\pm}$ is subsequently expressed in terms of a normalized net gain $g_{\pm, \text{net}} = g_{\pm} / g_{\text{th}} - 1$. In both sets of figures, we show three representative time steps: In Figs. 6(a) and 7(a), we depict the optical wave within the cavity after reflection from the left facet. The peak of the forward-traveling pulse is clearly located within a net

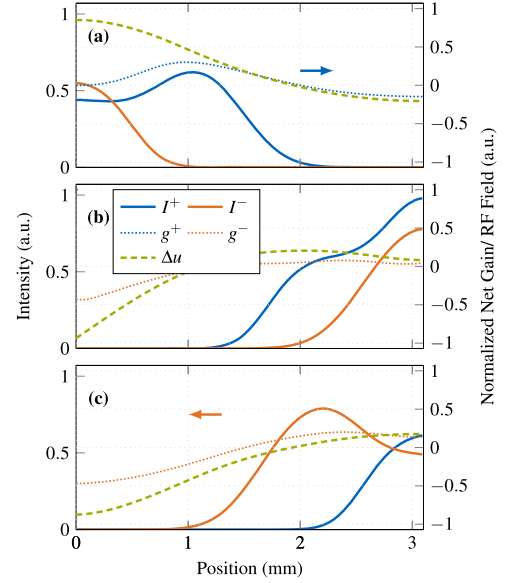


FIG. 6. Intracavity dynamics in a Fabry-Pérot cavity, obtained from simulations using the full MLT equations: The forward and backward traveling waves are shown with solid blue and orange lines, respectively. The corresponding gain is visualized as dotted curves, and the RF bias field is displayed as dashed green lines. Upon reflection from the left facet, the backward field changes direction, as shown in (a). The pulse is partially reflected again at the right facet, illustrated in (b), and travels back in the opposite direction, as can be seen in (c).

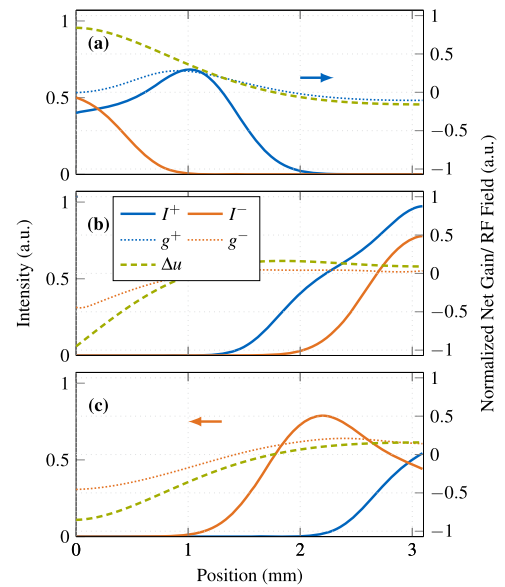


FIG. 7. Intracavity dynamics in a Fabry-Pérot cavity, obtained from simulations using the simplified model: The forward and backward traveling waves are shown with solid blue and orange lines, respectively. The corresponding gain is visualized as dotted curves, and the RF bias field is displayed as dashed green lines. Upon reflection from the left facet, the backward field changes direction, as shown in (a). The pulse is partially reflected again at the right facet, illustrated in (b), and travels back in the opposite direction, as can be seen in (c).

gain window, generated by the RF modulation. In contrast, the negative sign of the RF wave on the opposite end of the cavity introduces a net loss, which suppresses the optical field in that region. In Figs. 6(b) and 7(b), the pulses are shown directly at the right waveguide facet, and Figs. 6(c) and 7(c) illustrate the now backward traveling pulse. Again, the peak intensity resides within a gain window, while the field closer to the left facet is suppressed by a negative net gain. Thus, on average, the pulse experiences a net gain window when traveling through a resonantly modulated cavity, enabling the formation of a periodic pulse train.

IV. SIMULATION RESULTS

In order to demonstrate our model's ability to accurately describe the physical behavior of real-world semiconductor lasers under RF modulation, we dedicate this section to simulation results of two recently published devices. First, we examine an RF-modulated, mid-IR ring QCL, which mimics a quantum walk and Bloch oscillations in the Fourier domain.^{24,26} Second, we investigate a planarized THz Fabry-Pérot QCL that was actively mode-locked to produce picosecond pulses.²⁰ For both structures, the necessary active region characteristics were self-consistently extracted from carrier transport modeling by means of coupled Schrödinger-Poisson (SP) and density matrix ensemble Monte Carlo (EMC) simulations.^{66–68} The slope values of the Hamiltonian, dipole moment operator, and scattering/dephasing rates from Eq. (8) were obtained via an additional SP-EMC run at a different DC bias point.⁶⁹

A. Quantum walk frequency comb

Recently, it was demonstrated that the build-up of a frequency comb can be used to mimic a quantum walk⁷⁰ on a synthetic lattice

provided by the longitudinal laser modes of a ring QCL.²⁴ Here, the coupling between the lattice sites is induced by injecting an RF signal at the cavity round trip rate.²⁴ Moreover, this synthetic lattice has also been proposed as an emulator for a variety of phenomena from solid-state physics, such as Bloch oscillations.²⁶ This emulation is facilitated by detuning the voltage modulation frequency f_m from the cavity round trip rate, which effectively produces an artificial electric field in the picture of the synthetic lattice.²⁶ In the original work,²⁶ two regimes were described: for a detuning below a critical “ionization” value f_{ion} , the spectrum quickly converges to a broad steady state, while for higher detunings, the Bloch oscillations of the spectral intensity appear over time.

In this section, we present simulation results of a mid-IR ring QCL sample of circumference $L = 5.655$ mm, published in Ref. 24. As in the original publication, we assume the ring to be completely defect-free, resulting in a unidirectional, single-mode operation of the free-running device.^{24,71} First, we concentrate on the resonant injection of an RF signal,²⁴ which means that the modulation frequency f_m is close to the repetition rate f_{RT} of the device. Figure 8 visualizes the build-up of the comb, initialized with a single laser mode after the modulation is turned on. Here, the laser undergoes the quantum walk, exhibiting the characteristic ballistic expansion until it stabilizes after ~ 250 ns to a final bandwidth of roughly 2 THz with a Bessel-like spectrum. The corresponding time domain data have an almost constant intensity profile, while its instantaneous frequency is heavily modulated and can thus be considered an example of an FM comb. From the direct comparison of Figs. 8(a) and 8(b), we find excellent agreement between simulation results and experimental data. Next, we focus on the off-resonant case,²⁶ naturally included in our model by choosing a detuning $\Delta f = |f_{RT} - f_m|$ of the modulation frequency from the round trip rate of the ring cavity. In the following, we will show that it is possible to reproduce the two aforementioned detuning regimes with our

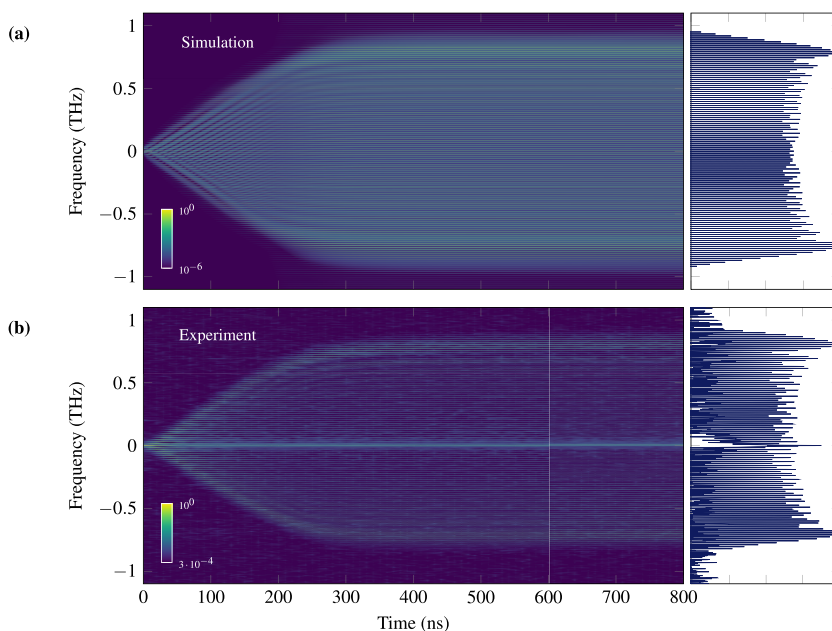


FIG. 8. Temporal build-up of an FM frequency comb in a ring laser, showing a quantum walk behavior: (a) simulation results obtained from our Maxwell-density matrix model and (b) experimental results from Refs. 24 and 65. The plots on the right side show the steady-state intensity spectra on a logarithmic scale.

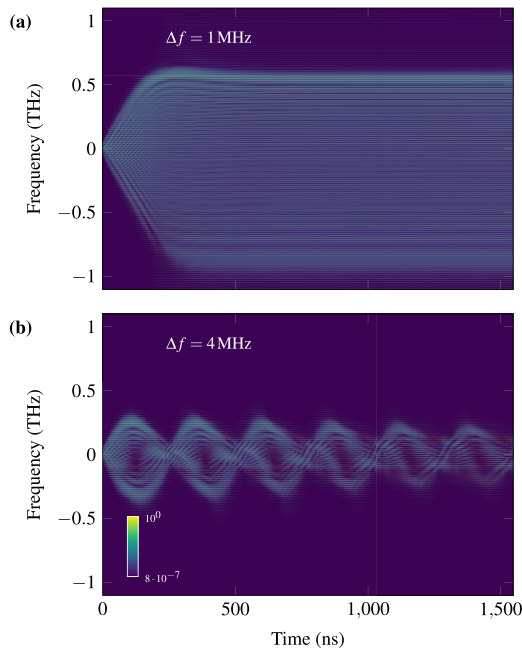


FIG. 9. Simulation results from a ring laser for detuned injection: (a) injection with a detuning of $\Delta f = 1$ MHz, resulting in the formation of a broad steady-state spectrum and (b) injection with a detuning of $\Delta f = 4$ MHz, leading to Bloch oscillations.

model. Simulation results for the two detunings $\Delta f = 1$ MHz and $\Delta f = 4$ MHz are displayed in Figs. 9(a) and 9(b), respectively. For $\Delta f = 1$ MHz, the modulation frequency lies below the critical threshold for “ionization” f_{ion} . Therefore, the spectrum quickly stabilizes to a broad steady state. In contrast, $\Delta f = 4$ MHz $> f_{\text{ion}}$ exceeds this threshold and results in damped Bloch oscillations. Consistent with the experimental and previous theoretical observations,²⁶ we find an oscillation period close to $T_{\text{Bloch}} = 1/\Delta f$ and a reduction in the oscillation amplitude with increased detuning. We note that in contrast to previous theoretical work,²⁴ where only the ideal lossless case with $a_m = 0$ was considered, our simulations above [see Figs. 8(a), 9(a), and 9(b)] include losses which are unavoidable for real-world devices. This is especially relevant for mid-IR QCLs, where RF losses as high as $a_m = 55 \text{ cm}^{-1}$ were reported,⁵⁶ leading to a strongly

damped bias field $\Delta u(z, t)$. Notably, for these high losses, the amplitude of the modulation signal U_m is approximately a factor of eight higher than for lossless simulations yielding intensity spectra with comparable bandwidth.

B. Active mode-locking

In active mode-locking (AML), the frequency of the loss modulation f_m is centered around the repetition rate of the laser cavity or its m th multiple. While the former is called fundamental mode-locking, the latter is known as harmonic mode-locking.¹ The out-coupled field forms a pulse train with a periodicity of $1/(mf_{\text{RT}})$ in time domain, which corresponds to a frequency comb with mode spacing mf_{RT} . In the context of semiconductor lasers, AML can be achieved by injecting the device with an RF signal.^{57,72,73}

In this section, we investigate an AML structure employing a planarized waveguide of length $L = 2.7$ mm, published in Ref. 20. In order to validate our simulations, we performed detailed measurements of the temporal and spectral operation characteristics. For this purpose, shifted wave interference Fourier transform (SWIFT) spectroscopy was employed to reconstruct the temporal pulse shapes and assess the comb coherence.^{74,75} For the SWIFT setup, a hot electron bolometer⁷⁶ was used as fast THz detector. This detector type possesses a high sensitivity at the cost of reduced stability over time, which explains the spurious intensity fluctuations outside the main pulse [see Fig. 10(a)]. Moreover, the intensity spectrum was obtained using a Fourier transform infrared spectrometer. To obtain the shortest possible pulses, the modulation frequency is chosen to be near resonance with the device’s fundamental repetition rate f_{RT} . We note that the experimental repetition rate $f_{\text{RT}} = 14.43$ GHz varies substantially from the calculated cold cavity resonance at approximately $f_{\text{RT}} = c_0/(2nL) \approx 15.42$ GHz, assuming a refractive index $n = 3.6$. The reasons for this are, for example, the cleaving of the experimental laser waveguide, which introduces an uncertainty in its length, hard to control thermal and bias effects, and the influence from the active region’s quantum system. For a close match to the experimental results, we adjust the refractive index n leading to a resonance near 14.43 GHz. With this, we find close agreement between the simulated optical intensities in frequency and time domain and the experimental data, as displayed in Figs. 10(a) and 10(b). In particular, our model is able to reproduce the key properties of mode-locked lasers, i.e., the pulse shape and duration, characterized by a FWHM of 5.4 ps in both simulation and experiment. Furthermore, in Fig. 11, we show the intracavity pulse dynamics of the simulated optical intensity $I^\pm = c_0 \epsilon_0 n |E_\pm|^2/2$, where

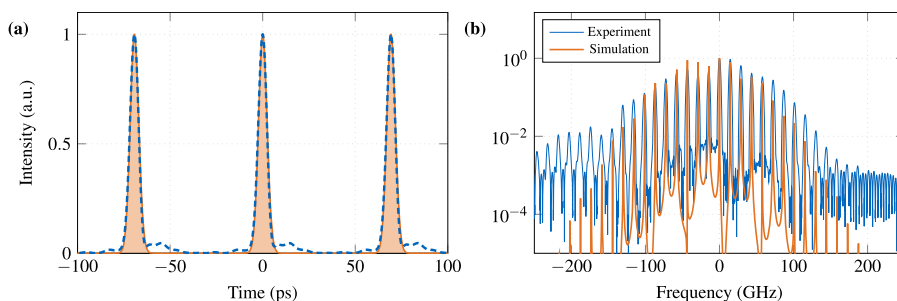


FIG. 10. Results of an actively mode-locked QCL from a Fabry-Pérot cavity: (a) pulse shapes in time domain and (b) corresponding intensity spectra on a logarithmic scale. The experimental data are shown in blue, and the simulation results are plotted in orange.

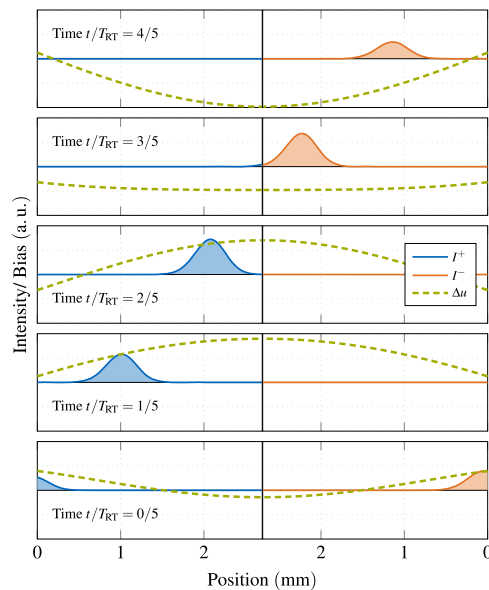


FIG. 11. Intracavity dynamics of the simulated optical field and the RF bias wave in an unfolded cavity view for a single round trip. The left column visualizes the forward, and the right column the backward traveling wave in blue and orange, respectively. The RF wave is shown as a dashed green line.

ϵ_0 is the vacuum permittivity and the RF bias field Δu induced by external microwave modulation at $z = 0$, in an unfolded cavity representation. Similarly, as discussed in Sec. III C, a co-propagation of the optical pulse along with the microwave modulation is visible throughout the whole device.

V. CONCLUSION

In this paper, we have presented a self-consistent model for the description of strongly RF-modulated semiconductor lasers. This model constitutes a generalization of the well-known Maxwell-density matrix equations, which are supplemented by transmission line equations governing the RF bias field. The latter have been analytically solved for the two most important cavity geometries, namely a Fabry-Pérot and a ring configuration, under the assumption of weak back-action from the optical onto the RF field. Conditions for the validity of this approximation have been investigated by comparing our simulation results with those obtained from the full MLT equations. In this way, we efficiently include microwave-optical co-propagation effects and take the voltage dependence of simulation inputs, such as the Hamiltonian or the dipole moment operator, into account. We have applied our model to real-world devices and have found close agreement between simulation results and experimental data. In particular, we have demonstrated that the model is able to reproduce a wide range of amplitude- and frequency-modulated waveforms induced by RF injection, including the Bessel-like spectra, Bloch oscillations, and short-pulse trains. Furthermore, the proposed approach could be beneficial for investigating other microwave photonic devices, such as multiple-quantum-well traveling-wave modulators,⁷⁷ and may serve as a

starting point for compact (semi-)analytical models. In conclusion, our approach will be valuable for the targeted design and optimization of various strongly modulated quantum-engineered structures.

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AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

Author Contributions

Michael A. Schreiber: Conceptualization (equal); Formal analysis (equal); Investigation (equal); Methodology (equal); Project administration (equal); Software (equal); Validation (equal); Visualization (equal); Writing – original draft (equal); Writing – review & editing (equal). **Urban Senica:** Conceptualization (equal); Formal analysis (equal); Investigation (equal); Methodology (supporting); Validation (equal); Visualization (supporting); Writing – original draft (supporting); Writing – review & editing (equal). **Johannes Stowasser:** Conceptualization (supporting); Formal analysis (supporting); Investigation (equal); Methodology (supporting); Validation (equal); Writing – original draft (supporting); Writing – review & editing (lead). **Lukas Seitner:** Conceptualization (supporting); Formal analysis (equal); Investigation (equal); Methodology (supporting); Software (equal); Validation (equal); Visualization (supporting); Writing – original draft (supporting); Writing – review & editing (supporting). **Michael Haider:** Conceptualization (equal); Formal analysis (equal); Funding acquisition (equal); Investigation (equal); Methodology (equal); Project administration (equal); Software (supporting); Supervision (equal); Validation (equal); Visualization (equal); Writing – original draft (supporting); Writing – review & editing (equal). **Giacomo Scalari:** Conceptualization (equal); Formal analysis (equal); Funding acquisition (lead); Investigation (equal); Methodology (supporting); Project administration (lead); Resources (lead); Supervision (lead); Validation (equal); Writing – review & editing (equal). **Christian Jirauschek:** Conceptualization (equal); Formal analysis (equal); Funding acquisition (equal); Investigation (equal); Methodology (equal); Project administration (equal); Resources (equal); Software (equal); Supervision (equal); Validation (equal); Writing – review & editing (equal).

DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

APPENDIX: DENSITY MATRIX EQUATIONS

In this appendix, we provide important details about the time evolution equations for the density matrix elements in our simulation model. As in Sec. II A, the states $|n\rangle$ at the corresponding energies E_n constitute a basis for the Hilbert space of the quantum system. The resulting transition frequencies are given by $\omega_{mn} = (E_m - E_n)/\hbar$. In addition to its diagonal elements $E_n = \langle n|\hat{H}_0|n\rangle$, the unperturbed Hamiltonian may also contain nonzero off-diagonal elements $\hbar\Omega_{mn} = \langle m|\hat{H}_0|n\rangle$, which, e.g., represent tunneling transitions between closely aligned states ($|\omega_{mn}| \ll \omega_c$) in QCL active regions.⁶⁶

Interference effects between two counter-propagating waves can lead to SHB, caused by an inversion grating in the laser cavity. Carrier diffusion, which counteracts the SHB, can be included into the density matrix equations by adding diffusion terms, $\partial_t \rho_{mn} = \dots + D_{mn} \partial_z^2 \rho_{mn}$, where D_{mn} denotes the corresponding diffusion coefficients.⁵¹

Next, we want to transform the Lindblad equation into the SVEA/RWA. To this end, we write

$$\rho_{mn}(z, t) = \rho_{mn}^0(z, t) + \rho_{mn}^+(z, t)e^{2ik_c z} + \rho_{mn}^-(z, t)e^{-2ik_c z} \quad (\text{A1})$$

for the diagonal elements, where ρ_{nn}^0 denotes the average inversion and $\rho_{nn}^\pm = (\rho_{nn}^\mp)^*$ are the respective amplitudes of the forward and backward traveling components of the inversion grating, thereby accounting for the presence of SHB. By inserting this ansatz into Eq. (3) and omitting rapidly oscillating terms, we obtain

$$\begin{aligned} \partial_t \rho_{nn}^0 &= 2 \sum_{i \neq n} \Im \{ \Omega_{ni} \rho_{ni}^0 \} - \sum_{\omega_{ni} > 0} \Im \{ \eta_{in}^- \epsilon_{ni}^+ + \eta_{in}^+ \epsilon_{ni}^- \} \\ &+ \sum_{\omega_{ni} < 0} \Im \{ \eta_{ni}^+ \epsilon_{ni}^- + \eta_{ni}^- \epsilon_{ni}^+ \} + \sum_{i \neq n} r_{in} \rho_{ii}^0 - r_n \rho_{nn}^0 \end{aligned} \quad (\text{A2})$$

and

$$\begin{aligned} \partial_t \rho_{nn}^\pm &= i \sum_{i \neq n} (\Omega_{in} \rho_{ni}^\pm - \Omega_{ni} \rho_{in}^\pm) + \frac{i}{2} \sum_{\omega_{ni} > 0} [\epsilon_{ni}^+ \eta_{in}^\pm - (\epsilon_{ni}^-)^* \eta_{in}^\pm] \\ &+ \frac{i}{2} \sum_{\omega_{ni} < 0} [(\epsilon_{ni}^-)^* \eta_{in}^\pm - \epsilon_{ni}^+ \eta_{in}^\pm] + \sum_{i \neq n} r_{in} \rho_{ii}^\pm - r_n \rho_{nn}^\pm - 4k_c^2 D_{nn} \rho_{nn}^\pm, \end{aligned} \quad (\text{A3})$$

where $\epsilon_{mn}^\pm = \mu_{mn} E_\pm / \hbar$. Regarding the off-diagonal density matrix elements, we must distinguish between states which are associated with near-resonant transitions ($\omega_{mn} \approx \omega_c$) and closely aligned states ($|\omega_{mn}| \ll \omega_c$). In the former case, we make for $\omega_{mn} > 0$ the ansatz

$$\rho_{mn}(z, t) = \eta_{mn}^+(z, t)e^{i(k_c z - \omega_c t)} + \eta_{mn}^-(z, t)e^{i(-k_c z - \omega_c t)}. \quad (\text{A4})$$

We obtain

$$\begin{aligned} \partial_t \eta_{mn}^\pm &= i(\omega_c - \omega_{mn}) \eta_{mn}^\pm + i \sum_{i \neq n, \omega_{mi} > 0} \Omega_{in} \eta_{mi}^\pm - i \sum_{i \neq m, \omega_{mi} > 0} \Omega_{mi} \eta_{in}^\pm \\ &+ \frac{i}{2} \sum_i (\epsilon_{mi}^\pm \rho_{ii}^0 + \epsilon_{mi}^\mp \rho_{ii}^\pm) - \frac{i}{2} \sum_i (\epsilon_{in}^\pm \rho_{mi}^0 + \epsilon_{in}^\mp \rho_{mi}^\pm) \\ &- \gamma_{mn} \eta_{mn}^\pm - k_c^2 D_{mn} \eta_{mn}^\pm \end{aligned} \quad (\text{A5})$$

for $\omega_{mn} > 0$, and use $\eta_{mn}^\pm = (\eta_{nm}^\mp)^*$ for the remaining elements. In the latter case, the ansatz

$$\rho_{mn}(z, t) = \rho_{mn}^0(z, t) + \rho_{mn}^+(z, t)e^{2ik_c z} + \rho_{mn}^-(z, t)e^{-2ik_c z} \quad (\text{A6})$$

yields

$$\begin{aligned} \partial_t \rho_{mn}^0 &= -i\omega_{mn} \rho_{mn}^0 + i \sum_{i \neq n} \Omega_{in} \rho_{mi}^0 - i \sum_{i \neq m} \Omega_{mi} \rho_{in}^0 \\ &+ \frac{i}{2} \sum_{\omega_{in} > 0} [(\epsilon_{mi}^+)^* \eta_{in}^+ + (\epsilon_{mi}^-)^* \eta_{in}^-] + \frac{i}{2} \sum_{\omega_{in} < 0} (\epsilon_{mi}^- \eta_{in}^+ \\ &+ \epsilon_{mi}^+ \eta_{in}^-) - \frac{i}{2} \sum_{\omega_{in} > 0} [(\epsilon_{in}^+)^* \eta_{mi}^+ + (\epsilon_{in}^-)^* \eta_{mi}^-] \\ &- \frac{i}{2} \sum_{\omega_{mi} < 0} (\epsilon_{in}^+ \eta_{mi}^+ + \epsilon_{in}^- \eta_{mi}^-) - \gamma_{mn} \rho_{mn}^0, \end{aligned} \quad (\text{A7})$$

and

$$\begin{aligned} \partial_t \rho_{mn}^\pm &= -i\omega_{mn} \rho_{mn}^\pm + i \sum_{i \neq n} \Omega_{in} \rho_{mi}^\pm - i \sum_{i \neq m} \Omega_{mi} \rho_{in}^\pm \\ &+ \frac{i}{2} \sum_{\omega_{in} > 0} (\epsilon_{mi}^-)^* \eta_{in}^+ + \frac{i}{2} \sum_{\omega_{in} < 0} \epsilon_{mi}^+ \eta_{in}^+ - \frac{i}{2} \sum_{\omega_{mi} > 0} (\epsilon_{in}^-)^* \eta_{mi}^+ \\ &- \frac{i}{2} \sum_{\omega_{mi} < 0} \epsilon_{in}^+ \eta_{mi}^+ - \gamma_{mn} \rho_{mn}^\pm - 4k_c^2 D_{mn} \rho_{mn}^\pm, \end{aligned} \quad (\text{A8})$$

with $\rho_{mn}^\pm = (\rho_{nm}^\mp)^*$. The polarization in the SVEA has the form⁵¹

$$p_\pm = \frac{n_{3D} \omega_c^2}{\epsilon_0 k_c c^2} \Gamma \sum_{\omega_{mn} > 0} \mu_{nm} \eta_{mn}^\pm, \quad (\text{A9})$$

where n_{3D} denotes the 3D electron density and Γ the overlap factor.

Finally, the current density through the active region of a QCL, as needed for the comparison with the full MLT equations in Secs. III B and III C, is given by

$$J = -en_{3D} L_{\text{period}} \sum_{m,n=1}^N \rho_{mm}^0 (r_{m,n+N} - r_{m,n-N}), \quad (\text{A10})$$

where e denotes the elementary charge and L_{period} is the length of one active region period.

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