Coherence of resonant-tunneling transport in terahertz quantum-cascade lasers

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We develop simple density-matrix models to describe the role of coherence in resonant-tunneling (RT) transport of quantum-cascade lasers (QCLs). Specifically, we investigate the effects of coherent coupling between the lasing levels with other levels on the transport properties and gain spectra. In the first part of the paper, we use a three-level density-matrix model to obtain useful analytical expressions for current transport through the injector barrier in a QCL. An expression for the slope discontinuity in the current-voltage characteristics at the lasing threshold is derived. This value is shown to be a direct measure of the population inversion at threshold, and contradicts the previously held belief of it being indicative of ratio of the laser level lifetimes. In the second part of the paper, we use density matrices to compute the gain spectrum for a resonant-phonon terahertz QCL design. The large anticrossing of the doublet of lower radiative levels is reflected in a broad gain linewidth due to a coherent RT assisted depopulation process. At certain bias conditions, the gain spectrum exhibits double peaks which is supported by experimental observations.

I. INTRODUCTION

The role of sequential resonant-tunneling (RT) in semiconductor quantum-wells for charge transport [1] as well as light amplification [2] has been discussed since the early 1970s. Subsequently, multiple proposals were introduced in the 1980s to predict intersubband lasing in semiconductor superlattice structures. With the advent of a unique RT based charge injection scheme, a unipolar mid-infrared (IR) intersubband laser, the so-called quantum-cascade laser (QCL), was first demonstrated in 1994 [3]. Mid-IR QCLs have since undergone rapid progress and room-temperature continuous-wave operation is now obtained over the $\lambda \sim 4 - 10 \, \mu m$ spectrum. Based on similar design principles, the operating frequency range of these devices has also been extended to terahertz frequencies ($\nu \sim 1 - 5 \, THz$, $\lambda \sim 60 - 300 \, \mu m$) [4]. However, due to additional challenges associated with the charge transport in these low-frequency devices, terahertz QCLs are still required to be cryogenically cooled [5, 6, 7]. It then becomes increasingly important to better understand the transport processes in terahertz QCLs to improve the existing designs, with a goal to ultimately achieve room-temperature operation.

The best temperature performance for terahertz QCLs is obtained with the resonant-phonon (RP) designs [5, 9], and operation up to 186 K without magnetic field [10], and 225 K with magnetic field [11] has been demonstrated. For QCLs, almost universally across all different designs and operating frequencies, RT plays an important role in the electrical injection process to populate the upper radiative level [12, 13]. For the resonant-phonon terahertz QCLs (RPTQCLs), RT also plays an important role in the lower level depopulation. Newer designs with RT based extraction have also been demonstrated recently achieving very low threshold current densities [14, 15]. The radiative levels in a terahertz QCL have small energy separation in the range of $\hbar \nu \sim 4 - 20 \, meV$ ($\nu \sim 1 - 5 \, THz$). The potential barriers in the multiple quantum-well (QW) structure are therefore kept thick to obtain tightly-coupled levels in order to maintain selectivity of the injection as well as the depopulation processes. This makes the coupling energies (as characterized by the anticrossing energy $2\hbar \Omega_{ij}$ for the coupled levels $i$ and $j$) similar in value to the low-temperature energy level broadening, which is expected to be of the order of a few meV. Consequently, the loss of coherence (or dephasing) in the RT process has a significant bearing on the electron transport across the barriers [10].

In this paper, simple density-matrix models are used to incorporate the important role of coherence in the RT transport of QCLs. We consider the case of tight binding for intermodule transport, since the intermodule energy anticrossings $2\hbar \Omega_{ij}$ are typically much smaller than the intramodule energy level separations, where each module can consist of one or more QWs and the QCL structure is a periodic repetition of one or more such modules. In the first part of the paper, we use a density-matrix model similar to the 2-level model first proposed by Kazarinov and Suris [17] and then later also discussed in Refs. [12, 18, 19] among others. We modify the model to extend to 3 levels to describe a QCL in a more general sense, and derive analytical expressions for current transport across the injector barrier both below and above the lasing threshold. Despite the simplicity of the model, we can gain useful information about QCL operation from the derived results that includes information about the possible temperature degradation mechanisms in RPTQCLs. The results presented in this section are applicable to mid-IR QCLs as well. In the second part of the paper, we use a similar model to estimate the optical gain spectrum of RPTQCLs. A coherent RT assisted depopulation process is stipulated to be the cause of broad gain bandwidths that are typically observed in these lasers [20].
scattering mechanisms that contribute to quantum transport, the electron wavepackets undergo dephasing, which manifests itself as broadening of the energy levels. The tunnel-coupling between the levels of the same module is strong, therefore, dephasing has a relatively negligible effect on the intramodule intersubband transport \cite{16}. However, the intermodule transport across the injector barrier is critically affected by the dephasing time of the wavepackets since the $1' \rightarrow 3$ tunneling time (half of the inter-well \textit{Rabi} oscillation period $\pi/\Omega_{1'3}$) is now longer and of the same order. To incorporate the role of coherence in the $1' \rightarrow 3$ RT transport, we use density-matrix (DM) rate equations corresponding to the tightbinding basis states of Fig. 1(b) \cite{16}. The time evolution of the $3 \times 3$ DM for this basis set can be written as

\[
\frac{d}{dt} \rho_{(1',3,2)} = -\frac{i}{\hbar} \left[ \bar{H}_{\text{ext}}, \rho_{(1',3,2)} \right] - \frac{i}{\hbar} \left[ \bar{H}', \rho_{(1',3,2)} \right]
\]

where, $\bar{H}'$ includes various radiative and non-radiative perturbation potentials to the conduction-band potential $\bar{H}_{\text{ext}}$. The advantage of writing the DMs with the tightbinding basis of Fig. 1(b) is two-fold. First, it allows inclusion of dephasing phenomenologically by means of decay of the coherences associated with levels $1'$ and $3$ due to non-zero off-diagonal terms in $\bar{H}_{\text{ext}}$ corresponding to those levels. Second, whereas the eigenstates of $\bar{H}_{\text{ext}}$ depend sensitively on the externally applied electric bias because of coupling between spatially separated states, the chosen basis states remain more or less independent of the bias in the range of interest (i.e. close to the “design bias” corresponding to the $1' - 3$ alignment), which keeps the form-factors for various intramodule scattering rate calculations approximately invariant of bias. In a first order approximation, we assume RT to be independent of the electron wavevector in the plane of the QWs. The subband lifetimes are assumed to be averaged over the electron distribution within a subband and are to be calculated within the Fermi’s golden rule approximation.

Expanding equation (1), we then obtain

\[
\frac{d}{dt} \rho_{(1',3,2)} = -\frac{i}{\hbar} \left[ \bar{H}_{\text{ext}}, \rho_{(1',3,2)} \right] - \frac{i}{\hbar} \left[ \bar{H}', \rho_{(1',3,2)} \right] \]

\[
\rho_{ii} + \frac{\rho_{i3}}{\tau_{31}} - \frac{\rho_{i3}}{\tau_{31}} \rho_{33} - \frac{\rho_{33}}{\tau_{31}} \rho_{i3} - \frac{\rho_{i2}}{\tau_{12}} \rho_{12} - \frac{\rho_{12}}{\tau_{12}} \rho_{i2} - \frac{\rho_{i2}}{\tau_{21}} \rho_{21} - \frac{\rho_{21}}{\tau_{21}} \rho_{i2}
\]

In the equation above, $\rho_{(1',3,2)} \equiv \left( \rho_{1'1'}, \rho_{1'3}, \rho_{1'2}, \rho_{31}, \rho_{33}, \rho_{32}, \rho_{12}, \rho_{21}, \rho_{22} \right)$ where $\rho_{ii} (\equiv n_i)$ is taken as the number of electrons per module in level $i$ and $\rho_{ij}$ is the coherence (also known as polarization) term for levels $i, j$. In $\bar{H}_{\text{ext}}$, the diagonal terms are the level energies given by $\bar{H}_{nn} = \langle n | \bar{H}_{\text{ext}} | n \rangle \approx E_n$, and the level anticrossings are represented in the off-diagonal terms as $\bar{H}_{mn} = \langle m | \bar{H}_{\text{ext}} - \bar{H}_{tb} | n \rangle \approx -\hbar \Omega_{mn}$. 

\[\text{FIG. 1: Plot of the magnitude squared envelope wavefunctions for a 3-level QCL design with two different sets of basis functions. Plot (a) is for the "extended" scheme, where energy splitting due to the injector anticrossing $2\Omega_{1'3}$ is visible, and the wavefunctions are calculated for a potential profile $\hat{H}_{\text{ext}}$ as it appears in the figure. Plot (b) is for the "tightbinding" scheme, where the potential $H_{tb}$ is formed by making the barriers at the boundaries of a module sufficiently thick to confine the wavefunctions within the module.}\]
For the lifetimes, \( \tau_{ij} \) is the intersubband scattering time from \( i \to j \), \( \frac{1}{\tau_{ij}} = \frac{1}{\tau_{31}} + \frac{1}{\tau_{21}} + \frac{1}{\tau_{23}} \) is the dephasing rate for the coherence term \( \rho_{ij} \) that consists of lifetime broadening terms as well as a phenomenological broadening term \( T_{\gamma}^{\ast} \) due to interface-roughness and impurity scattering \([10]\), and \( \tau_{st} \) is due to the radiative stimulated emission above the lasing threshold \((\to \infty \text{below threshold})\). The backscattering times \( \tau_{23} \) and \( \tau_{12} \) can also be included in equation (2) if relevant for a particular design. Note that \( \Omega_{32} = 0 \) for the chosen cases since subbands 3 and 2 are the eigenstates of the tightbinding potential \( H_{tb} \) in Fig. (1b). By such a choice, the role of coherence in \( 3 \to 2 \) transport cannot be included. This does not introduce a large error in estimating the current flow since 3 and 2 are strongly coupled. In other words, if tightbinding bases were chosen for the radiative subbands 3 and 2 across the middle “radiative” barrier of the two-well module, \( \Omega_{32} \) would be large and the Rabi oscillation period \( \pi/\Omega_{32} \) would be much smaller than the dephasing time \( \tau_{32} \) for the \( 3 \to 2 \) tunneling, making \( \tau_{32} \) inconsequential for the \( 3 \to 2 \) transport.

As a simpler alternative to more advanced methods, equation (2) can model some aspects of QCL transport fairly accurately. Although it could be solved numerically, we seek analytical expressions that could provide a greater understanding about the effect of various parameters on the transport. Toward that goal, we assume \( \Omega_{1/2} \approx 0 \) akin to a unity \( 1' \to 3 \) injection selectivity. This assumption is in general valid for mid-IR designs due to a large radiative level separation \( E_{32} = (E_3 - E_2) \), and also becomes reasonable for the diagonal terahertz designs \([10]\). Within this approximation, equation (2) can be reduced to that with \( 2 \times 2 \) matrices as follows

\[
\frac{d}{dt} \tilde{\rho}(1',3) = -i \left[ \begin{pmatrix} E_{1'}/\hbar & -\Omega_{1'3} \\ -\Omega_{1'3} & E_3/\hbar \end{pmatrix}, \tilde{\rho}(1',3) \right] \\
+ \begin{pmatrix} \rho_{33} \tau_{31} & \rho_{32} \tau_{31} & -\rho_{1'3} \tau_{32} \\ -\rho_{1'3} \tau_{32} & \rho_{33} - \rho_{22} \tau_{32} \end{pmatrix} \tag{3}
\]

where, \( \tilde{\rho}(1',3) = \begin{pmatrix} \rho_{1'1'} & \rho_{1'3'} \\ \rho_{3'1'} & \rho_{3'3'} \end{pmatrix} \), \( \tau_{ij} \equiv \tau_{ij3} \), \( \tau_{33} \equiv \frac{\rho_{33} \tau_{31}}{\tau_{31} + \rho_{33} \tau_{32}} \), and \( \frac{\rho_{33} \tau_{31}}{\tau_{31} + \rho_{33} \tau_{32}} \) from equation (2) is substituted by \( \frac{\rho_{33} \tau_{31}}{\tau_{31} + \rho_{33} \tau_{32}} \) in equation (3), which holds when \( \Omega_{1/2} = 0 \) as a statement of current continuity. Additionally, we can write the following equation for \( \rho_{22} \) below and above the lasing threshold

\[
\rho_{22} = \begin{cases} \frac{\rho_{33} \tau_{31}}{\tau_{32}} & \text{... (} I < I_{th} \) \\
\rho_{33} - \Delta n_{th} & \text{... (} I \geq I_{th} \) \tag{4}
\end{cases}
\]

where, \( \Delta n_{th} = (\rho_{33} - \rho_{22})I_{th} \) is the population inversion at threshold that is assumed to remain constant beyond threshold. Equations (3) and (4) can be solved analytically for steady-state \((\frac{d}{dt} \to 0)\). With the constraint \( n_{tot} = (\rho_{11} + \rho_{22} + \rho_{33}) \), where \( n_{tot} \) is the total number of electrons per module and is a constant, the following expressions are obtained for the current \( I \) \([22]\)

\[
I \equiv |e| \left( \rho_{33} \frac{\tau_{31}}{\tau_{31} + \rho_{22} \tau_{21}} + \rho_{22} \frac{\tau_{21}}{\tau_{31} + \rho_{22} \tau_{21}} \right) = \begin{cases} \\
|e| n_{tot} \left[ \frac{4\Omega^2_{1'3'} \tau_{31} + 2 \Omega^2_{1'3'} \tau_{32}}{4\Omega^2_{1'3'} \tau_{31} + 2 \Omega^2_{1'3'} \tau_{32}} \left( 1 + \frac{\tau_{31}}{\tau_{32}} \right) + \Delta^2_{1'3'} \tau_{32}^2 \right] + 1 & \text{... (} I < I_{th} \) \\
|e| n_{tot} \left[ \frac{2 \Delta n_{th}}{6 \Omega^2_{1'3'} \tau_{31} + 2 \Omega^2_{1'3'} \tau_{32}} \left( 1 + \frac{\tau_{31}}{\tau_{32}} \right) + \Delta^2_{1'3'} \tau_{32}^2 \right] + 1 & \text{... (} I \geq I_{th} \) \tag{5}
\end{cases}
\]

where, \( e \) is the unit charge and \( \hbar \Delta_{1'3} = E_{1'} - E_3 \) is the energy detuning between levels \( 1' \) and \( 3 \) that is a function of the externally applied electrical bias. For the case of ultra-short lifetime of the lower radiative state \((\tau_{21} \ll 2\tau_{32})\), the below-threshold term in equation (5) becomes

\[
I = \frac{|e| n_{tot}}{2\tau_{31}} \left( \frac{4\Omega^2_{1'3'} \tau_{31} + 2 \Omega^2_{1'3'} \tau_{32}}{4\Omega^2_{1'3'} \tau_{31} + 2 \Omega^2_{1'3'} \tau_{32}} \left( 1 + \frac{\tau_{31}}{\tau_{32}} \right) + \Delta^2_{1'3'} \tau_{32}^2 \right) + 1 \text{... (} \tau_{21} < 2\tau_{32} \text{... (} I < I_{th} \) \tag{6}
\]

which reproduces the commonly used expression in literature \([2, 12]\).

Since \( \tau_{21} \ll 2\tau_{32} \) typically holds for a QCL design, the below-threshold term for the 3-level model in equation (6) does not provide any new insight from equation (5). However, the advantage of the model lies in describing transport above threshold. It is instructive to write expressions for maximum current \( I_{max} \), which flows at the \( 1' \to 3 \) resonance \((\Delta_{1'3} = 0)\) for the case of a coherent RT process, i.e. a large injector coupling \( \Omega_{1'3} \) \([12, 24]\). The following expressions are obtained for \( I_{max} \) and the level populations when threshold could not
be attained

\[ I_{\text{max}} = \frac{|e| n_{\text{tot}}}{2\tau_3 (1 + \frac{\tau_{21}}{2\tau_{32}})} \]

\[ n_3 = n_1 = n_{\text{tot}} \left( 1 - \frac{1}{2 + \frac{\tau_{21}}{\tau_{32}}} \right) \]

\[ \Delta n = n_3 - n_2 = n_{\text{tot}} \left( 1 - \frac{\tau_{21}}{2 + \frac{\tau_{21}}{\tau_{32}}} \right) \]

\[ \ldots (4\Omega_1^2 \tau_{13} \tau_3 > 1, \quad I_{\text{max}} > I_{\text{th}}) \] (7)

The results in equation (7) are slightly different than that obtained using a two-level model in Ref. 12 as a consequence of adding an additional level (i.e. the lower laser subband 2) in these calculations. However, the commonly used two-level model result \( I_{\text{max}} = |e| n_{\text{tot}}/(2\tau_3) \) is recovered in the limit \( \tau_{21} \ll \tau_{32} \) as it is to be expected. Equation (7) suggests that \( I_{\text{max}} \) for coherent injection is independent of \( \Omega_1^3 \), and therefore the thickness of the injector barrier, and is limited by the upper state lifetime \( \tau_3 \). Typical values of \( \Omega_1^3 \) that bring a QCL within this limit could be determined from Fig. 2(a). The value of \( I_{\text{max}} \), however, is different if enough population inversion could be attained prior to the \( 1^s \rightarrow 3 \) resonance and the device starts lasing, in which case stimulated emission lowers the upper state lifetime. In such a scenario, the maximum current is limited by the lower state lifetime \( \tau_{21} \) instead, and is given by

\[ I_{\text{max}} = \frac{|e| n_{\text{tot}}}{3\tau_{21}} \left[ 1 - \frac{2\Delta n_{\text{th}}}{n_{\text{tot}}} \right] \left( 1 + \frac{\Delta n_{\text{th}}}{n_{\text{tot}}} \right) \]

\[ n_3 = n_1 = \frac{n_{\text{tot}} + \Delta n_{\text{th}}}{3} \]

\[ \ldots (6\Omega_1^2 \tau_{13} \tau_{21} > 1, \quad I_{\text{max}} > I_{\text{th}}) \] (8)

Equation (8) implies that a QCL with a large injector coupling \( \Omega_1^3 \) and a short lower state lifetime \( \tau_{21} \) can possibly obtain a large dynamic range in current due to a large \( I_{\text{max}} \) (see Figs. 3 and 31). However, it may be noted that for coherent injection, the gain linewidth of the QCL becomes additionally broadened as the injector coupling \( \Omega_1^3 \) is increased. Consequently, a larger \( \Delta n_{\text{th}} \) is required to attain a certain value of peak gain, which mitigates the increase in the value of \( I_{\text{max}} \). This will become more clear in section III from the gain spectrum calculations for some specific cases.

Approaching threshold, the value of current that must flow through the QCL structure to establish a population inversion of \( \Delta n_{\text{th}} \) is calculated to be

\[ I_{\text{th}} = \frac{|e| \Delta n_{\text{th}}}{\tau_3 (1 - \frac{\tau_{21}}{\tau_{32}})} \] (9)

While the above expression for \( I_{\text{th}} \) can also be derived from a simple rate equation analysis, the minimum value of \( \Omega_1^3 \) needed for a current \( I_{\text{th}} \) to flow through the structure is derived from the present 3-level DM model as

\[ 4\Omega_1^2 \tau_{13} \tau_3 > \frac{2\Delta n_{\text{th}}}{n_{\text{tot}} - 2\Delta n_{\text{th}} - (n_{\text{tot}} + \Delta n_{\text{th}}) \frac{\tau_{21}}{\tau_{32}}} \] (10)

This result is obtained from equation (9) as a necessary condition for the two expressions to have the same value for some particular bias \( \Delta_1^3 \). An estimate of the minimum value of \( \Omega_1^3 \) required to meet this condition can be obtained from the plots in Fig. 3(b). Figure 3(b) can also be interpreted in a different way, since it determines the maximum value of population inversion that can be attained for a given \( \Omega_1^3 \). For example, in the limit \( \tau_{21} \rightarrow 0 \), a maximum of \( \Delta n = n_{\text{tot}}/2 \) can be obtained if \( 4\Omega_1^2 \tau_{13} \tau_3 \gg 1 \).

A. Current-voltage characteristics for typical parameters

To gauge the effect of various parameters on QCL’s performance, Fig. 3 shows calculation of the current-voltage (I-V) and differential-resistance-voltage (R-V, \( R = \frac{dV}{dI} \)) characteristics for a range of parameters using the analytical expressions in equation (5). The I-Vs show a discontinuity in slope at the occurrence of the lasing threshold, as was first discussed in detail in Ref. 12. However, any discussion about the differential resistance in the present context is left until later. For the I-Vs the main features to be noted are the values of the threshold current density \( J_{\text{th}} \) and the maximum current density \( J_{\text{max}} \). In general for any design, the goal is to obtain a larger dynamic range for lasing \( J_{\text{max}}/J_{\text{th}} \) while also keeping the value of \( J_{\text{th}} \) low. A larger dynamic range leads to greater amount of the optical power output, and also a higher operating temperature \( T_{\text{max}} \). As it is to be expected, the plots show that the laser performance improves by making \( \tau_{21} \) and \( \tau_{32} \) larger, and \( \tau_{21} \) smaller.

We now compare the 3-level model I-Vs in Fig. 3 to those experimentally measured for two different RTPQCL designs. Fig. 4 shows typical results from a 4-level design \( 14, 26, 27 \) and a 5-level \( 18, 19, 8 \) RTPQCL respectively. The structures in Fig. 4(a) and 4(b) can be qualitatively analyzed with the 3-level model of this section by using the following expression for the effective lifetime of the lower laser level 2, which is depopulated through RT into 2a, and subsequently through electron-longitudinal-optical (e-LO) phonon scattering into the injector level(s) (i.e. the resonant-phonon scheme). The following expression can be derived using a 2-level density-matrix for levels 2 and 2a exclusively and assuming \( 2 \rightarrow 2a \) tunneling to be the only mechanism for carrier injection into level 2a. 22

\[ \tau_{2,\text{eff}} = \tau_{2a} \left( \frac{2\Omega_2^2 \tau_{2a} \tau_2 + \Delta_2^2 \tau_{2a} \tau_2 + 1}{2\Omega_2^2 \tau_{2a} \tau_2} \right) \] (11)
FIG. 2: (a) A plot of the factor $4\Omega_{r,3}^2 \tau_1 \tau_3$ to determine the regime of RT transport through the injector barrier ($\gg 1$ coherent, $\ll 1$ incoherent). A phenomenological value of $T_2 = 0.75$ ps is assumed. (b) A related plot to determine the maximum value of population inversion ($n_3 - n_2$) that can be attained for a given $\Omega_{r,3}$, calculated using equation (13). The top axis converts $\Delta n$ on the bottom axis to corresponding values of peak gain for the following typical parameters: $n_{tot}/\text{Volume} = 5 \times 10^{15}$ cm$^{-3}$, $f_{32} = 0.5$, $\Delta \nu = 1.0$ THz, and using the expression $g \approx 7 \times \left(\frac{[\Delta n/(10^{15}$ cm$^{-3})] f_{32}}{(\Delta \nu/1$ THz$)} [\text{cm}^{-1}]\right)$ for GaAs material [6] that assumes a Lorentzian gain linewidth of $\Delta \nu$ (note that $f_{32}$ is the oscillator strength of the radiative transition).

FIG. 3: Calculations of the current density ($I/\text{Area}$) as a function of the energy detuning $\hbar \Delta_{1/3}$ (which is proportional to the external bias voltage $V$, as in equation (12), and its inverse slope $\frac{\Delta I}{\Delta \hbar \Delta_{1/3}}$ (which is proportional to the differential resistance $R$, as in equation (13). The calculations are done for a range of parameters using equation (13) for the 3-level model. Following default values are chosen corresponding to the typical values for RPTQCL designs: $2\hbar \Omega_{r,3} = 1.5$ meV, $T_2 = 0.75$ ps, $g_{th} = 40$/cm [22], $\tau_{21} = 0.5$ ps, $\tau_{32} = 3.0$ ps, $\tau_{31} = 5.0$ ps. A doping density $n_{tot}/\text{Volume} = 5 \times 10^{15}$ cm$^{-3}$ is used. The radiative transition is assumed to have a Lorentzian linewidth of $\Delta \nu = 1.5$ THz (the broad linewidth is based on the findings of section III) and an oscillator strength of $f_{32} = 0.6$ to determine the population inversion $\Delta n_{th}$ required to attain a particular value of threshold gain $g_{th}$. The thin (red) portion of the curves corresponds to $I < I_{th}$, while the thick (blue) region is for $I > I_{th}$ where the occurrence of threshold is marked by a discontinuity in $R$. Each of the subplots show the variation of the $I$-$V$s and the $R$-$V$s when only a single parameter is changed, the others being kept at the values mentioned above. Note that additional linewidth broadening due to coherent effects (discussed in section III) is not considered for calculations of the curves above threshold.
The effective lower-level lifetime $\tau_{2,\text{eff}}$, which is also equivalent to the tunneling time through the collector barrier, is plotted for three different values of the collector anticoercin: $2h\Omega_{2,2a}$ in Fig. 5. The best performing RPTQCLs have large collector anticoercis in the range of $2h\Omega_{2,2a} \sim 4 - 5$ meV, in which case $\tau_{2,\text{eff}}$ varies little in the operating bias range close to the $2 - 2a$ resonance ($h\Delta_{2,2a} = 0$). For example, $2h\Omega_{2,2a} \sim 4.7$ meV for the 4-level QCL in Ref. 10 and the energy detuning $h\Delta_{2,2a}$ approximately varies from $-2$ meV to $2.5$ meV in operating bias range of the design. As seen from Fig. 5(a), $\tau_{2,\text{eff}}$ changes little within such a range of detuning.

We can similarly take the combined population $n_{\text{tot}} = n_{1'} + n_2 + n_3$ to be approximately bias independent. The population of level $2a$ is likely to be negligible due to its very short lifetime $\tau_{2a} \sim 0.2$ ps, and that of level $1a$ in Fig. 3(b) is likely to vary negligibly with bias in the operating bias range of interest due to the typically large values of the intra-injector anticoercing $2h\Omega_{1a,1} \sim 4 - 5$ meV in the 5-level design Fig. 4(b). Given the bias independence of $n_{\text{tot}} = n_{1'} + n_2 + n_3$ and the lower-level lifetime $\tau_{2,\text{eff}}$ for the resonant-phonon designs in Fig. 4 we can now qualitatively compare the 3-level model I-Vs in Fig. 3 to the experimental continuous-wave (cw) I-Vs in Fig. 4. For the latter, it can be noticed that $J_{\text{max}}$, which is characterized by the occurrence of a negative differential resistance (NDR) region in the I-V, changes little up until the maximum operating temperature of the laser $T_{\text{max,cw}}$. However, beyond $T_{\text{max,cw}}$, the value of $J_{\text{max}}$ increases with temperature. This characteristic is best described by the calculated I-Vs in Fig. 3(a) since the above-threshold current expression in equation 5 is independent of the upper state to lower state lifetime $\tau_{32}$ to a first order. Hence, it is likely that one of the dominant temperature degradation mechanism for RPTQCLs is a reduction in the upper state ($u$) to lower state ($l$) lifetime, which is mostly attributed to the ther-
mally activated LO phonon scattering from the upper state \(5, 6\). The recently developed terahertz QCL design with a very diagonal radiative transition is based on this observation to effectively increase the \(u \to l\) lifetime at high temperatures \(10\). Additionally, it seems less likely that an increase in the effective lifetime of the lower state (potentially due to \(1 \to 2\) thermal backfilling or increased dephasing for the \(2 \to 2n\) RT that affects \(\tau_{2,\text{eff}}\) as in Fig. \(5\)), or a broadening of the gain linewidth \(28\) are more dominant temperature degradation mechanisms than that mentioned above; otherwise, the observed experimental behavior would have corresponded more closely with Figs. \(3\text{e}\) or \(3\text{c}\), respectively. That is, the peak current density \(J_{\text{max}}\) would decrease at elevated temperatures.

The two-well design of Fig. \(1\) which features an intrawell-phonon (IP) depopulation scheme as opposed to the RP depopulation scheme of Fig. \(4\) has also been experimentally realized recently \(23\). The design-bias band diagram of the realized structure is shown in Fig. \(6\text{a}\) including higher energy parasitic levels that are believed to contribute to electron transport at elevated temperatures. The experimental \(I\text{-}V\)s and \(R\text{-}V\)s from a representative ridge laser in cw operation are shown in Fig. \(6\text{b}\). The temperature variation of the \(I\text{-}V\)s shows that \(J_{\text{max}}\) for this IP QCL decreases slightly with temperature up to \(T \sim 45\) K and subsequently increases steeply with temperature until and beyond the \(T_{\text{max,cw}} \sim 63\) K. This unique dependence of \(J_{\text{max}}\) with \(T\), also shown explicitly in the inset of Fig. \(6\text{b}\), is different from that of the RP QCLs in Fig. \(4\) and is attributed to the onset of a temperature degradation mechanism that is in addition to the reduction in \(\tau_{3,2}\) due to thermally activated e-LO phonon scattering from \(3 \to 2\). It is postulated that the lifetime of the upper state 3 decreases additionally due to absorption of non-equilibrium (hot) LO phonons via \(3' \to (4',5)\) scattering \(28\). Any such scattered electrons quickly relax back eventually into the injector level of a neighboring module due to the short lifetime of the parasitic levels 4 and 5 (\(\tau_{4'} \sim \tau_3 \sim 0.3\) ps). Such a leakage mechanism can be considered approximately as an effective reduction in \(\tau_{31}\) in order to apply the results of the 3-level model to explain the behavior in Fig. \(6\text{b}\), which then becomes consistent with calculated \(I\text{-}V\) behavior in Figs. \(3\text{b}\). Note that the upper laser state in the RP designs is spatially isolated from the wide injector well(s) and hence from the higher energy parasitic levels \(6\). Hence, the aforementioned hot-phonon mediated leakage mechanism is weaker for the RPTQCLs as compared to the IP QCL structure of Fig. \(6\text{a}\).

### B. Discontinuity in differential resistance at threshold

The onset of lasing in a QCL is characterized by a slope-discontinuity in its \(I\text{-}V\) characteristics \(12\). This is a manifestation of the increased rate of carrier flow due to the stimulated emission process from the upper to the lower state, such that the population inversion is kept constant beyond threshold. The relative change in the differential resistance \(R = dV/dI\) of the device at threshold is a useful parameter since it is easily and accurately measurable, and is shown below to be directly proportional to the value of \(\Delta V_{\text{th}}\). We can relate the externally applied bias voltage across all the periods of the QCL to the energy detuning \(\hbar \Delta V_{1-3}\) as

\[
V = \frac{\hbar \Delta V_{1-3} N_p}{f_V |e|} \tag{12}
\]

where, \(N_p\) is the number of repeated periods in the QCL structure, and \(f_V\) is the fraction of per module voltage bias \(V/N_p\) that appears as the energy difference between levels 1' and 3. \(f_V\) is typically a slowly varying non-linear function of the applied voltage \(V\) and is a characteristic of a particular design as shown in Fig. \(7\). For the main

![FIG. 6: (a) Conduction band diagram of a recently demonstrated two-well terahertz QCL design, labeled TW246 \(22\). Only three levels (1, 2 and 3) participate in transport at low temperatures; however, at higher temperatures additional parasitic levels (4 and 5) are also likely to contribute to the current flow. (b) Experimental cw \(I\text{-}V\)s and \(R\text{-}V\)s at different heat-sink temperatures from a 20 \(\mu\)m x 1.56 mm metal-metal ridge laser with a \(T_{\text{max,cw}} \sim 63\) K. The lasing threshold is marked by a discontinuity in the \(R\) curves that is shown more clearly in an expanded view in the lower inset. The upper inset shows the variation of fractional discontinuity in \(R\) at threshold \(\delta_{\text{frac}}\) and of \(J_{\text{max}}\) with temperature.](image-url)
result presented in this section, the particular form of \( f_V \) is inconsequential and it is assumed to be a constant in the bias range right below and above the threshold. Using equation (12) the differential resistance \( R \) becomes

\[
R = \frac{dV}{dI} \approx \frac{\hbar N_p}{f_V |e|} \frac{dE_{1/3}}{dI}
\]

(13)

FIG. 7: Detuning energy \( \hbar \Delta_{1/3} \) as a function of the voltage per QCL module \( (V/N_p) \) in equation (12) for the tightbinding wavefunctions of the 4-level resonant-phonon design of Fig. 4(a) and the 3-level intrawell-phonon design of Fig. 5(a) respectively. Small circles represent calculated values, which are overlaid with straight line fits to the data points close to the \( 1^\prime \)–\( 3 \) resonance. The fits indicate that \( \hbar \Delta_{1/3} \) is linearly related to \( V/N_p \) close to the \( 1^\prime \)–\( 3 \) resonance (i.e. \( f_V \) in equation (12) is a constant). Typically, lasing threshold occurs after the \( 1^\prime \)–\( 2 \) resonance \( (\sim 30 \text{mV/module}) \) beyond which the current continues to increase up to the \( 1^\prime \)–\( 3 \) resonance when \( J_{\text{max}} \) occurs.

In equation (13), we have dropped the term corresponding to \( df_V/dI \) since \( f_V \) is approximately a constant as can be seen from Fig. 7. The calculations in Fig. 7 are done without accounting for band-bending due to dopant-carrier segregation, which is typically insignificant due to the low-doping in such QCL structures. The value of \( df_V/dI \) is likely to be negligible in comparison to the leading term of equation (13) even if band-bending were found to be significant for a particular design. We can now derive analytical expressions for the ratio as well as the fractional change in differential resistance just below \( (R_{th}^-) \) and above \( (R_{th}^+ \) threshold using equation (5) to calculate \( dR/df_V \). The individual expressions for \( R_{th}^+ \) and \( R_{th}^- \) are complicated; however, the ratio \( R_{th}^- / R_{th}^+ \) and hence the fractional change in \( R \) at threshold \( \Delta R_{th} / R_{th} \) is expressed in a surprisingly concise form as (22)

\[
\frac{R_{th}^+}{R_{th}^-} = \left[ 1 - \frac{2\Delta n_{th}}{n_{tot}} \left( \frac{1 - \frac{\tau_{21}}{\tau_{31}}}{1 + \frac{\tau_{21}}{\tau_{31}}} \right) \right]
\]

(14)

\[
\frac{\Delta R_{th}}{R_{th}} = \frac{R_{th}^- - R_{th}^+}{R_{th}^-} = \frac{2\Delta n_{th}}{n_{tot}} \left( 1 - \frac{\tau_{21}}{\tau_{31}} \right)
\]

(15)

Note that equation (15) is derived for the case of unity injection efficiency, i.e. \( \Omega_{1/2} \approx 0 \) in the 3 x 3 DM equation (2). Hence, within the approximation that the current flow due to the \( 1^\prime \)–\( 2 \) channel is negligible in comparison to the \( 1^\prime \)–\( 3 \) channel at threshold, the expression derived for \( \Delta R_{th} / R_{th} \) holds true irrespective of the nature of the RT transport (coherent or incoherent) across the injector barrier. At low temperatures, \( \tau_{31} \ll \tau_{21} \), and hence \( \Delta R_{th} / R_{th} \approx 2\Delta n_{th} / n_{tot} \) gives an absolute measurement of the population inversion in the laser as a fraction of the combined populations of the injector level \( 1^\prime \) and the laser levels 3 and 2 \( (n_{tot} \equiv n_{1^\prime} + n_2 + n_3) \).

The slope efficiency of a QCL’s optical power output is written as

\[
\frac{dP_{\text{out}}}{dI} = \frac{N_p \hbar \omega_0}{|e|} \frac{\alpha_m}{(\alpha_w + \alpha_m)} \eta
\]

(16)

where \( \omega_0 \) is the lasing frequency, \( \alpha_m \) is the radiative (mirror) loss in the cavity, \( \alpha_w \) is the material (waveguide) loss, and \( \eta \) is the internal quantum efficiency of the QCL structure. \( \eta < 1 \) due to the fact that \( n_3 \), and hence the non-radiative component of the current \( I \) \( (\approx |e| n_3/\tau_3) \), continues to increase with \( I \) above threshold (even as \( \Delta n = n_3 - n_2 \) remains fixed at \( \Delta n_{th} \), which causes the current above threshold \( (I = I_{th}) \) to be not entirely due to radiative transitions. An expression for \( \eta \) is derived as

\[
\eta = \frac{1 - \frac{\tau_{21}}{\tau_{31}}}{1 + \frac{\tau_{21}}{\tau_{31}} + \frac{d\Delta n_{th}}{dI} |l = l_{th}^+|} = \frac{1}{|e| \left( \frac{\tau_{21}}{\tau_{31}} + \frac{\tau_{31}}{\tau_{31}} \right)}
\]

(17)

where,

\[
\frac{d\Delta n_{th}}{dI} |l = l_{th}^+| = \frac{1}{|e|} \frac{\tau_{21}}{\tau_{31}}
\]

(18)

Equation (17) for \( \eta \) can also be derived from a rate equations model since \( n_3 \) can be expressed in terms of \( I \) regardless of the nature of \( 1^\prime \)–\( 3 \) RT transport. In literature [12, 20], \( \Delta R_{th} / R_{th} \) has similarly been derived from a rate equations approach, arguing that \( n_3 \propto \Delta_{1/3} \), and hence the applied voltage \( V \), in which case \( \Delta R_{th} / R_{th} \) becomes same as \( \eta \) (for unity injection efficiency), and hence an indicator of the ratio of laser level lifetimes \( \tau_{21}/\tau_{32} \). However, the expression for \( \Delta R_{th} / R_{th} \) in equation (15) is starkly different from that of \( \eta \) in equation (17). While \( \eta \to 1 \) for \( \tau_{21} \to 0 \), \( \Delta R_{th} / R_{th} \to 2\Delta n_{th} / n_{tot} \). Also, \( \eta \) strongly depends on the upper state to lower state lifetime \( \tau_{32} \), whereas \( \Delta R_{th} / R_{th} \) is independent of \( \tau_{32} \). Hence, the result derived with the 3-level DM model has important implications in the way the slope discontinuity is interpreted for the \( I-V \) of a QCL at threshold. In essence, \( \Delta R_{th} / R_{th} \) is an indicator of the population inversion at threshold and not the ratio of level lifetimes, which are two different aspects of laser operation.

By means of Fig. 8 we now show that the assumption \( n_3 \propto \Delta_{1/3} \) which is the basis of the previously held
belief of $\Delta R_{th}$ being equivalent to $\eta$, is incorrect. For the conventional resonant-tunneling diode (RTD) structures, carriers tunnel from the three-dimensional states in the emitter into the quasi-two-dimensional states in the well. Considering only first-order tunneling processes (i.e., conservation of in-plane momentum in tunneling through the barriers), the current flow is proportional to the Fermi energy $\mu_E$ in the emitter and hence the applied voltage $V$ (as shown in Fig. 8(a), see Ref. [31] for example). In such a case, the population $n_1$ of the subband 1 in Fig. 8(a) will indeed be proportional to $V$. However, for a semiconductor superlattice structure of which QCLs are specific examples, the current flow will be negligible if the subbands are significantly off-resonance in the neighboring quantum-wells even if the carrier distributions overlap in energy. This is because total energy cannot be conserved in such a tunneling process since the in-plane momentum conservation needs to be satisfied. The applied bias field is in the $z$ direction and hence affects the bottom energy of the subbands and their $z$-wavefunctions, however, the quasi-Fermi levels within the respective subbands represent the in-plane carrier distribution and are not directly affected by the applied voltage $V$. As a result, the subband populations cannot be assumed to be directly proportional to $V$. Instead, the subband populations and their thermal distributions (and hence the respective quasi-Fermi levels) are determined by the various intersubband and intrasubband scattering processes and also by the resonant-tunneling current flow induced by the coupling of the subband wavefunctions across the barriers as determined by the anticrossing energies $\hbar \Omega_{ij}$ and detuning energies $\hbar \delta_{ij}$. Note that higher order corrections to the resonant-tunneling current flow that relax the requirement of in-plane momentum conservation are not included in this simplified picture [18, 32].

![Illustrative band diagrams for (a) double-barrier resonant-tunneling diode structure [30] that consists of a single quantum-well sandwiched between degenerately doped emitter and collector regions, and (b) a superlattice structure [1] that consists of multiple repeated quantum-wells of which only three wells are shown. In (a), the shown Fermi distributions (indicated by thin red lines) for the carrier populations apply to a quasi-continuous carrier distribution in three-dimensions, whereas in (b), the shown carrier distribution applies only to the two-dimensional momentum space in the $x-y$ plane (since the carriers are confined in the $z$ direction), and is typically Maxwell-Boltzmann like (i.e. the Fermi energy $E_{F}$ of the subbands is indicated by thick horizontal lines). In (a), $V$ is the voltage applied between the emitter and the collector that appears as the difference between the respective Fermi energies, and in (b) $V$ represents the voltage per repeated module of the superlattice that appears as the difference in the energy of the bottom of the subbands.

![Variation of the fractional change in differential resistance at threshold $\Delta R_{th}/R_{th}$ with $\tau_{31}$ calculated using the expression in equation (15) with same typical values of different parameters as in Fig. 8. Figure 9 shows typical variation of $\Delta R_{th}/R_{th}$ with $\tau_{31}$ according to equation (15), which shows that $\Delta R_{th}/R_{th}$ decreases rapidly as $\tau_{31}$ becomes smaller and approaches $\tau_{21}$. The trend in Fig. 9 could be compared to the experimental variation of $\Delta R_{th}/R_{th}$ with temperature for the two-well QCL shown in the upper inset of Fig. 6(b), which indicates a steady degradation of its effective $\tau_{31}$ with temperature due to a predicted hot-phonon effect [24]. Also note that $J_{max}$ and $\Delta R_{th}/R_{th}$ in Fig. 8(b) have a correlated behavior where $J_{max}$ increases as $\Delta R_{th}/R_{th}$ decreases. This validates the expression in equation (15) for operation above threshold, which suggests $J_{max} \propto \left( 1 - \frac{\Delta R_{th}}{R_{th}} \right)$, where $J_{max}$ is the current flowing at $\lambda' = 3$ resonance ($\Delta \lambda' = 0$) and equation (15) is used for substitution. For this IP QCL also, gain bandwidth broadening with temperature is less likely to be the dominant temperature degradation mechanism. Otherwise, the value of $\Delta R_{th}/R_{th}$ should increase according to equation (15) with the requirement of a larger population inversion to reach threshold.

III. OPTICAL GAIN SPECTRUM OF RESONANT-PHONON TERAHERTZ QCLS

Terahertz QCL designs with RP depopulation typically have broad gain linewidths. The spontaneous emission spectra from one of the earliest such designs had a $\sim 2$ THz full-width half-maximum (FWHM) linewidth.
for a $\sim$ 4 THz QCL active region $^{19}$. Experimental spontaneous emission data for some of the more recent high performance designs $^{10, 33}$ is not available because of the difficulty in observing sub-threshold optical signal in metal-metal waveguides $^{34}$, both because of the low loss in these waveguides that causes lasing soon after the upper level is populated with electrons, and also due to the poor out-coupling efficiency of such cavities $^{35}$. However, simultaneous lasing of modes separated by frequencies greater than 0.5 THz $^{20, 36}$ suggests that large gain exists over a broad bandwidth that is a significant fraction of the center frequency in a homogeneously grown RPTQCL design (in contrast to heterogeneous cascade designs that have been used to realize broad gain bandwidths at mid-infrared frequencies $^{37}$).

In this section, we use density-matrices to numerically estimate the optical gain spectrum in a RPTQCL design and find reasons for broadening of the gain spectrum. Similar to the $I-V$ calculations in section $^{11}$, the simplified DM calculations are shown to be an effective method to understand the role of various design parameters toward the optical response of a terahertz QCL gain medium, as opposed to the nonequilibrium Green’s function technique that incorporates a full quantum theory of gain $^{38, 39}$. Similar calculations have been used recently to determine the optimal injector coupling in mid-infrared QCLs $^{40}$, and also to describe the electrical transport characteristics of RT extraction based terahertz QCL structure $^{14}$. We consider the simplest RP design with 4-levels per QCL period as shown in Fig. $^{10}$.

To compute the gain (or loss) spectrum, the linear response to a sinusoidal electric field perturbation of the form $\mathbf{E} = \bar{z}\mathbf{E}(e^{i\omega t} + e^{-i\omega t})$ is calculated by incorporating the electric-dipole interaction term for coherent coupling of the radiative levels. Only the electric-field component in the growth direction $\bar{z}$ is considered due to the intersubband polarization selection rule. The time evolution of the DM for the 4-level design is then written as $^{22}$

$$
\frac{d}{dt} \begin{pmatrix} \rho_{1'1'} \\ \rho_{1'4} \\ \rho_{4'1'} \\ \rho_{4'4} \\ \rho_{2'2} \\ \rho_{2'1'} \\ \rho_{1'2} \\ \rho_{2'4} \\ \rho_{4'2} \\ \rho_{4'3} \\ \rho_{3'4} \\ \rho_{3'2} \end{pmatrix} = \frac{i}{\hbar} \begin{pmatrix} E_{1'} & -\Omega_{1'4} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\Omega_{1'4} & E_4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & E_{1'} & -\Omega_{2'1'} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\Omega_{2'1'} & E_{4'} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & E_{1'} & -\Omega_{3'4} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\Omega_{3'4} & E_{2'} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & E_{2'} & -\Omega_{4'2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\Omega_{4'2} & E_{4'} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & E_{2'} & -\Omega_{4'3} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\Omega_{4'3} & E_{1'} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & E_{1'} \end{pmatrix} \rho_{(1',4,3,2)} + \begin{pmatrix} \frac{\rho_{1'1'} + \rho_{2'2}}{2} & \frac{\rho_{3'1'}}{2} + \frac{\rho_{4'3'}}{2} & \frac{\rho_{4'1'}}{2} + \frac{\rho_{1'4}}{2} & \frac{\rho_{2'3}}{2} & \frac{\rho_{4'2'}}{2} & \frac{\rho_{2'4}}{2} & \frac{\rho_{4'3'}}{2} & \frac{\rho_{1'4'}}{2} & \frac{\rho_{3'2'}}{2} & \frac{\rho_{4'1'}}{2} & \frac{\rho_{2'3}}{2} & \frac{\rho_{4'2'}}{2} \end{pmatrix}
$$

Equation (19) is written similarly as equation (2) with additional modifications due to the sinusoidal electric-field perturbation. We consider linear response within the rotating-wave approximation (i.e. $|\omega - \omega_{34}| \ll \omega$) in which case the affected coherences can be explicitly written to have a sinusoidal time variation as shown with the slowly-varying amplitudes $\rho_{mn}$. The radiative levels 3 and 4 are now coherently coupled through the off-diagonal electric-dipole interaction term $|e| \mathbf{r} \cdot \mathbf{E}$ that has an amplitude $|e|z_{43}\mathbf{E}$, where $z_{43} = (4|\bar{z}|3)$ is the dipole-matrix element for the said tightbinding levels. Since $(1',4)$ and $(3,2)$ are coherently coupled due to non-zero $\Omega_{1'4}$ and $\Omega_{32}$ terms respectively, the coherences corresponding to $(1',3)$, $(1',2)$, and $(4,2)$ acquire a time-harmonic character due to the time-harmonic $(4,3)$ coherent coupling. The sinusoidal component of the coherences is written explicitly in the ansatz $\rho_{(1',4,3,2)}$, in which case $\rho_{1'1'} = 0$ in the steady-state for the slowly varying amplitudes $\rho_{mn}$. Note that $\rho_{(1',4,3,2)}$ on the right-side of equation (19) is the same as the left-side matrix appearing with the time derivative.

We made some simplifying approximations in writing equation (19). Similar to before, for simplicity of calculations, we assume a unity injection efficiency ($\Omega_{1'3} \approx 0$), also a unity collection efficiency ($\Omega_{42} \approx 0$), and neglect the backscattering terms $\tau_{12}$ and $\tau_{34}$. For non-zero $\Omega_{1'3}^{\text{LO}}$.
and/or $\Omega_{12}$, equation (19) will become more complicated since some of the non-harmonic terms in the $\tilde{h}(1, 4, 3, 2)$ matrix will additionally acquire time-harmonic character and similarly some of the time-harmonic coherences will additionally acquire a constant value in the steady-state, thereby effectively increasing the number of independent variables to be solved for the system (currently 16 for the written equation). Also, a parameter $\tau_{41}$ is included to incorporate the effect of any indirect parasitic scattering channels from 4 to 1, since direct $4 \rightarrow 1$ transport is otherwise only allowed via inter-sub-module tunneling across the collector barrier for the chosen set of tight-binding basis functions. We can now solve this equation, which, in addition to yielding values of current and level populations, also yields the electrical polarization $\tilde{\mathbf{P}}(t)$ induced due to the external optical field $\mathbf{E}$ as

$$\mathbf{P} = \epsilon_0 \chi(\omega) \mathbf{E} e^{i\omega t} + \text{c.c.}$$

$$= -\frac{|\epsilon|}{V_{ac}} \frac{\epsilon_{243}}{\epsilon_{0}\epsilon_{243}} \left[ \rho_{43}(\omega) + \rho_{34}(-\omega) \right] e^{i\omega t} + \text{c.c.} \right\}$$

where $V_{ac}$ is the volume of the active region. The induced electrical susceptibility $\chi(\omega)$ becomes

$$\chi(\omega) = \chi'(\omega) + i\chi''(\omega)$$

$$= -\frac{|\epsilon|}{V_{ac}\epsilon_0} \left[ \rho_{43}(\omega) + \rho_{34}(-\omega) \right]$$

which is independent of the amplitude $\mathbf{E}$ for small values. The optical gain coefficient $g(\omega)$ (in meter$^{-1}$) is related to the imaginary part of the susceptibility $\chi''(\omega)$ as

$$g(\omega)|_{\chi' = \chi''(\omega)} < n_t^2 = \frac{\chi''(\omega)}{n_t} \frac{\omega}{c}$$

where $n_t$ is the refractive index of the medium. In the following, we show results of the computed optical gain spectrum as a function of several different parameters of interest.

A. Optical gain spectrum as a function of injector anticrossing

Figure 11 shows the numerically computed gain spectra for the 4-level RPTQCL design as modeled by equation (19) for different values of injector anticrossing $2\Delta\Omega_{14}$. For the $4 \rightarrow 3$ radiative transition, the FWHM frequency linewidth due to scattering is given by $\Delta\nu_{\text{scatt}} \approx \frac{1}{2} \left[ \frac{1}{2\tau_{43,\text{eff}}} + \frac{1}{2\tau_{43}} + \frac{1}{\tau_{41}} \right]$, which yields a value of 0.67 THz ($h\Delta\nu_{\text{scatt}} \approx 2.75$ meV) for the chosen parameters. The value of $T_{23} = 0.75$ ps was assumed for the above value of the linewidth to approximately agree with those observed typically for bound-to-continuum THz QCLs [41, 42, 43] whose linewidths are more likely to be scattering limited. As $2\Delta\Omega_{14}$ becomes as large as $h\Delta\nu_{\text{scatt}}$, injector transport becomes more coherent and the gain spectrum becomes additionally broadened due to anticrossing splitting of the linewidth as can be seen from Fig. 11. Also note that the population inversion $\Delta n$ approaches the maximum value given by equation (7) for coherent injection, which, for the present case yields $\Delta n_{\text{max}} \approx \frac{1}{2} \frac{\Delta \nu_{\text{scatt}}}{\Delta \nu_{\text{eff}}} n_{\text{tot}} \approx 0.28 n_{\text{tot}}$. The area under the gain curve is proportional to the population inversion $\Delta n_{43}$, therefore, any additional broadening decreases the peak gain. This suggests that a value of $2\Delta\Omega_{14}$ much larger than $h\Delta\nu_{\text{scatt}}$ might in fact diminish the performance of a design. However, as will be shown in the next section, RPTQCL designs anyway have broad linewidths due to a coherent RT assisted depopulation process, in which case having $2\Delta\Omega_{14} > h\Delta\nu_{\text{scatt}}$ is less likely to cause additional broadening of the gain linewidth. Consequently, the injector anticrossing value for the RPTQCL designs is chosen based on other design parameters such as the $1' \rightarrow 3$ parasitic current leakage [40] rather than the concerns about gain broadening.

B. Optical gain spectrum as a function of collector anticrossing

Figures 12(a) and 12(b) show the computed gain spectra for different values of collector anticrossings $2\Delta\Omega_{23}$, and energy detuning $h\Delta\nu_{\text{23}}$, respectively. The best RPTQCL designs typically have collector anticrossing values in the range of $4 - 5$ meV. This is to maintain a short effective lower state lifetime so as to maximize $J_{\text{max}}/J_{\text{th}}$, since $J_{\text{max}} \propto \tau_{\text{lower}}^{-1}$ for coherent injection (equation 8), al-

![Figure 11: Computed gain spectra for the 4-level structure of Fig. 10 for different injector anticrossings $2\Delta\Omega_{14}$, evaluated at $1' \rightarrow 4$ resonance ($\Delta_{14} = 0$). Levels 3 and 2 are also taken to be at resonance ($\Delta_{32} = 0$) and a small value of $2\Delta\Omega_{23} = 2$ meV is chosen to limit additional broadening due to a coherent 3 $\rightarrow$ 2 RT process (as shown in Fig. 12b). All other parameters have same equivalent values as in Fig. 3, except $\tau_{21} = 0.2$ ps that results in an effective lower state lifetime $\tau_{3,\text{eff}} \approx 1$ ps, which can also be estimated from the equivalent of equation (11). Also, $E_{43} = 16.5$ meV (4 THz). The values of FWHM linewidth $\Delta\nu_{\text{23}}$ and population inversion $\Delta n_{43} = n_{43} - n_{3}$ obtained as a result of the calculation are also indicated alongside each of the curves.](image-url)
As seen from Fig. 12(b), note that linewidth broadening
broad linewidths associated with RPTQCLs [19, 20, 36].

splitting of the gain spectrum due to the coherent R T
ing $\nu$ the 2

For example, linewidth of $1 \times 10^{-3}$ ps. This shows that the anticrossing
of detuning ($\Delta_{14}$) which is direct, and due to $4 \leftrightarrow 3$ coherent
coupling) is considerably detuned from the stronger
4 \rightarrow 3 radiative transition (which is direct, and due to
4 \leftrightarrow 3 coherent coupling), and hence contributes neg-
ligibly to the gain. For a coherent 3 \rightarrow 2 RT process
(i. e. large $\Omega_{32}$), the peak gain occurs at a frequency

though at the cost of a broader linewidth. For example,
the 2$h\Omega_{32} = 5$ meV spectrum in Fig. 12(a) has a FWHM
linewidth of 1.8 THz, a value almost twice as large as
the scattering linewidth $\Delta\nu_{\text{scat}} \sim 1$ THz (calculated using
$\tau_{1,\text{eff}} \sim 0.3$ ps). This shows that the anticrossing
splitting of the gain spectrum due to the coherent RT
assisted depopulation process is the main cause of the
broad linewidths associated with RPTQCLs [19, 20, 36].

As seen from Fig. 12(b), note that linewidth broadening
happens only close to the 3 \rightarrow 2 resonance at $h\Delta_{32} \approx 0$.
For $|h\Delta_{32}| > 0$ and $|h\Delta_{32}| < E_{43}$, the width of the spectrum
remains narrow, since the 4 \rightarrow 2 radiative transition
(which is indirect, and due to $4 \leftrightarrow 3$ and $3 \leftrightarrow 2$ coherent
coupling) is considerably detuned from the stronger
4 \rightarrow 3 radiative transition (which is direct, and due to
4 \leftrightarrow 3 coherent coupling), and hence contributes neg-
ligibly to the gain. For a coherent 3 \rightarrow 2 RT process
(i. e. large $\Omega_{32}$), the peak gain occurs at a frequency

$\omega_{\text{peak}} > E_{43}/h$ for $h\Delta_{32} < 0$ and $\omega_{\text{peak}} < E_{43}/h$ for
$h\Delta_{32} > 0$. The frequency shift of $\omega_{\text{peak}}$ away from $E_{43}/h$
is due to the energy splitting due to the 3\rightarrow 2 anticrossing
close to resonance.
at 8 V to 15.7 meV (3.8 THz) at the 1′ − 4 resonance bias of 12 V due to the large value of the Stark shift in a diagonal radiative transition. However, the peak gain occurs close to a frequency of 4 THz at almost all bias conditions for the calculated spectra. This behavior is due to the coherent nature of the depopulation process. The 3 − 2 energy detuning $\hbar \Delta_{32}$ also varies linearly with the applied bias, from $-4.7$ meV at 8 V to 2.4 meV at 12 V. Consequently, as shown by the calculations in Fig. 12(b), the gain peak is pushed to higher frequencies than the radiative separation $E_{43}$ at low-bias that effectively masks the Stark shift in $E_{43}$. This is affirmed from the lasing spectra in Fig. 13(b) that shows that the $\sim 3.9$ THz mode is excited at all bias. In contrast, the Stark shift is clearly emphasized in the lasing mode spectrum of the diagonal bound-to-continuum terahertz QCLs due to the different depopulation mechanism in such designs.

As an evidence of the broad gain linewidth in this QCL, at some middle-bias points, additional lasing spectra are excited close to a frequency of 3.3 THz that leads to simultaneous cw lasing of modes separated by $\sim 0.6$ THz. This behavior could be attributed to the double-peaked gain spectra that emerges close to the 3 − 2 resonance ($\Delta_{32} \approx 0$), for which, this design, happens at the middle-bias points. It may be noted that we have observed similar dual-frequency lasing behavior in some versions of the 5-level RPTQCL design of Fig. 11(b). Whether or not this happens depends on the relative alignment of the injector and collector anticrossings as a function of the applied electrical bias.

We should note that recently a much smaller FWHM linewidth of $\sim 0.6$ THz has been measured for a similar 4-level RPTQCL design using a THz time-domain spectroscopy technique, which could be due to the following reasons. The QCL structure in Ref. 44 has a smaller collector anticrossing $2m_3 \sim 3.7$ meV as opposed to a value of $2m_{32} \sim 4.7$ meV for the design in Ref. 10 that is analyzed in Fig. 13. Also, it is possible for a given QCL structure that the bias range of lasing operation may not sweep through its collector resonance ($\Delta_{32} = 0$) depending on the relative alignment of the injector and the collector anticrossings for the grown structure, in which case the gain spectra may not show additional broadening due to the 3 − 2 RT as seen from some specific calculations for non-zero $\hbar \Delta_{32}$ in Fig. 12(b). We would also like to note that the present calculations were done within a rotating-wave approximation ($|\omega - \omega_{43}| \ll \omega$), which becomes less accurate once the gain linewidth becomes a significant fraction of the center frequency. Hence, the true linewidths may be somewhat narrower than those calculated in this section. Nevertheless, within the assumptions considered, the close tracking of the calculated and experimental spectral characteristics of the 4-level RPTQCL design in Fig. 13 establishes the importance of the relatively simple density-matrix model developed in this section for estimating the optical gain spectrum of a terahertz QCL structure.

In conclusion, we have presented simplified density-matrix transport models to describe resonant-tunneling transport in terahertz QCLs. Due to the closely spaced energy levels in terahertz QCL structures, coherence plays an important role in the resonant-tunneling mechanism, which is incorporated well within the presented framework. A 3-level model was developed to derive current transport through the injector barrier of any general QCL design (which applies to mid-infrared QCLs as well). Useful expressions were derived for current flow above and below threshold that could directly be used to analyze the experimental behavior of some representative QCL designs. Based on experimental observations, we have been able to speculate about some of the dominant temperature degradation mechanisms in phonon-depululated terahertz QCL designs. We have extended the density-matrix model to estimate the gain spectra of resonant-phonon terahertz QCLs. A coherent resonant-tunneling assisted depopulation process is identified to be the primary cause of the broad gain bandwidths typically observed in such QCLs.

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