To My Parents
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CHAPTER I

INTRODUCTION: INTERSUBBAND STIMULATED EMISSION

A strong current injection exclusively into the upper subband of optically active multiple-quantum-well tunneling regions provides in the quantum cascade laser\textsuperscript{1,2,3} a finite population inversion and actual lasing at mid-infrared frequency $\omega_\Delta \approx 300$ meV. This seminal achievement culminates a quest for such intersubband stimulated emission which began in 1971 with a theoretical treatment by Drs. Kazarinov and Suris\textsuperscript{4} soon after the seminal work on superlattices by Esaki and Tsu.\textsuperscript{5}

The frequency $\omega_\Delta$ of the stimulated emission is given by the level (or subband) separation, $\Delta$, in the tunneling regions of the quantum cascade laser.\textsuperscript{1,2,3} A simple modification of the tunneling potential thus allows the (stimulated) intersubband emission to be tuned anywhere within the mid-infrared and down to the far-infrared (or Tera-Hertz) regime. This tunability has been demonstrated by the recent observation\textsuperscript{6} of spontaneous emission in such a quantum-cascade-laser design also at $\omega \approx 120$ meV.

There is a considerable interest in achieving such intersubband stimulated emission also in the far-infrared (or Tera-Hertz) regime, which we shall defines as fre-
frequencies $\omega \approx 10 \text{ meV}$. There is a wealth of recent and exciting experimental results involving Tera-Hertz radiation and we mention in particular the observation of spontaneous emission in superlattices excited by a strong nonequilibrium current flow,\cite{7,8} of coherent oscillations, or quantum beats, in optically excited double-quantum-well structures,\cite{9,10} of Bloch oscillations\cite{11,12} and photon-assisted tunneling\cite{13} in superlattices, and finially of dynamical screening effects in resonant-harmonic generation in a double-quantum-well structure.\cite{14}

In this dissertation we adapt the quantum-cascade-laser design\cite{1,2,3} and consider theoretically the intersubband decay and resulting population inversion in a double-quantum-well tunneling structure with the far-infrared subband separation, $\Delta \approx 11 \text{ meV}$. One may imagine this structure serves as an optically active region of a hypothetical far-infrared quantum cascade laser, but we emphasize that the design of a good waveguide confinement will be difficult due to the long wavelength of the far-infrared radiation.

The bottom panel of Figure 1.1 shows schematics of hypothetical far-infrared quantum-cascade-laser design presently investigated. The tunneling structure comprises a central asymmetric double-quantum-well region surrounding by two moderately doped injector layers serving as emitter and collector leads. The quantum-well region confines (more than) two resonant level $E_1$ and $E_2$ with subband separation $\Delta = E_2 - E_1 \approx 11 \text{ meV}$. The choice of this central region is motivated by the small intersubband decay, $1/\tau \approx 0.03 \text{ meV}$ at $T \leq 50 \text{ K}$, observed\cite{15} under weak optical pumping of the corresponding isolated double-quantum-well structure.\cite{14,15} Similar vanishing intersubband decay rates has been reported for quantum-well structures with corresponding far-infrared subband separations, see for example Refs. 16,17.
FIGURE 1.1 Schematic of far-infrared optically active tunneling structure (bottom panel) and examples of the *nonequilibrium* electron-electron scattering $\Gamma$ which dominates the intersubband decay. The hypothetical structure comprises, see bottom panel, a central $L_{QB} = 243 \ \text{Å}$ wide tunneling region (based on asymmetric double-quantum-well structure investigated in Ref. 15) *surrounded* by the $n$-doped (left/right) emitter/collector lead with band-edge $\phi_{L/R}$ and chemical potential $\mu_{L/R}$. A moderate voltage drop $V \equiv (\mu_L - \mu_R)/e \sim 20 \ \text{mV}$ ensures a current injection $\Gamma_e$, solid arrow, *exclusively* into upper resonant level $E_2$ and fast tunneling escape rates $\Gamma_{c1(2)}$, dashed-single(double)-dotted arrow, out from lower level $E_1$ (from $E_2$.). Lower panel shows tunneling potential, resonant levels (solid bars,) and wavefunctions $\Psi_{1,2}^\delta(x)$ at special voltage drop $V_{\text{sym}}$ where the quantum-confined Stark effect\textsuperscript{23} causes an avoided crossing in the subband separation $\Delta(V) \equiv E_2 - E_1 \geq 10.9 \ \text{meV}$ and restores a near-exact wavefunction inversion symmetry:\textsuperscript{24} $\Psi_{1(2)}^\delta(x_0 - x) \approx +(-)\Psi_{1(2)}^\delta(x - x_0)$ (where $x_0$ is the node of $\Psi_2^\delta(x)$.) For comparison the dashed bars shows positions of $E_{1,2}$ at $V = 0$. The *three pairs* of opposite transition arrows in the *top* panel illustrate the dominant decay of the current-injected upper-subband distribution (dotted dispersion curve,) namely the *nonequilibrium* scattering ($\Gamma$) between two upper-subband electrons which both decay to subband $E_1$. As indicated by the pair of solid arrows, the scattering $\Gamma$ occurs with the characteristic momentum transfer $q_\Delta = \sqrt{2m^*_e \Delta}$ and on average with no energy transfer.
Electron-electron scattering

\[ \Delta = E_2 - E_1 \]

\[ q_\Delta = (2m_e^{*}\Delta)^{1/2} \]

\[ F_{dc} = \frac{V_{sym}}{L_{QB}} \]

FIGURE 1.1
Such vanishing intersubband decay rates are possible at temperatures $T \leq 50$ meV because the optical phonon frequency ($\Omega_{LO} \approx 36$ meV in GaAs) exceeds the subband separation, $\Omega_{LO} > \Delta$. The optical-phonon emission is thus thermally activated with activation energy $15 \Omega_{LO} - \Delta \approx 25$ meV.

We may assume that the experimental value, $1/\tau < 0.03$ meV at $T \leq 50$ K (observed at weak optical pumping) constitute an approximate bound on the total single-electron decay, $\Gamma_{se}$, resulting with the strong current injection exclusively into the upper-subband of the Figure 1.1 tunneling structure.

We demonstrate that it straight forward to ensure intersubband population inversion if the intersubband decay was limited to $\Gamma_{se}$. However, we find that the current injection results in a very significant nonequilibrium electron-electron scattering ($\Gamma = \Gamma_{22 \rightarrow 11}$ and $\Gamma_{22 \rightarrow 21}$) which we evaluate for a complete upper-subband occupation below the emitter chemical potential.

The top panel of Fig. 1.1 illustrate typical intersubband scattering events contributing to $\Gamma$. Such processes involves two upper-subband electrons which both decay to the lower subband. This nonequilibrium scattering $\Gamma$ is given by an intersubband Coulomb matrix element which can be determined from existing measurements of a large equilibrium depolarization shift, $\Delta* - \Delta \approx 2$ meV, of the absorption peak, $\Delta*$, from the subband separation, $\Delta \approx 11$ meV.

In addition there is the nonequilibrium electron-electron scattering $\Gamma_{22 \rightarrow 12}$ which also involves two upper-subband electrons but where only one electron decays

---

* We define the total single-electron decay, $\Gamma_{se}$ as the intersubband decay resulting from everything but the electron-electron interaction. That is, we define $\Gamma_{se}$ as the intersubband decay resulting from impurity, interface-defect, acoustic-phonon scattering and from the thermally activated optical-phonon emission.
to the lower subband. This scattering is given by an intersubband Coulomb matrix element which we find essentially vanishes when, at a finite voltage drop, the so-called quantum-confined Stark effect\textsuperscript{23} restores an approximate wavefunction-inversion symmetry.\textsuperscript{24}

We demonstrate that the nonequilibrium electron-electron intersubband scattering $\Gamma (\Gamma_{22\rightarrow21})$ is never significantly reduced by screening, and, unlike the near-equilibrium electron-electron scattering,\textsuperscript{27,28} is \textit{not} (only partially) inhibited by Pauli exclusion, as we can assume population inversion and hence a vanishing lower-subband occupation.

Furthermore, in this dissertation we (1) identify a simple scaling of scattering rate $\Gamma$ with upper-subband occupation, (2) predict a very strong intersubband decay $\sim 2\Gamma \approx 10$ meV for an upper-subband sheet-density $N_L \approx 10^{11}$ cm$^{-2}$ comparable to that in the mid-infrared quantum cascade laser,\textsuperscript{1,3} (3) demonstrate that a smaller population inversion density ($\sim 0.25 \times 10^{11}$ cm$^{-2}$) \textit{can} be maintained at a moderate tunneling current density, and finally (4) predict, also for the combined nonequilibrium electron-electron intersubband decay rate, $2\Gamma + \Gamma_{22\rightarrow21}$, a dramatic bias dependence arising from the quantum-confined Stark effect.\textsuperscript{23}

Finally we note that the predicted strong nonequilibrium electron-electron intersubband scattering is relevant also for the study of possibility of continuous-wave Bloch oscillations in double-quantum-well resonant-tunneling structures as has recently been addressed in two theory studies:\textsuperscript{25,26} the strong electron-electron scattering may reduce the intersubband population inversion which is proportional\textsuperscript{26} to the predicted net stimulated emission of such Bloch oscillations.
I. A Detailed overview of dissertation

Here in Chapter I, we briefly discuss the resonant current flow both in the standard double-barrier resonant-tunneling diode,\textsuperscript{5,29,30,31} and in the two-level tunneling structure shown in Fig. 1. Specifically, we introduce simple rate equations to describe the current flow and demonstrate that population inversion requires that the tunneling escape rates out from the lower level exceeds the (nonradiative) intersubband decay. We estimate the tunneling rates into and out from the quasi-bound resonant levels for the potential shown in Figure 1.1 and demonstrate that it is straightforward to maintain a finite population inversion if the intersubband decay is limited to the total single-electron decay, $\Gamma_{sp}$ (approximately bounded by the experimental value, $1/\tau \approx 0.03$ meV.) Finally, we explain how even a moderate intersubband population inversion may result in a significant stimulated emission because (a) the optical transitions is concentrated around a single frequency $\omega_{\Delta}$ given by the subband separation $\Delta$, and (b) the quantum-well potential results in very large optical transition matrix elements.

In Chapter II, we discuss the mid-infrared Quantum Cascade Laser following Refs. 1,2,3. We describe the chemical composition and corresponding effective tunneling potential. In particular we discuss the current injection in the set of 25 active tunneling regions separated by interjacent so-called injector layers serving as emitter and collector leads. We also describe the total current flow and power dissipation at threshold conditions, that is, just before the onset of lasing. Moreover, we explain a simple theory estimate\textsuperscript{3} of the so-called (peak) material gain, i.e., the net amplification of the lasing mode if traveling exclusively within an (infinite) superlattice of the optically active regions with interjacent injector layers/leads. Finally,
we explain how Capasso and coworkers achieved a good waveguide confinement by surrounding the optically active 25-period superlattice by so-called cladding layers with a smaller index of refraction. This waveguide confinement both enhances the lasing intensity inside the optically active superlattice and prevents a potentially significant (impurity aided) free-carrier and plasmon reabsorption especially at the contact layers.

In Chapter III, we discuss the hypothetical far-infrared quantum-cascade-laser design in greater detail. We specify a possible chemical potential and describe the resulting potential as a function of the voltage drop \( V \) applied across the tunneling region. We determine the corresponding variation of the resonant levels and in particular identify an avoided crossing in the subband separation at voltage drop \( V_{sym} = 22.9 \) mV with potential shown in Figure 1.1. We also estimate the voltage-drop variation of the tunneling rates and estimate the range of voltage drops which ensures a current injection exclusively into the upper subband of the hypothetical tunneling structure. Moreover, we demonstrate that the voltage drop \( V_{sym} \) restores a near-exact wavefunction inversion symmetry in the still asymmetric potential. We determine the voltage-drop variation on this wavefunction-inversion symmetry and explain this quantum-confined Stark effect within a simple two-level model. Finally, we discuss the total single-electron intersubband decay rate, \( \Gamma_{se} \), which we, at temperatures \( T \leq 25 \) K, can assume bounded by the experimental value, \( 1/\tau \approx 0.03 \) meV.

In Chapter IV we provide a detailed study of the nonequilibrium electron-electron intersubband scattering \( \Gamma \equiv \Gamma_{22\rightarrow11} (\Gamma_{22\rightarrow12}) \) between two upper subband electrons which both decay (of which only one decays) to the lower subband. We
evaluate these nonequilibrium rates for a complete upper subband occupation below emitter chemical potential. We describe the effective Coulomb intersubband interaction and observe that this interaction (a) exhibits only a moderate variation with in the in-plane momentum transfer $q$ and (b) shows only a correspondingly moderate dependence on an effective Thomas-Fermi screening wavevector $q_{TF}$. We furthermore find that the nonequilibrium scattering $\Gamma$ is characterized by a matrix elements whose value at $q = 0$ can be extracted directly from the experimental observation$^{14,15}$ of a significant equilibrium depolarization shift.$^{19}$ Moreover, we identify a simple scaling of the scattering rate $\Gamma$ with the upper-subband occupation. In contrast, we find no scaling for the other nonequilibrium scattering, $\Gamma_{22 \rightarrow 21}$, when (at a finite occupation) the Pauli exclusion principle begins to restrict the availability of final upper-subband states.

We furthermore predict a significant wavefunction-symmetry variation of both $\Gamma$ and $\Gamma_{22 \rightarrow 21}$, and also of the combined electron-electron intersubband decay rate, $2\Gamma + \Gamma_{22 \rightarrow 21}$. We find that a very strong intersubband decay rate, $\sim 2\Gamma \sim 1.0$ meV, prevents an upper-subband occupation density $n_2 \approx 10^{11}$ cm$^{-2}$. Nevertheless, we demonstrate that a smaller finite intersubband population inversion, $\sim 0.25 \times 10^{11}$ cm$^{-2}$ can be maintained at a current density comparable with the current density of the mid-infrared quantum cascade laser.$^{1,3}$

In our concluding Chapter V we summarize our results and list of open questions. In particular, we observe that while a finite intersubband population can be maintained it does not guarantee that actual far-infrared lasing can be achieved. Especially the design of a good waveguide confinement of a potentially far-infrared lasing mode will be very difficult due to the very long wavelength.
Finally, in Appendix A we provide a formal derivation of the intersubband electron-electron scattering rates based on the Fermi golden rule. In particular, we demonstrate that the so-called direct and exchange contributions to the same-spin scattering cancel if the $q$-variation of intersubband Coulomb matrix element can be ignored. For the dominant opposite-spin scattering we derive the estimates evaluated in Chapter IV.

1.B The resonant-tunneling current flow

The standard resonant-tunneling diode comprises (for example) a central GaAs quantum-well layer separated from two outside $n$-doped GaAs leads by a pair of Al-GaAs tunneling-barriers. As schematically illustrated in the upper panel of Fig. 1.2, this variation of the chemical composition defines an effective double-barrier potential for the conduction-band electrons and the higher potential in the AlGaAs-barrier layers traps a resonant level $E_r$ in the central quantum-well. A typical width, 30–40 Å, of each barrier ensures a vanishing probability for tunneling from emitter to collector unless the electron energy matches that of the quasibound resonant level.

In the sample structure illustrated in Fig. 1.2, the resonant level $E_r$ is in equilibrium (top panel) located well above the chemical potential of the leads, $E_r > \mu_L = \mu_R$. However, as illustrated in the bottom panel of Fig. 1.2, a finite voltage drop $V$ applied across the tunneling region raises (lowers) the emitter (collector) Fermi sea and will result in a fast current injection rate, $\Gamma_e$, (tunneling escape rate, $\Gamma_c$), when the quasibound level is positioned between the emitter
FIGURE 1.2 Schematic band profile of a resonant-tunneling heterostructure diode in equilibrium (upper panel) and under resonant operating conditions (lower panel.) The effective double-barrier potential traps a quasibound resonant level $E_r$ between the emitter (‘L’) and collector (‘R’) leads with lower conduction band edge $\phi_{L/R}$ and chemical potential $\mu_{L/R}$. In Equilibrium, as illustrated in the upper panel, the resonant level is typically located above the chemical potential, $\mu_L = \mu_R$, and there is only a small linear-response conductivity. However, as illustrated in the lower panel, a finite applied bias raises (lowers) the emitter (collector) lead. Under these so-called resonant conditions the quasibound level is positioned within the emitter Fermi sea, $\mu_L > E_r > \phi_L$, and there is both a large resonant-tunneling current injection, $\Gamma_e$, from the emitter into the quasibound level and a large tunneling escape rate, $\Gamma_c$, from the resonant level out to the collector lead. The resulting resonant-tunneling current flow is proportional to the steady-state nonequilibrium occupation of the resonant level, $E_r$. 
Vanishing conductance

\[ E_r > \mu_L \]

Resonant-tunneling current

\[ \mu_L > E_r > \varphi_L \]

FIGURE 1.2
band-edge and chemical potential (above the collector chemical potential,)

\[ \phi_L < E_r < \mu_L, \]  

\[ (E_r > \mu_R). \]  

A significant current may flow under the resonant conditions, Eqs. (1) and (2), because the quasi-bound resonant level can be exploited by a finite (two-dimensional) density of electrons, which, in effect, tunnel in parallel. The electrons are free to move in the plane of the heterostructure, that is, perpendicular to the tunneling current flow. This motion can be characterized in-plane momentum \( \vec{k} \) and dispersion

\[ E_r + E|| (k) \equiv E_r + \frac{k^2}{2m^*_e}, \]  

given by the effective electron mass \( m^*_e \). All such subband states with an energy, Eq. (3), below the emitter chemical potential, \( \mu_L \), will contribute to the current flow. With just a moderate doping concentration, \( \sim 10^{17} \text{ cm}^{-3} \), giving a \( \mu_L/\mu_R - \phi_L/\mu_R \sim 10 \text{ meV} \) thickness of the emitter/collector Fermi sea, one can obtain a finite density of subband states,

\[ N_L = \frac{2m^*_e (E_r - \phi_L)}{2\pi} \sim 10^{11} \text{ cm}^{-2}. \]  

Under resonant conditions, Eqs. (1) and (2), the resulting current flow can be determined by a simple rate equation\(^ {32} \) for the electron occupation density, \( n \), of the resonant level. Specifically, since all subband states below the emitter chemical potential may tunnel in parallel, we have

\[ \frac{dn}{dt} = (N_L - n)\Gamma_e - n\Gamma_c. \]  

\[ (1) \]  

\[ (2) \]  

\[ (3) \]  

\[ (4) \]  

\[ (5) \]
The steady-state solution, $n^0 = N_L \Gamma_e / (\Gamma_e + \Gamma_c)$ (limited by $N_L$), of Eq. (5) then yields the current flow

$$J = e \Gamma_e (N_L - n^0) = e \frac{\Gamma_e \Gamma_c}{\Gamma_e + \Gamma_c}. \quad (6)$$

The discussion of the resonant-tunneling current flow is thus reduced to a determination of the rates $\Gamma_e$ and $\Gamma_c$, which, following Bardeen, may be obtained by the Fermi golden rule.

Adapting the approach described in Refs. 33, 34 we provide below a formal Fermi-golden-rule estimate for the tunneling rates as follows. We assume a simple voltage-drop dependence, $\phi_{L/R}(V) = \phi_{L/R}(V = 0) + \sqrt{eV}/2$, for the position of the emitter/collector lower band edge, exactly as illustrated in both Figure 1.1 and Figure 1.2, and express all energies from the position of the GaAs quantum-well potential at $V = 0$. For simplicity we also assume that the potential confining quasi-bound resonant level $E_r$ can be treated as symmetric and ignore the changes in the barrier potential $\phi_B$ with the finite voltage-drop $V$. For an electron of energy $E \ll (\phi_B - E)$ we then obtain the probabilities, $T_L(E)$ and $T_R(E)$, for tunneling from the quantum-well region to the emitter ('L') and to collector ('R') leads as

$$T_L(E) \approx 16 \Theta(E - \phi_L) \sqrt{E(E - \phi_L)} \frac{\phi_B - \phi_L}{\phi_B - E} \exp(-2L_B \sqrt{2m_e^* (\phi_B - E)}), \quad (7)$$

$$T_R(E) \approx 16 \Theta(E - \phi_R) \sqrt{E(E - \phi_R)} \frac{\phi_B - \phi_R}{\phi_B - E} \exp(-2L_B \sqrt{2m_e^* (\phi_B - E)}), \quad (8)$$

where $L_B$ denotes the barrier width.

The escape rate out from level $E_r$ can be estimate as a product of the tunneling probability, given by Eq. (8), and a tunneling attempt frequency. The thickness, $L_{QB}$, of the tunneling region (introduced in Figure 1.1) represent a simple measure
of the extension of the quasi-bound wavefunction in level $E_r$. Hence, we may estimate this tunneling attempt frequency$^{35,36}$ as the ratio of the resonant-level velocity $v_0 = \sqrt{2E_r/m_e^*}$ to $2LQB$. Thus we finally obtain the estimate

$$\Gamma_c = \frac{v_0}{2LQB} T_L(E_r) = \frac{\sqrt{2E_r/m_e^*}}{2LQB} T_L(E_r),$$

(9)

for the current injection rate and

$$\Gamma_c = \frac{v_0}{2LQB} T_R(E_r) = \frac{\sqrt{2E_r/m_e^*}}{2LQB} T_R(E_r),$$

(10)

for the tunneling escape rate.

We emphasize that we have in Eqs. (8) and (10) only obtained a qualitative estimate of the tunneling escape rate, $\Gamma_c$. We have for example not included the effects on the tunneling potential on the barrier height, nor have we treated possible electron charging effects. However, such quantitative corrections to $\Gamma_c$ (and $\Gamma_e$) can be offset by a change in the actual barrier thickness $L_B$ which has a dramatic affect on the tunneling probability, see Eq. (8).

We also note that the above simple treatment based on the rate equation, Eq. (5), clearly suggest that the predicted current flow at resonant conditions, Eq. (1), is very robust toward scattering. It is in fact under these resonant conditions possible to derive the rate equation independently of the strength of an interaction at the resonant level, provided the in-plane momentum transfer can be ignored.$^{36}$

The insensitivity toward scattering of the current flow at resonant conditions, Eq. (1) and (2), is in contrast to the situation in the so-called valley region of the current-voltage characteristics of a standard double-barrier resonant-tunneling diode. This valley region results at even higher voltage drops which pushes the
emitter lower band edge $\phi_L$ above the level $E_r$. As is evident from the estimate, Eq. (9), we then have $\Gamma_e \equiv 0$ and we expect no current injection directly into the lower subband. When the resonant-tunneling diode enters this region there is a dramatic drop in the current flow and a negative differential conductance is observed — a feature which has continued to sustain interest since its first observation in 1974. Twenty-nine Specifically, the negative differential conductance has possible application in the realization of very fast oscillations which should in principle be able to operate even at Tera-Hertz frequencies, i.e., in the far-infrared regime.

It has, however, proven difficult to prevent a small but finite inelastic tunneling also in the valley region. In particular a so-called phonon echo in the valley region has been identified with electrons which emits an optical-phonon emission while tunneling. Thirty, Thirty-one Such inelastic resonant tunneling has been the focus of several theory investigations, see for example Refs. Thirty-seven, Thirty-eight, Forty, Forty-one, Forty-two, Forty-three.

On the other hand, there is a large difference between the current flow at resonant conditions and in the valley current. Thus if, in a two-level resonant-tunneling structure, one can achieve both of the following conditions

$$\phi_L \leq E_2 \leq \mu_L, \quad (11)$$
$$\phi_L > E_1 > \mu_R, \quad (12)$$

one has at the same time a large current injection $\Gamma_e$ into upper level $E_2$ but only an insignificant current injection into $E_1$. Moreover, the condition, $E_1 > \mu_R$, ensures a fast tunneling escape rate $\Gamma_{e1}$ out from lower-level $E_1$ and the (almost) exclusive upper-subband current injection may then provide a finite intersubband population and far-infrared stimulated emission. This is particularly so in the
Figure 1.1 tunneling structure where achieving the conditions Eqs. (11) and (12) requires just a moderate voltage drop, $V \approx 12-30$ mV, and in particular the optical-phonon emission remains thermally activated.

I.C Intersubband population inversion in two-level tunneling structure

Figure 1.3 illustrates the (voltage-drop) dependent intersubband optical response of the Figure 1.1 two-level tunneling structure. The top panel shows the level positions, $E_1$ and $E_2$, and the emitter/collector Fermi sea (from lower band edge $\phi_{L/R}$ to chemical potential $\mu_{L/R}$) in equilibrium where only the lower level $E_1$ is occupied. As indicated by the solid upwards arrow, the tunneling structure will in equilibrium provide a significant intersubband absorption.

However, as illustrated in the bottom panel of Figure 1.4, the Figure 1.1 tunneling structure requires just a moderate voltage drop ($V \approx 12$ mV) to achieve the conditions, Eqs. (11) and (12), for the exclusive upper-subband current-injection. As we shall eventually demonstrate, the current injection may then maintain a finite population inversion in spite of a significant decay. As a consequence there will be a significant intersubband stimulated emission (indicated by the solid downward arrow) at a frequency $\omega_\Delta$ given by the subband separation $\Delta = E_2 - E_1$.

The bottom two panels of Figure 1.4 illustrate the scattering processes contributing to the total nonradiative* intersubband decay $\gamma_{nr}$. In particular the solid arrow in the bottom left panel illustrates the elastic impurity and interface-defect

* We consider the quantum-cascade-laser design in the absence of any external radiation and in particular below a possible threshold condition.
FIGURE 1.3 Schematics of intersubband optical response of the two-level resonant-tunneling structure shown in Figure 1.1. The top panel illustrate the equilibrium situation. Only the lower level (with equilibrium position $E^0_1$) is then occupied and the system exhibits a resonantly enhanced absorption (solid upward arrow) at a frequency given by the equilibrium subband separation $\Delta(V = 0) = E^0_2 - E^0_1$. The bottom panel illustrate that it takes only a moderate voltage drop ($V \gtrsim 12\text{ mV}$) to position the upper level within the emitter Fermi sea, $\phi_L < E_2 < \mu_L$, and the lower level below the emitter band edge but above the collector Fermi surface, $\phi_L > E_1 > \mu_R$. As a consequence there is then both an exclusive upper-subband current injection (left dashed-double-dotted arrow) and fast tunneling escape rates (right dashed-dotted arrows) out from both upper and lower resonant levels $E_2$ and $E_1$. The current injection may then provide a finite current population inversion which can result in a significant, resonantly enhanced, stimulated emission (solid downward arrow) at a frequency $\omega_\Delta$ given by the subband separation $\Delta = E_2 - E_1$, see also top panel of Figure 1.4.
Absorption

\[ \mu_L \rightarrow \mu_R \]
\[ \varphi_L \rightarrow \varphi_R \]

Emission

\[ \mu_L \rightarrow \mu_R \]
\[ \varphi_L \rightarrow \varphi_R \]

FIGURE 1.3
FIGURE 1.4 Intersubband scattering event, bottom two panels, and resonantly enhanced intersubband stimulated emission with an exclusive upper-subband current injection, top panel. The solid arrow in the bottom left panel illustrate the intersubband decay due to impurity and interface defect scattering. The dashed-dotted arrow, also in the bottom left panel, illustrate that the decay due to acoustic-phonon can be considered as essentially elastic (the actual average energy transfer is $\sim 0.5 \text{ meV} \ll \Delta$ and the panel shows a very exaggerated electron-acoustic-phonon energy-transfer for clarity.) The pair of opposite transition arrows in the bottom right panel illustrate the nonequilibrium electron-electron scattering (also illustrated in top panel of Figure 1.1.) Finally, the top panel explain why the intersubband optical transitions is resonantly enhanced around single frequency, $\omega_{\Delta} \sim \Delta$, because of the vanishing optical in-plane momentum transfer and because the subbands are described by parallel parabolae. It is, as a consequence, possible for a moderate upper-subband occupation density $\sim 10^{11} \text{ cm}^{-2}$ (dotted dispersion curve,) injected ($\Gamma_e$) below emitter chemical potential $\mu_L$, to provide a significant intersubband stimulated emission.
FIGURE 1.4
scattering, the dashed arrow also in the bottom left panel illustrates the almost elastic electron acoustic-phonon scattering, and finally the pair of opposite solid transition arrows in the lower right panel illustrates a nonequilibrium electron-electron scattering event (also illustrated in the top panel of Figure 1.1.) This total nonradiative decay $\gamma_{nr} = \gamma_{nr}(n_2, n_1)$ will in general depend on the upper- and lower-subband occupation densities, $n_2$ and $n_1$.

Generalizing the rate equation, Eq. (5), we may estimate the resulting upper- and lower-subband occupation densities, $n_2$ and $n_1$, from the two-level rate equation

$$\frac{dn_2}{dt} = (N_L - n_2)\Gamma_e - n_2\Gamma_{c2} - \gamma_{nr}(n_1, n_2), \tag{13}$$

$$\frac{dn_1}{dt} = -n_1\Gamma_{c1} + \gamma_{nr}(n_1, n_2), \tag{14}$$

involving the total nonradiative decay $\gamma_{nr}$, the current injection rate $\Gamma_e$, and the tunneling escape rates $\Gamma_{c1}$ and $\Gamma_{c2}$ out from level $E_1$ and $E_2$, respectively. In this two-level rate equation the maximum upper-subband occupation density, $N_L$, is given by

$$N_L = \frac{2m^*_e(E_2 - \phi_L)}{2\pi} \sim 10^{11} \text{ cm}^{-2}, \tag{15}$$

in complete analogy with the single-level case, see Eq. (4).

Assuming first that the intersubband decay is linear in $n_2$, we introduce an intersubband decay rate, $\Gamma_{nr}$, defined by

$$\gamma_{nr} \equiv n_2\Gamma_{nr}. \tag{16}$$

Inserting this assumption in the two-level rate-equation, Eqs. (13) and (14), we find the steady-state occupation densities

$$n_2 = N_L \frac{\Gamma_e}{\Gamma_e + \Gamma_{c2} + \Gamma_{nr}}, \tag{17}$$

$$n_1 = N_L \frac{\Gamma_e \Gamma_{nr}}{(\Gamma_e + \Gamma_{c2} + \Gamma_{nr})\Gamma_{c1}}. \tag{18}$$
The resulting steady-state intersubband population inversion and current density are

\[ \Delta n \equiv (n_2 - n_1) = n_2(1 - \frac{\Gamma_{nr}}{\Gamma_{c1}}), \]
\[ J \equiv e\Gamma_e(N_L - n_2) = e\Gamma_eN_L\frac{\Gamma_{c2} + \Gamma_{nr}}{\Gamma_e + \Gamma_{c2} + \Gamma_{nr}}. \]

In particular, we observe that maintaining population inversion requires that the lower-level escape rate \( \Gamma_{c1} \) exceeds the intersubband decay rate \( \Gamma_{nr} \).

For the potential shown in Figure 1.1 we estimate tunneling escape rates as follows. The voltage drop \( V_{sym} = 22.9 \text{ mV} \) positions the upper (lower) quasibound-resonant level at \( E_2 \approx 51 \text{ meV} \) (\( E_1 \approx 40 \text{ meV} \)) and the lower collector emitter at \( \phi_L \approx 25 \text{ meV} \) (relative to the GaAs potential at \( V = 0 \)). Assuming a \( L_B = 30 \text{ Å} \) (\( \phi_B = 214 \text{ meV} \)) barrier width (barrier potential height) we estimate (from Eqs. (8) and (10)) the tunneling escape rates

\[ \Gamma_{c2}^s \approx 1.0 \text{ meV}, \]
\[ \Gamma_{c1}^s \approx 0.5 \text{ meV}. \]

If the total nonradiative decay rate \( \Gamma_{nr} \) was bounded by the recent experimental observation of just a small decay rate, \( 1/\tau \leq 0.03 \text{ meV} \) (at temperatures \( T \leq 50 \text{ K} \)) it would be straightforward to maintain a finite population inversion \( \gg 10^{11} \text{ cm}^{-2} \). Unfortunately we find that the nonequilibrium current injection results in a very significant nonequilibrium electron-electron scattering which significantly reduces the resulting population inversion and which is the main focus of the dissertation.
In this final section we discuss the resulting intersubband stimulated emission. In particular we explain how an intersubband population inversion of \( \sim 10^{11} \text{ cm}^{-2} \) can provide a significant stimulated emission because (a) the optical transitions occur around a single frequency \( \omega_\Delta \) set by the subband separation \( \Delta = E_2 - E_1 \), and (b) the confinement within the quantum-well structure results in very large optical transition matrix elements.

For a detailed account of the intersubband stimulated emission it is necessary to again consider the electron motion parallel to the heterostructure layers, i.e., perpendicular to the current flow. In the absence of any scattering, this in-plane motion is independent of the electron tunneling and can be characterized by a (two-dimensional) momentum \( \vec{k} \) and dispersion

\[
E_{||}(\vec{k}) = \frac{k^2}{2m_e^*}.
\]  

Both the upper and lower levels thus give rise to a subband of states

\[
\langle x; \vec{p} | \Psi_{2(1)}; \vec{k} \rangle = \frac{1}{\sqrt{A}} e^{i\vec{k} \cdot \vec{p}} \Psi_{2(1)}(x)
\]  

with energies

\[
E_{2(1)}(k) = E_{2(1)} + E_{||}(k),
\]  

illustrated by the pair of parabolas in the top panel of Fig. 1.4. We assume for simplicity that the fast lower-subband escape rate \( (\Gamma_{c1}) \) ensures a vanishing lower-subband occupation, whereas the exclusive upper-subband current injection \( (\Gamma_e) \) provides the finite upper-subband occupation (dotted dispersion curve in Figure 1.4) \( n_2 = \Delta n \sim 10^{11} \text{ cm}^{-2} \).
The intersubband optical transitions are described by dipole matrix elements

\[
\langle \Psi_1; \vec{k}_f | x | \Psi_2; \vec{k}_i \rangle = \delta_{\vec{k}_f, \vec{k}_i} \langle \Psi_1 | x | \Psi_2 \rangle, \tag{26}
\]

\[
\langle \Psi_1 | x | \Psi_2 \rangle \equiv \int \Psi_1(x) x \Psi_2(x) dx \tag{27}
\]

with a vanishing in-plane momentum transfer. Hence, as illustrated by the set of downward optical transition arrows in Figure 1.4, all upper-subband electrons will contribute to the stimulated at a frequency \(\omega_\Delta \sim \Delta\). This is in contrast with the standard inter-band semiconductor laser where the population inversion is distributed over a range of possible transition energies, see Refs. 44, 45.

In addition, the quantum-confinement provides very large numerical values of the optical transitions matrix elements, Eq. (27). In fact for the Figure 1.1 tunneling structure the quantum confinement results in a very significant oscillator strength,

\[
f_{21} = 2m^*_e \Delta |\langle \Psi_2 | x | \Psi_1 \rangle|^2 \approx 0.46 \tag{28}
\]

with dipole matrix element \(\langle \Psi_2 | x | \Psi_1 \rangle \approx 50 \text{ Å}\). A correspondingly large oscillator strength, and the fact that the optical transition is concentrated around one transition frequency, allows just a \(\Delta n \sim 10^{11} \text{ cm}^{-2}\) population inversion density in the mid-infrared quantum cascade laser\(^1\),\(^3\),\(^2\) to provide a significant stimulated emission and actual lasing.
REFERENCES


 CHAPTER II

THE MID-INFRARED QUANTUM CASCADE LASER

In this chapter we discuss in detail the seminal achievement by Dr. F. Capasso and his collaborators J. Faist, D. L. Sivco, C. Sirtori, A. L. Hutchinson, and A. Y. Cho of intersubband population inversion and net stimulated emission (gain) in the mid-infrared quantum cascade laser.\textsuperscript{1,2,3}

The entire quantum-cascade-laser heterostructure, grown on a $n^+$-doped substrate, comprises a total of more than 500 AlInAs and GaInAs semiconductor layers. A net stimulated emission results in a set of 25 optically-active tunneling regions separated by so-called injector layers. These injector layers serve, at threshold condition (only,) as emitter and collector leads for the active tunneling regions whose working principle is as discussed in Section I.C.

The optically active 25-period superlattice of tunneling regions and interjacent injector layers is located within a waveguide core formed by surrounding cladding layers with a lower index of refraction. The variation of the index of refraction within the quantum cascade laser is designed to achieve a significant concentration of the lasing mode intensity within the optically active superlattice and thus increase the effective gain. In addition, the waveguide confinement also prevents a potential
dramatic (plasmon) reabsorption in the heavily-doped top contact layers and in the InP substrate.

The lasing frequency $\omega_\Delta$ is given by the mid-infrared (conduction-)subband separation $\Delta = 295 \text{ meV}$ between two optically active quasi-bound states of the tunneling regions. This lasing frequency corresponds to the (vacuum) wavelength, $\lambda_\Delta = 4.26 \mu\text{m}$, that is, within one of the infrared transmission windows of the atmosphere. In addition, spontaneous intersubband emission at wavelengths, $\lambda \approx 10 \mu\text{m}$ (in the other infrared atmospheric window,) has also been reported in a modified quantum-cascade-laser design.

In the original\(^1\) (subsequent\(^3\)) 12 $\mu\text{m} \times 0.72 \text{ mm} \ (14 \ \mu\text{m} \times 1.2 \text{ mm})$ cleaved mesa cavity realization the mid-infrared quantum cascade laser produced a peak optical power of 8.5 (30) mW in 20 (80) ns current pulses with repetition frequency 1 (50) kHz and with a threshold heat loss $P_{th} \sim 4 \text{ W}$. A recent paper\(^5\) reports an even better performance within a slightly modified mid-infrared quantum-cascade-laser design. In addition, the seminal achievement of actual intersubband lasing\(^1,2,3\) have fostered interest in the quantum-cascade-laser design also at QUEST, University of California, Santa Barbara, see for example Ref. 6.

The outline of this chapter is as follows. We first describe the chemical composition of the quantum-cascade-laser heterostructure\(^1,2,3\) in general and of the optically active superlattice in particular. We explain how the digitally-graded-alloy injector layers can serve as emitter (and collector) leads for the (optically active) tunneling regions at and around the threshold conditions. Following the discussion in Section I.C we obtain a simple description of the current flow and estimate the resulting population inversion. We also discuss the threshold conditions which in particu-
lar require that the voltage drop across each superlattice period exceeds the lasing frequency, $\omega_{\Delta} \sim 295 \text{ meV}$.

In addition we describe a theory-estimate\textsuperscript{3} for the peak material gain, that is, the gain which would arise if the lasing mode is traveling within a (hypothetical) infinite superlattice of back-to-back tunneling regions and interjacent injector layers. We discuss the waveguide confinement which results from the variation of the index of refraction within the quantum-cascade-laser heterostructure, and explain how this confinement both increases the peak effective gain and limits the internal reabsorption. We furthermore compare threshold estimates for the effective gain with the internal loss and with the estimated rate by which the (stimulated) intersubband radiation escapes the lasing cavity.

II.A Chemical composition and tunneling potential

The quantum-cascade-laser heterostructure comprises a total of more than 500 alternating Ga\textsubscript{0.48}In\textsubscript{0.52}As and Al\textsubscript{0.47}In\textsubscript{0.53}As layers, grown on an InP substrate. It provides a net mid-infrared intersubband gain (at 295 meV) in just a 25-period superlattice of optically active tunneling regions and interjacent so-called injector layers. A build-in waveguide formed by layers with a low index of refraction partially confines the emitted radiation and increases the effective gain. This waveguide confinement also prevents a potentially dramatic (plasmon) reabsorption in the top heavily-doped contact layers or in the $n^+$-doped InP substrate.

Table 2.1, reproduced from Table 1 of Ref. 1, shows the chemical compositions on a course-grained level. Specifically, the structure comprises a central waveguide core region which includes a 25-periods superlattice (entry listed $\times 25$) formed by
TABLE 2.1 Overall chemical composition of the quantum-cascade-laser heterostructure formed by more than 500 alternating layers of Ga$_{0.48}$In$_{0.52}$As and Al$_{0.47}$In$_{0.53}$As. The structure provides a net mid-infrared intersubband gain in just 25 periods of optically active regions with neighboring injector layers. Table 2.2 list the chemical composition of the active regions and Figure 2.2 shows schematics of resulting tunneling potential inside this optically active superlattice which is here represented by the single entry marked ‘×25.’ The injector layers themselves comprises a multitude of layers (not listed here,) resulting in a graded effective potential designed to counter the large internal field necessary to achieve threshold conditions, see text. The optically active superlattice is located within a waveguide core with a larger effective index of refraction, $n_{\text{mode}} = 3.26$, than for the surrounding AlInAs waveguide-cladding layers described by $n_{\text{clad}} \approx 3.15$. This difference in index of refraction is increased by the inclusion in the waveguide core of two 3000 Å GaInAs layers. The variation in the index of refraction provides a partial confinement of the lasing mode within the waveguide core (see panel (a) of Figure 2.1) and thus concentrates the intensity within the optically active superlattice where the lasing mode can further stimulate the intersubband transitions. Finally, the structure includes set of top contact layers which are heavily $n$-doped to prevent a large contact resistance and hence a significant power dissipation by the necessary strong threshold current (listed in Table 2.3.)
<table>
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<th>Material</th>
<th>Doping [cm$^{-3}$]</th>
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<td>10000</td>
</tr>
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</tbody>
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TABLE 2.2 Chemical composition, potential, effective electron mass, and individual layer thickness of the optically active regions within the quantum-cascade-laser heterostructure. These triple-quantum-well resonant-tunneling regions (with effective potential shown in Figure 2.2) comprises alternating layers of AlInAs and GaInAs with effective electron masses $m_e^*$ given in terms of the free-electron mass $m_0$. Note the very large conduction-band discontinuity, 520 meV, between the AlInAs and the GaInAs layers allows a triple-quantum-well potential which can confine the energetic upper resonant level $E_4$ in the very narrow (8 Å) first quantum-well, see Figure 2.2.
<table>
<thead>
<tr>
<th>Description</th>
<th>Active region</th>
<th>Effective potential</th>
<th>$m^*_e/m_0$</th>
<th>Layer thickness [Å]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Emitter tunneling barrier</td>
<td>Al$<em>{0.48}$In$</em>{0.52}$As</td>
<td>520 meV</td>
<td>0.078</td>
<td>45</td>
</tr>
<tr>
<td>First (level $E_4$) quantum well</td>
<td>Ga$<em>{0.47}$In$</em>{0.53}$As</td>
<td>0 meV</td>
<td>0.043</td>
<td>8</td>
</tr>
<tr>
<td>Second tunneling barrier</td>
<td>Al$<em>{0.48}$In$</em>{0.52}$As</td>
<td>520 meV</td>
<td>0.078</td>
<td>35</td>
</tr>
<tr>
<td>Second quantum well</td>
<td>Ga$<em>{0.47}$In$</em>{0.53}$As</td>
<td>0 meV</td>
<td>0.043</td>
<td>35</td>
</tr>
<tr>
<td>Third tunneling barrier</td>
<td>Al$<em>{0.48}$In$</em>{0.52}$As</td>
<td>520 meV</td>
<td>0.078</td>
<td>30</td>
</tr>
<tr>
<td>Third quantum well</td>
<td>Ga$<em>{0.47}$In$</em>{0.53}$As</td>
<td>0 meV</td>
<td>0.043</td>
<td>28</td>
</tr>
<tr>
<td>Collector tunneling barrier</td>
<td>Al$<em>{0.48}$In$</em>{0.52}$As</td>
<td>520 meV</td>
<td>0.078</td>
<td>30</td>
</tr>
</tbody>
</table>

§ As specified in Figure 1 of Ref. 3.
optically active tunneling regions and neighboring so-called injector layer. Table 2.2 list the detailed chemical composition of the optically active triple-quantum-well tunneling regions.

The waveguide core also includes two 3000 Å GaInAs layers which serve to increase the effective index of refraction, \( n_{\text{mode}} = 3.26 \), of the waveguide core compared with the value, \( n_{\text{clad}} \approx 3.15 \), for the surrounding waveguide-cladding layers of AlInAs. This variation of the index of refraction results in a partial waveguide confinement of the lasing mode which increases the effective gain, see Section II.D.

Finally the quantum-cascade-laser heterostructure includes a set of top contact layers. All of these layers are heavily n-doped to prevent a large contact resistance and thus a significant power dissipation by the necessary strong threshold current flow. The partial waveguide confinement prevent a potentially dramatic (plasmon) reabsorption in these top contact layers and in the n\(^+\)-doped InP substrate.

The bottom panel (b) of Figure 2.1 shows the detailed conduction-band potential of the superlattice of optically active triple-quantum-well tunneling regions (identified by the set of four thicker tunneling barriers) and the interjacent injector layers. Also shown are moduli squared of (quasi-bound) wavefunctions 2–4 (mostly contained within triple-quantum-well tunneling region) and 0–1 (extending throughout the injector layers.) The intersubband lasing results at \( \omega_\Delta \approx 295 \text{ meV} \) from stimulated emission between quasi-bound levels 4 and 3 (formed as a combination of 3' and 3") within the tunneling regions.

We emphasize that the injector layers are themselves formed as a digital alloy, that is, by alternating AlInAs and GaInAs layers. A spacial grading of the relative thickness of the AlInAs and GaInAs layers ensures — at the threshold internal
FIGURE 2.1 [Reproduced with kind permission from Ref. 3] Detailed tunneling potential for superlattice of optically active regions with interjacent digital-alloy injection layers (panel (b)) and partial confinement of resulting lasing mode (panel (a).) The bottom panel (b) shows detailed design of both optically active regions (identified by set of four thicker tunneling barriers) and of digital-alloy injector layers [with voltage drop shown right to left — opposite convention used elsewhere in dissertation.] The panel (b) also shows the moduli squared of the quasi-bound wavefunctions either (mostly) confined in the $(LQB = 211 \text{ Å})$ active region (curves denoted 2-4) or extended throughout the $(Linj = 186 \text{ Å})$ injection layers (curves denoted 0 and 1.) The optical transition occurs from level 4 to level 3 (arising as a linear combination of shown wavefunction moduli squared 3' and 3'') The schematic in Figure 2.2 explains the current flow within each superlattice period. A repeated upper-subband current injection in all periods of the superlattice requires a strong internal field, $F_{dc} \sim 100 \text{ kV/cm}$, so that the potential drop $eF_{dc} \times (LQB + Linj)$ across each superlattice period is slightly larger than the optical transition frequency $\omega_\Delta \approx \Delta = E_4 - E_3 \approx 295 \text{ meV}$. A fast current transport within the injector layers is nevertheless possible because the digital grading, as shown here, ensures a large density of extended states (spaghetti of wavefunction moduli squared) exactly at the shown energies for the threshold internal field $F_{dc}$. The top panel (a) (or insert) shows how the waveguide cladding layers provides a finite confinement of the lasing mode intensity (left axis) in the waveguide core due to the variation of the effective index of refraction (right axis.) This confinement, discussed further in Figure 2.3, concentrates a significant fraction, $\Phi \sim 0.5,$ of the lasing-mode intensity within the optically active superlattice (denoted ‘MQW’) and thus increases the effective gain. In addition, the confinement prevents a potentially dramatic (plasmon) reabsorption in the heavily-doped top contact layers and in the substrate.
FIGURE 2.1
field $F_{dc} \sim 100 \text{ kV/cm}$ with illustrated resulting potential (only) — a fast electron transport between the triple-quantum-well tunneling regions. In particular, the large density of injector-layer states (spaghetti of moduli squared wavefunctions) is by design positioned exactly to allow a fast exit out from level 3 of the upstream tunneling region and a strong current injection into level 4 of the downstream tunneling region. In effect, the injector layers serve (at threshold conditions only) as both emitter and collector leads for the tunneling regions whose working principle is thus as described in Section I.C.

Consider finally the top panel (a) (or insert) of Figure 2.1 which illustrates how the lower (average) index of refraction (right axis) of the waveguide cladding layers ensures a partial confinement of the lasing mode (left axis) within the waveguide core. This waveguide confinement, explained schematically in Section II.D below, concentrates a significant fraction, $\Phi \sim 0.5$, of the lasing-mode intensity within the optically active superlattice (denoted ‘MQW’) and thus increases the effective gain. In addition, the confinement prevents a potentially dramatic (plasmon) reabsorption in the heavily-doped top contact layers and in the substrate.

II.B The threshold current flow and power dissipation

The bottom panel of Figure 2.2 shows schematics of the effective tunneling potential and current flow within the optically active superlattice at threshold conditions. The detailed potential within the injector layers (shown in Figure 2.1) is here in Figure 2.2 substituted by an effective potential (dotted lines) formed as the weighted average of the individual AlInAs and GaInAs layer in the digital alloy. The spacial variation of the detailed injector-layer compositions results — in
FIGURE 2.2 Schematics of threshold current flow within active tunneling regions and through injector layers (bottom panel) realized by build-in grading of effective injector-layer potential (dotted lines in top panel.) The detailed realization of this effective tunneling potential as a digital allow is shown in Figure 2.1. The lasing transition, indicated by wavy arrow in bottom panel, results between levels $E_4$ and $E_3$. The lasing threshold requires a significant internal field, $F_{dc} \sim 100$ kV/cm, to ensure a repeated current injection ($\Gamma_e \approx 3$ meV, estimated in Ref. 1) exclusively into the top optically active level 4 of subsequent active tunneling regions, see text. The digital grading of the injector layers (dotted lines in top panel) is designed to cancel this strong applied field and provide an almost constant effective injector-layer potential indicated by the dotted lines in bottom panel. The flat effective potential provides a finite density of extended states in the injector layers (as shown in Figure 2.1) which thus serves as both emitter and injector leads. The large density of extended states results in particular in a fast effective escape rate ($\Gamma_{cB} \sim 1.0$ meV, see Ref. 1) out from lower optically active level $E_3$ (via an optical-phonon emission to level $E_2$.) However, only a small escape rate ($\Gamma_{cA} \sim 0.1$ meV, see again Ref. 1) results for upper level $E_4$. 
FIGURE 2.2

<table>
<thead>
<tr>
<th>Undoped</th>
<th>n-doped</th>
<th>Undoped</th>
</tr>
</thead>
<tbody>
<tr>
<td>Active Region</td>
<td>Digitally Graded Injector</td>
<td>Active Region</td>
</tr>
<tr>
<td>('Lead')</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
the absence of an internal field — in the graded (or sawtooth) effective potential illustrated by dotted lines in the top panel.

The lasing transition, indicated by wavy arrow in bottom panel, results between levels $E_4$ and $E_3$ with frequency $\omega_D \approx \Delta \equiv E_4 - E_3$. The lasing threshold requires (a) a strong current injection $\Gamma_e$ into upper level $E_4$, and (b) a fast (effective) lower-level escape rate $\Gamma_{cB}$ out from lower optically active level $E_3$ throughout the 25 period superlattice.

An electron leaving lower level $E_3$ in an upstream active region [to the left of central injector layer in Figure 2.2] must in particular be able to enter to the upper-level $E_4$ in the downstream neighboring-period active region [to the right in Figure 2.2] as illustrated in Figure 2.2. The lasing threshold thus requires a significant internal field, $F_{dc} \sim 100 \text{ kV/cm}$, to ensure that the potential drop across one superlattice period, $(L_{QB} + L_{Inj})$, exceeds the optical transition energy, $F_{dc} \times (L_{QB} + L_{Inj}) > \omega_D$, and thus allows the repeated current injection.

The digital grading of the injector layers (illustrated in the top panel) is designed to cancel this strong necessary internal field and provide an almost flat effective injector-layer potential (dotted lines in bottom panel) around the actual threshold conditions (only.) As discussed in Figure 2.1, the digital alloy provides in particular a finite density of states which extend throughout the injector layers. These states allow the injector layers to serve as emitter and collector leads and provides both a fast current injection $\Gamma_e$ into level $E_4$ and a fast (effective) escape rate out from level $E_3$ (via an optical-phonon emission to level $E_2$.) A smaller escape rate $\Gamma_{cA}$, out from upper level $E_4$ results in part because this level must traverse two tunneling barriers to reach the injector layer. Table 2.3 list reported estimates for
these tunneling rates and for the nonradiative intersubband decay rate* $\Gamma_{nr}$.

The working principle of the active regions (near threshold conditions) are as discussed in Section I.C with the injector layers serving as emitter and collector leads. We may in particular estimate the (threshold) current flow from the two-level rate equation

$$\frac{dn_A}{dt} = (N_L - n_A)\Gamma_e - n_A\Gamma_{cA} - n_A\Gamma_{nr}, \quad (1)$$

$$\frac{dn_B}{dt} = -n_B\Gamma_{cB} + n_A\Gamma_{nr}. \quad (2)$$

where the maximum upper-subband occupation density, $N_L \sim 1.5 \times 10^{11}$ cm$^{-2}$ (as listed in Table 2.3) may be estimated as follows. Denoting the lower-band edge of the injector layer $\phi_L$ and assuming a quasi-Fermi level $\mu_L$ determined by the $N_{3D} = 1.5 \times 10^{17}$ cm$^{-3}$ injector-layer doping concentration yields $\mu_L - \phi_L \sim 10$ meV. Within the quantum-well we use the low effective electron mass, $m^*_e = 0.043m_0$, and find that the value $\mu_L - E_2 \sim 10$ meV corresponds to $N_L \sim 1.5 \times 10^{11}$ cm$^{-3}$.

The steady-state solution of the rate equation, Eqs. (1) and (2), yields a resulting current density

$$J = e\Gamma_e N_L \frac{\Gamma_{cA} + \Gamma_{nr}}{\Gamma_e + \Gamma_{cA} + \Gamma_{nr}}, \quad (3)$$

and population inversion

$$\Delta n = \frac{J}{e(\Gamma_{cA} + \Gamma_{nr})} \left(1 - \frac{\Gamma_{nr}}{\Gamma_{cB}}\right). \quad (4)$$

* This nonradiative intersubband decay is ascribed$^1$ to optical-phonon-emission processes. In contrast to the strong optical-phonon induced decay $E_3 \rightarrow E_2$ (which helps provides the fast effective escape rate out from quasi-bound level $E_3$,) the transition $E_4 \rightarrow E_3$ is not resonant with the optical-phonon frequency. The nonradiative optical-phonon induced decay $E_4 \rightarrow E_3$ is thus characterized by a large in-plane momentum transfer which ensures just a moderate value of the electron-optical-phonon interaction matrix element (given for example in Ref. 8) and a small value,$^1$ $\Gamma_{nr} \sim 0.15$ meV, for the estimated decay.
TABLE 2.3 Physical characteristics of the mid-infrared quantum cascade laser realized both as a 12 μm x 0.72 mm cleaved mesa\(^1\) (information indicated by †) and as a 14 μm x 1.2 mm cleaved mesa\(^3\) (information indicated by ‡.) A significant internal electric field, \(F_{dc} \sim 100\) kV/cm, is required to achieve the threshold/lasing conditions with a fast current injection exclusively into upper subband \(E_4\) of the active regions. At such internal fields the \(L_{inj} = 186\) Å wide injector ('L') can serve as an emitter lead with quasi-Fermi sea of thickness, \(\mu_L - \phi_L \sim 10\) meV given by the injector layer doping concentration \(N_{3D} = 1.5 \times 10^{17}\) cm\(^{-3}\). The resonant-tunneling current injection may thus provide a population inversion density bounded by \(N_L = 1.5 \times 10^{11}\) cm\(^{-2}\), with the actual threshold population inversion being determined by the listed estimates for current injection rate \(\Gamma_c\), tunneling escape rates, \(\Gamma_{cA}\), and \(\Gamma_{cB}\), and and nonradiative intersubband decay rate \(\Gamma_{nr} \sim 0.15\) meV. The table also described the threshold current flow and large applied bias (given by the necessary strong threshold internal field \(F_{dc}\).) The significant resulting power dissipation caused the original realizations of the quantum cascade laser to be operated in pulsed mode.\(^9\) Finally the table also documents the increase of peak optical power which results with the longer mesa realization, Ref. 3. This increase arises in part because of the smaller cavity emission rate, \(\alpha_M\), see Table 2.4.
## TABLE 2.3

| Description: | Symbol | Quantum Cascade Laser

<table>
<thead>
<tr>
<th>Configuration:</th>
<th>12 µm × 0.72 mm (14 µm × 1.2 mm) mesa</th>
</tr>
</thead>
<tbody>
<tr>
<td>Threshold internal field</td>
<td>( F_{dc} )</td>
</tr>
</tbody>
</table>

| Width of active regions | \( L_{QB} \) | 211 Å |
| Width of injector layers | \( L_{Inj} \) | 186 Å |
| Injector doping density | \( N_{3D} \) | \( 1.5 \times 10^{17} \) cm\(^{-3}\) |
| Injector Fermi sea | \( \mu_L - \phi_L \) | \( \sim 10 \) meV |
| Density of tunneling states | \( N_L \) | \( \sim 1.5 \times 10^{11} \) cm\(^{-2}\) |

| Emitter tunneling-in rate | \( \Gamma_e \) | \( \sim 3 \) meV |
| Upper level escape rate | \( \Gamma_{eA} \) | \( \sim 0.1 \) meV |
| Lower level escape rate | \( \Gamma_{eB} \) | \( \sim 1 \) meV |
| Nonradiative decay rate | \( \Gamma_{nr} \) | \( \sim 0.15 \) meV |

| Threshold current density | \( J_{th} \) | 11 (5.35) kA/cm\(^2\) |
| Threshold current | \( I_{th} \) | 0.95 (0.9) A |
| Threshold applied bias | \( V_{th} \) | 8 (9.4) V |
| Threshold power dissipation | \( P_{th} \) | \( \approx 3.8 \) (4.2) W |
| Pulse duration | — | 20 (80) ns |
| Repetition frequency | — | 1 (50) kHz |
| Peak optical power | — | \( \gtrsim 8.5 \) (30) mW |

\( \dag(\ddagger) \) Reported in Ref. 1 (Ref. 3).

\( \S(\|) \) Listed (estimated) under threshold/lasing conditions.
The lasing threshold arises when the intersubband stimulated emission resulting from the population inversion, Eq. (4), exceeds both the internal loss and the rate of emission from the lasing cavity, see Section II.E.

The original two realizations were formed as a 12 \( \mu \text{m} \times 0.72 \text{ mm} \) (reported in Ref. 1) and a 14 \( \mu \text{m} \times 1.2 \text{ mm} \) (reported in Ref. 3) etched mesa with cleaved ends serving as cavity mirrors. For these structures the lasing threshold did require a very significant threshold current density, \( J_{th} \), and also actual current flows, \( I_{th} \approx 0.9 \text{ A} \), as listed in Table 2.3. Because furthermore, a large threshold bias, \( V_{th} \approx 8 \text{ V} \), is mandated by the necessary large internal field, \( F_{dc} \approx 100 \text{ kV/cm} \), such large current flows results in a very significant threshold power dissipation \( P_{th} \approx 4 \text{ W} \). As a consequence, the first realizations of the quantum cascade laser was thus operated in the pulsed operation modes described in Table 2.4.\(^9\)

Finally we emphasize a potential technological advantage\(^3,10\) of the intersubband optical transitions in the quantum cascade laser, namely the observed small temperature-dependence of the threshold current.\(^3\) The threshold current in standard inter-band semiconductor laser\(^11,12\) exhibit a finite temperature variation.\(^13\) This variation results in part because the spontaneous and stimulated emission involves electrons (holes) distributed within a positive-(negative-)mass conduction (valence) band and can occur at all frequencies larger than the band gap. Only a fraction of the total population inversion contributes to the actual lasing mode and this fraction decreases with temperature (as the electrons and holes are heated to more energetic conduction- and valence-band states respectively.) A higher temperature thus forces a larger total population inversion and a larger threshold current (which we assume is given by the combined nonradiative and radiative electron-hole
combination rate for the total population inversion.)

In contrast, one expects a smaller threshold-current temperature dependence in the quantum-cascade-laser design because the intersubband spontaneous and stimulated emission are concentrated around just a single (lasing) frequency $\omega_\Delta \sim \Delta$. In particular, the contribution to the stimulated emission at $\omega_\Delta$ from an upper-subband electron is (almost) independent of the initial in-plane momentum and is not (significantly) affected by a thermal smearing of the upper- and lower-subband electron distributions.

In practice some temperature dependence of the intersubband threshold current does result because (a) the enhanced optical emission rate reduces the population inversion, (b) the enhanced intra- and inter-subband scattering increases the linewidth of the luminescence spectra and thus reduces the peak gain (see Section II.C) and because (c) the tunneling escape rate out from the lower optically active level decreases with temperature since some of the final collector states becomes occupied. Nevertheless, the threshold-current temperature dependence of the intersubband quantum cascade laser remains small at $T \lesssim 100$ K, as shown in the top insert of Figure 3 in Ref. 3.

II.C The peak material gain

The material gain is defined as the stimulated emission rate for the lasing mode if traveling exclusively within a superlattice of optically active tunneling regions and the interjacent injector layers (both described in Section II.A.) We report here a simple estimate of the peak material gain, $\gamma_{\text{mat}}$, based on a theoretical$^3$ deter-
mination of the total spontaneous emission. Our discussion follows essentially the
treatment in Ref. 14.

To estimate the material gain we consider a fictitious material made up entirely
of back-to-back active-region/injector-layer periods. We assume for this material
a homogeneous dielectric constant, $\varepsilon_r = n_r^2$, and describe the electromagnetic field
by the (quantized) vector potential

$$\vec{A}(\vec{r}, t) = \sum_{\vec{q}, \eta} \left( \frac{2\pi c^2}{L^3 \omega \varepsilon_r} \right)^{1/2} \vec{\xi}(\vec{q}, \eta) \times \exp(i\vec{q} \cdot \vec{r}) \left[ a_{\vec{q}, \eta} e^{-i\omega t} + \text{h.c.} \right],$$

(5)

where $\vec{\xi}(\vec{q}, \eta)$ denotes the polarization of the cavity mode $(\vec{q}, \eta)$. We consider a bulk
'cavity' of volume $L^3$ where the spacial dimension is $L$ much larger than the wave-
length $\lambda_\Delta \sim 4$ mu of the lasing mode. We also assume Transverse-Electro-Magnetic
(TEM) modes with polarization perpendicular to the direction of propagation.

The optical transition between an initial upper-subband state, $|\Psi_4, \vec{k}_i\rangle$, and a
final lower subband state, $|\Psi_3, \vec{k}_f\rangle$, is described by dipole matrix element

$$\langle \Psi_4, \vec{k}_i | (y, z) | \Psi_3, \vec{k}_f \rangle \propto \langle \Psi_4 | \Psi_3 \rangle = 0,$$

(6)

and

$$\langle \Psi_4, \vec{k}_i | x | \Psi_3, \vec{k}_f \rangle = \delta_{\vec{k}_i, \vec{k}_f} \langle \Psi_4 | x | \Psi_3 \rangle$$

$$= \delta_{\vec{k}_i, \vec{k}_f} \int dx \Psi_4(x) x \Psi_3(x).$$

(7)

where we have ignored the optical in-plane momentum transfer. Within this simpli-
fied description it is thus, for a given radiation mode $(\vec{q}, \eta)$, only the $x$-component
(parallel to the current flow) of the electric field

$$E(\vec{r}, t) = -\frac{1}{c} \frac{\partial A_x}{\partial t} \propto \xi_x(\vec{q}, \eta),$$

(8)

which causes the intersubband transition.
On the other hand, a cavity mode \((\vec{q}, \eta)\) polarized in the \(\hat{x}\)-direction (i.e., with \(\xi_x(\vec{q}, \eta) = 1\)) does result in the very significant interaction

\[
H_{\vec{q}, \eta}(t) = e_x i \sum_{\vec{q}, \eta} \left( \frac{2\pi \omega_{\vec{q}}}{L^3 \omega_{\vec{q}e_r}} \right)^{1/2} \xi_x(\vec{q}, \eta) \left[ a_{\vec{q}, \eta} \exp(-i\omega_{\vec{q}} t) + \text{h.c.} \right].
\]

(9)

In particular, the dipole matrix element characterizing this interaction, Eq. (9), is estimated\(^3\) at \(\langle \Psi_4|x|\Psi_3 \rangle \approx 10 \text{ Å} \) corresponding to a very significant oscillator strength

\[
f_{43} = 2m_e^*(E_4 - E_3)|\langle \Psi_4|x|\Psi_3 \rangle|^2 \approx 0.4.
\]

(10)

Such large (resonant) values of the oscillator strength result because the quantum-confinement concentrates the total oscillator strength on just a few possible optical transitions — an important build-in advantage of intersubband optical transitions which is thus exploited in the quantum-cascade-laser design.

For a single electromagnetic mode \((\vec{q}, \eta)\) of energy \(\omega_{\vec{q}} = |\vec{q}|c/\eta_r\) and containing \(n_{\vec{q}, \eta}\) photons we next evaluate the transition rate between occupied upper-subband initial state \((\Psi_4, \vec{k}_i)\) and empty lower-subband final state \((\Psi_3, \vec{k}_f)\). Using the Fermi golden rule we find

\[
\Gamma_{(\vec{k}_i)}\rightarrow(\vec{k}_f) (n_{\vec{q}, \eta}) = 2\pi \left| \langle \Psi_4, n_{\vec{q}, \eta}|H_{\vec{q}, \eta}(t)|\Psi_3, n_{\vec{q}, \eta} + 1 \rangle \right|^2 \delta_{\vec{k}_i, \vec{k}_f} \delta(\Delta - \omega_{\vec{q}})
\]

(11)

Note that within the above simple treatment the optical transition rate is independent of \(\vec{k}_i = \vec{k}_f\), and in particular independent of any thermal smearing of the upper-subband initial distribution. This observation helps account for the observed small temperature dependence of the threshold current — an potentially technological advantage\(^10\) briefly discussed in Section II.B.

For every pair, \((|\Psi_4, \vec{k}_i|, |\Psi_3, \vec{k}_f|)\), of an occupied upper-subband initial state with a corresponding empty lower-subband final state, we obtain the intersubband
transition rate Eq. (11) as a sum

$$\Gamma_{4\rightarrow3}(\vec{q}, \eta) = \Gamma_{43}^{sp}(\vec{q}, \eta) + \Gamma_{43}^{st}(\vec{q}, \eta),$$  \hspace{1cm} (12)

$$\Gamma_{43}^{sp}(\vec{q}, \eta) = \left(\frac{e^2}{\epsilon_r}\right) |\langle \Psi_4 | x | \Psi_3 \rangle|^2 \frac{(2\pi)^2}{L^3} |\xi_x(\vec{q}, \eta)|^2 \omega_q \delta(\Delta - \omega_q),$$  \hspace{1cm} (13)

$$\Gamma_{43}^{st}(\vec{q}, \eta) = n_{\vec{q}, \eta} \Gamma_{43}^{sp}(\vec{q}, \eta),$$  \hspace{1cm} (14)

of a spontaneous ($\Gamma_{43}^{sp}(\vec{q}, \eta)$) and a stimulated ($\Gamma_{43}^{st}(\vec{q}, \eta)$) emission rate. Using the standard result,

$$\sum_{\eta} \int d\Omega_q \xi_x(\vec{q}, \eta)^2 = \frac{8\pi}{3},$$  \hspace{1cm} (15)

we sum Eq. (13) over all modes inside our $L^3$ cavity and thus estimate the integrated spontaneous emission rate

$$\Gamma_{43}^{sp} = \sum_{\vec{q}, \eta} \Gamma_{43}^{sp}(\vec{q}, \eta)$$

$$= \frac{4}{3} \left(\frac{e^2}{\epsilon_r}\right) \left(\frac{n_r}{c}\right)^3 \Delta^3 |\langle \Psi_4 | x | \Psi_3 \rangle|^2,$$  \hspace{1cm} (16)

expressed in terms of the fine-structure constant $\alpha$, and the (unscaled) Bohr radius and Rydberg, $a_0, \text{Ry}$.

In a simple theoretical estimate of the integrated spontaneous emission rate for the mid-infrared quantum cascade laser we use $\Delta = 295 \text{ meV}$, $\langle \Psi_4 | x | \Psi_3 \rangle = 10 \text{ Å}$, and take for the assumed homogeneous index of refraction $n_r$ the value, $n_r = n_{\text{mode}} = 3.26$, that is, the estimated effective (or average) index of refraction for the lasing mode. Inserting these numbers we find

$$\Gamma_{43}^{sp} = \frac{1}{\tau_{sp}} \approx 3 \times 10^{-5} \text{ meV}.$$  \hspace{1cm} (17)
corresponding to the small spontaneous decay time $\tau_{sp} \approx 14$ ns. This estimate is in good agreement with the value $\tau_R = 13$ ns reported in Ref. 1.

The above results Eqs. (13), (14), and (16) assume that there is only one possible transition energy, namely the subband separation $\Delta$. However, the actual luminescence (i.e., the spontaneous emission) is observed within a distribution of energies,

$$\Gamma_{43}^{sp}(\omega) \equiv \Gamma_{43}^{sp} \frac{a(\omega)}{2\pi},$$

(18)
described by a line-shape function $a(\omega)/2\pi$ normalized to unity. Figure 4 of Ref. 3 shows this line-shape function (see the low-current curve) which is of course still strongly peaked at a frequency $\omega_\Delta$ given by the subband separation $\Delta$. For the quantum cascade laser one can assume a Lorentzian form

$$a(\omega) = \frac{2\Gamma_\phi}{(\omega - \omega_\Delta)^2 + \Gamma_\phi^2},$$

(19)
of with a $2\Gamma_\phi = 22$ meV full-width-half-maximum value at $T = 10$ K, see Ref. 3.

Following Ref. 14 we account for this line-shape of the spontaneous emission rate, Eq. (18), by assuming that $a(\Delta')/2\pi$, describes the distribution of energy differences in the optically active pairs comprising the occupied initial upper-subband state and corresponding empty final lower-subband state. Such a distribution of transition energies arises because (a) the inter- and intra-subband scattering leads to a broadening of both the initial and final subband states, (b) the optical momentum transfer is not exactly zero causing the optical transition energy ($\Delta$) to depend on the initial electron in-plane momentum even when assuming parallel parabolic subbands, and finally because (c) the assumption of such parabolic subbands is only approximate. The large line-width observed in the quantum cascade laser is
in Ref. 3 ascribed primarily to the strong interface scattering in the narrow 8 Å quantum well containing the most energetic level 4.

Rather than Eqs. (13) and (14), the intersubband spontaneous and stimulated emission into mode \( (\vec{q}, \eta) \) may thus be approximated by the averaged rates

\[
\Gamma_{43}^{sp}(\vec{q}, \eta) = \frac{\omega_{\vec{q}}}{L^3} \left( \frac{e^2}{\varepsilon_r} \right) |\langle \Psi_4 | x | \Psi_3 \rangle|^2 2\pi a(\omega_{\vec{q}}),
\]

\[
\Gamma_{43}^{st}(\vec{q}, \eta) = n_{\vec{q}, \eta} \Gamma_{43}^{sp}(\vec{q}, \eta),
\]

arising by integrating Eqs. (13) and (14), respectively, over the assumed distribution of the parameter \( \Delta' \). We note that summing Eq. (20) over all modes of frequency \( \omega \) reproduces the experimentally observed result Eq. (18).

Using the above described heuristic approach we find for the lasing mode polarized in the \( \hat{x} \)-direction and having \( n_\Delta \) photons of frequency \( \omega_\Delta \), a stimulated emission rate

\[
\Gamma_{43}^{st}(n_\Delta) = W_{3D}(n_\Delta) \Gamma_{43}^{sp} \left( \frac{3\pi e^2}{2n_\Delta^2 \omega_\Delta^3} \right) a(\omega_\Delta).
\]

This rate is directly proportional to the total integrated spontaneous emission rate \( \Gamma_{43}^{sp} \) estimated above and to the energy density

\[
W_{3D}(\omega_\Delta) = \frac{n_\Delta \omega_\Delta}{L^3},
\]

of the lasing mode inside the \( L^3 \) cavity.

To provide a simple estimate of the peak material gain \( \gamma_{mat} \) we consider the propagation of the lasing mode in the in-plane direction (perpendicular to the current flow.) We denote by \( \hat{y} \) the direction of this in-plane propagation and assume the following spacial variation

\[
E(y, t) = \frac{1}{2} \left[ E_0 e^{i(q_\Delta y - \omega_\Delta)} + \text{c.c.} \right] \exp \left( \gamma_{mat}(\omega_\Delta)y/2 \right),
\]
\[ W_{3D}(y, \omega_\Delta) = \frac{1}{8\pi} \epsilon_r |E_0|^2 \exp(\gamma_{\text{mat}}(\omega_\Delta)y), \]

\[ S(y, \omega_\Delta) = \frac{\varkappa}{n_r} W_{3D}(y, \omega_\Delta) = \frac{\varkappa}{8\pi n_r} |E_0|^2 \exp(\gamma_{\text{mat}}(\omega_\Delta)y), \]

for the lasing mode electric field, energy density and radiation intensity, respectively.

The amplification of the radiation intensity

\[ \frac{dS(y, \omega_\Delta)}{dy} = \gamma_{\text{mat}}(\omega_\Delta)S(y, \omega_\Delta) \]

is just the lasing frequency \( \omega_\Delta \) times the net number of emission processes (i.e., emission minus absorption) produced within a unit volume containing \( 1/(L_{QB} + L_{Inj}) \) periods and having the total population inversion

\[ \Delta n_{(3D)} = \frac{\Delta n}{L_{QB} + L_{Inj}}. \]

The resulting material gain,

\[ \gamma_{\text{mat}}(\omega_\Delta) = \Delta n_{(3D)} \frac{\Gamma_{43}^{sp}(\omega_\Delta)}{\varkappa} \frac{\omega_\Delta}{S(y, \omega_\Delta)} \]

\[ \approx \left( \frac{3\pi c^2}{2n_r^2 \omega_\Delta^2} \right) \frac{\Delta n}{(L_{QB} + L_{Inj})} \Gamma_{43}^{sp} a(\omega_\Delta), \]

is proportional to the intersubband population inversion density \( \Delta n \) and, assuming a constant nonradiative decay rate \( \Gamma_{nr} \), proportional to the current density \( J \), see (4). Following Refs. 1 and 3 we can thus introduce the so-called normalized gain coefficient

\[ \gamma_{\text{mat}} \equiv gJ, \]

for which we above have derived the theoretically estimated

\[ g \approx \left( 1 - \frac{\Gamma_{nr}}{\Gamma_{cB}} \right) \frac{3\pi c^2 \Gamma_{43}^{sp} a(\omega_\Delta)}{2n_r^2 \omega_\Delta^2 (L_{QB} + L_{Inj}) e(\Gamma_{cB} + \Gamma_{nr})}. \]

Assuming \( \Gamma_{nr} \ll \Gamma_{cB} \) (valid for the mid-infrared quantum cascade laser) and using Eq. (16) to estimate \( \Gamma_{43}^{sp} \), the above expression Eq. (29) is identical to the
theory estimate provided in Ref. 3. The reported numerical value of this theory-
estimate is $g \approx 29 \text{ cm/kA}$. For comparison we note that Ref. 1 reports the esti-
mate $g \approx 9 \text{ cm/kA}$ based on an experimental measurement of the total integrated
luminescence $\Gamma_{43}^{sp}$ at the lasing threshold. Both values are reported in Table 2.4.

Finally, we emphasize that the peak stimulated emission, the peak material
gain, and hence the normalized gain coefficient is all proportional to the peak value
$a(\omega_\Delta) = 2/\Gamma_\phi$, of the line-shape function. That is, the peak gain is *inversely* pro-
portional to the full-width-half-maximum line-width $2\Gamma_\phi$. In the original quantum-
cascade-laser design discussed above this broadening was large primarily because
the optical active transition originates in the very narrow first quantum well (see
Figure 2.2) and thus very sensitive to interface scattering, see Ref. 3. We note in
particular that an significant improvement of the peak material gain was achieved
in a modified design\textsuperscript{5} in which the optical transitions occurs between two levels of a
wider quantum wells and that this improvement can be explained\textsuperscript{10} by the expected
reduced interface scattering.*

\textbf{II.D The waveguide confinement}

The discussion in the previous section addressed only the material $\gamma_{mat}$, that
is, the gain in a hypothetical infinite superlattice comprising back-to-back active-
region/injector-layer periods. However, the vacuum wavelength of the lasing mode

\textsuperscript{*} One can hope that the material gain in the hypothetical *far-infrared* quantum-
cascade-laser design introduced in Chapter I also will benefit from a narrower line-
width because the optical transitions results between quasi-bound levels in relative
wide quantum wells. We note in particular that the experimentally observed absorp-
tion line-width in the corresponding isolated quantum-well structure investigated
in Refs. 15, 16 is $2\Gamma_\phi \approx 1 \text{ meV}$ at low temperatures, $T \sim 10 \text{ K}$. 
is $\lambda_\Delta = 4.2 \mu m$ which inside the waveguide core (with effective index of refraction $n_{\text{mode}} = 3.26$) corresponds to the modified wavelength, $\lambda_\Delta/n_{\text{mode}} \approx 1.3 \mu m$. This modified wavelength is, however, comparable to the total extension of the 25-period superlattice, $25 \times (L_{QB} + L_{Inj}) \approx 1 \mu m$ and the estimated material gain must be adjusted to predict the effective (actual) gain arising within the optically active, but finite, superlattice.

Following the treatment in Ref. 17 one can estimate the resulting (reduced) effective gain $\gamma_{\text{mat}}$ (defined as the actual gain resulting from the 25-period superlattice of the quantum-cascade-laser heterostructure) simply by weighting the peak material gain by the fraction $\Phi$ of the lasing-mode intensity actually inside the finite superlattice,

$$\gamma_{\text{eff}} \approx \Phi \gamma_{\text{mat}}. \quad (31)$$

The design of a good waveguide, allowing a significant value of this so-called waveguide-confinement factor $\Phi$, is thus an important part of the quantum-cascade-laser heterostructure. This is particularly so because a large value of $\Phi$ not only increases the effective gain, Eq. (31), but at the same time also limits the reabsorption $\alpha_I$ in the regions outside the waveguide core as discussed in Section II.E. A detailed account for the large value $\Phi \approx 0.46$ reported in Ref. 1 is beyond the present scope but we include below a simple discussion.

Consider the radiation field for the lasing mode

$$E(\vec{R}; t) = \left[ E_{ac}(\vec{R}) \exp(-i\omega t) + c.c \right], \quad (32)$$

which we (thanks to the waveguide cladding layers) shall assume propagates entirely in the in-plane direction $\hat{y}$, see Figure 2.3. We also assume for simplicity that the
FIGURE 2.3 Waveguide confinement of mid-infrared lasing mode $q_{rad}$ explained by variation in effective index of refraction. The top panel shows the lasing mode which we assume polarized in the tunneling/growth direction ($\hat{x}$) perpendicular to the waveguide plane and propagating in the in-plane $\hat{y}$-direction indicated by wavevector $q_{rad}$. The middle and lower panels show the variation of effective index of refraction $n_r(x)$ within the quantum-cascade-laser heterostructure and resulting waveguide confinement potential, $\phi_\omega(x) = -n_r(x)^2(\omega^2/c^2)$, which enters into an approximate HelmHoltz equation for the lasing-mode radiation field $E_{ac}$, see text. As indicated by the dotted line in the middle panel, we assume for the waveguide core a constant index of refraction, $n_{mode} = 3.26$, estimated $^3$ as the effective index of refraction for the lasing mode $q_{rad} = n_{mode}(\omega\Delta/c)$. The middle panel also illustrate how the inclusion of two 3000 Å GaInAs layers, with large index of refraction $n_r > 3.4$, increases $^7$ this effective waveguide-core index of refraction, $n_{mode} = 3.26$, compared with the index of refraction, $n_{clad} \approx 3.15$, of the surrounding waveguide-cladding layers. For the approximate waveguide confinement potential, shown in the bottom panel, the larger difference, $n_{mode}^2 - n_{clad}^2$, implies a deeper potential and a shorter decay length, $1/\kappa \sim c/(\omega\Delta\sqrt{n_{mode}^2 - n_{clad}^2}) \approx 0.4$ µm, of the lasing mode into the cladding layers.
FIGURE 2.3
radiation constitute a TE-mode\textsuperscript{18} and is polarized entirely in the growth direction \( \hat{x} \) (as indicated in Figure 2.3.) The \( x \)-component of the electric field can be written

\[
E_{ac}(\vec{R}) = E_0(x, z)e^{i\vec{q}_{rad}(x)y}.
\]

Here the radiation wavevector,

\[
\vec{q}_{rad}(x) \equiv n_r(x)\frac{2\pi}{\lambda_\Delta},
\]

is given by the vacuum wavelength \( \lambda_\Delta \) of the lasing mode but assumed modified by the index of refraction \( n_r(x) \) for the specific heterostructure layer at position \( x \). However, for the waveguide-guide region we shall assume just a constant index of refraction, \( n_{\text{mode}} = 3.26 \), given as the estimated\textsuperscript{3,7} effective value for the lasing mode, \( q_{rad} = n_{\text{mode}}(\omega_\Delta/c) \).

The spacial (\( x \)) variation of the index of refraction \( n_r(x) \) results in a corresponding variation of the background dielectric constant \( \varepsilon_r(x) \equiv n_r(x)^2 \). In addition there is also a plasmon contribution to the dielectric constant arising from the finite conductivity \( \sigma(x) \) of the heterostructure layer at position \( x \). Within a simple Drude description we have

\[
\sigma(x; \omega) = \frac{\sigma_0(x)}{1 - i\omega\tau},
\]

\[
\sigma_0(x) = N_{3D}(x)\frac{e^2/\varepsilon_0(x)}{m_c^*(x)},
\]

where \( m_c^* (N_{3D}(x)) \) represents the local effective mass (carrier concentration) and \( 1/\tau \sim 1 \text{ meV} \) denotes the relaxation rate. The local plasmon frequency

\[
\Omega_{pl}(x) = \left(\frac{4\pi N_{3D}(x)e^2}{\varepsilon_0(x)m_c^*}\right)^{1/2}
\]

\[
= 4\text{Ry}^*(x)\sqrt{N_{3D}(x)\pi a_s^2}
\]
expressed in terms of the local scaled Rydberg, \( \text{Ry}^*(x) \), and scaled Bohr radius, \( a^*(x) \), remains, however, much smaller than the lasing frequency \( \omega_\Delta \) in all but the top contact layers.

We shall consequently approximate the Helmholtz equation for the lasing mode simply by

\[
-\frac{\partial^2}{\partial x^2} E_0(x;z) - \frac{\omega^2}{c^2} n_r(x)^2 E_0(x;z) = -q_{\text{rad}}(x)^2 E_0(x;z)
\]

where we have also ignored the \( x \)-variation of \( q_{\text{rad}} \).

Finally, if we also assume a wide mesa (with extension in direction \( z \) larger than the modified wavelength, \( \lambda/n_{\text{mode}} = 2\pi/q_{\text{rad}} \)) we arrive at the one-dimensional eigenvalue problem:

\[
-\frac{\partial^2}{\partial x^2} E_0(x) - \frac{\omega^2}{c^2} n_r(x)^2 E_0(x) = -q_{\text{rad}}^2 E_0(x),
\]

defined by the effective radiation-mode quantum-well confinement potential

\[
\phi_\omega(x) = -n_r(x)^2 \frac{\omega^2}{c^2},
\]

schematically illustrated in the lower panel of Figure 2.3.

The eigenvalues, \( \varepsilon \equiv -q_{\text{rad}}^2 \), of this potential problem defines the lasing mode which is confined within the waveguide core but does 'leak' through evanescent tails out into the waveguide cladding layers. The actual lasing mode wavevector \( q_{\text{rad}} \) is given by \( n_{\text{mode}} \) and the following effective potential barrier

\[
\Delta \phi_\omega = \frac{\omega^2}{c^2} \left( n_{\text{mode}}^2 - n_{\text{clad}}^2 \right)
\]

determines the radiation decay in the waveguide cladding layers with index of refraction \( n_{\text{clad}} \approx 3.15 \). While this one-dimensional treatment is far from exact we
use the Helmholtz equation in the cladding layers:

$$\frac{d^2}{dx^2} E_0 e^{\pm kx} + \Delta \Phi \sim 0,$$

(42)

to provide an order of magnitude estimate of the radiation decay length

$$\frac{1}{\kappa} \sim \frac{(c/\omega)}{\sqrt{n_{mode}^2 - n_{clad}^2}} = \frac{1}{2\pi} \frac{\lambda_\Delta}{\sqrt{n_{mode}^2 - n_{clad}^2}}.$$  

(43)

Using the reported Quantum Cascade Laser heterostructure parameters we find a decay length $1/\kappa \sim 0.4 \mu m$ — significantly smaller than than the width of the waveguide cladding ($\sim 1 \mu m$).

The above discussion is of course only schematic. However, it does illustrate the significant waveguide confinement, $\Phi = 0.46$, achieved in the quantum-cascade-laser design simply by including waveguide cladding layers with a lower average index of refraction.*

II.E The threshold optical characteristics

In Section II.C above we derived a formal estimate for the peak material gain, $\gamma_{mat} = g_{th}$. In the previous Section II.D we discussed the so-called waveguide-confinement factor, $\Phi$, giving the fraction of the lasing mode intensity concentrated within the optically active superlattice. The peak threshold effective gain is thus $\Phi g_{th}$. We conclude our discussion of the mid-infrared quantum cascade laser by a

* At the same time, however, it is also clear that such a waveguide confinement becomes increasingly more difficult for longer wavelengths. It may in particular be very difficult to achieve a good waveguide confinement in a hypothetical far-infrared quantum cascade laser. Such a discussion is beyond the scope of this dissertation.
comparison of the estimated peak material and effective gains with the estimated loss, $\alpha_I$, and net emission rate, $\alpha_M$, out from the end mirrors of the lasing cavity. The comparison in summarized in Table 2.4.

The design of a good waveguide confinement, i.e., a large value of $\Phi$, using the variation of the index of refraction is an important element in the quantum-cascade-laser design. In Section II.C above we derived a formal estimate for the peak material gain, $\gamma_{mat} = gJ_{th}$. For the threshold current reported for the Ref. 1 (Ref. 3) cleaved mesa realization this estimate yield the threshold material gain $gJ_{th} = 99(155) \text{ cm}^{-1}$. Using the estimated value, $^3 \Phi \sim 0.5$, for the waveguide-confinement factor we predict a peak threshold effective gain of

$$\Phi gJ_{th} \sim 45 \ (78) \text{ cm}^{-1}, \tag{44}$$
directly proportional to $\Phi$.

A good waveguide confinement ($\Phi$) is also important in limiting the internal reabsorption $\alpha_I$ of the lasing mode. Specifically, the top contact layers and the InP substrate are heavily doped and has a plasmon energy comparable with the lasing frequency. However, the potentially dramatic plasmon reabsorption is avoided because only a vanishing part of the lasing mode intensity penetrate through the waveguide cladding layers.* As a consequence, the total internal loss is estimated at just $\alpha_I \approx 9 \ (20) \text{ cm}^{-1}$ in Ref. 1 (Ref. 3.)

Summarizing the above results, the amplification of the lasing-mode intensity $S(y; \omega_\Delta)$ is at threshold described by a net gain

$$\frac{dS(y, \omega_\Delta)}{dy} = [\Phi gJ_{th} - \alpha_I] > 0, \tag{45}$$

* The moderate doping concentration, $\leq 10^{18} \text{ cm}^{-3}$ of the cladding layers yields plasmon frequencies, $\omega_p \leq 43 \text{ meV}$ and causes no plasmon reabsorption.
2.4 Threshold optical characteristics the quantum cascade laser realized both as a 12 µm x 0.72 mm cleaved mesa\(^1\) (indicated by †) and as a 14 µm x 1.2 mm cleaved mesa\(^3\) (indicated by ‡). A simple two-level rate-equation description (see text) provides an estimate for the threshold density population inversion, \(\Delta n_{th}\). Also listed are estimates for the optical transition matrix element, \(\langle \Psi_4|x|\Psi_3 \rangle \approx 10 \, \text{Å}\), between level \(E_4\) and \(E_3\). Such a large transition matrix element is possible because the quantum-confinement concentrates a very large oscillator strength, \(f_{43} = 2m_e^* \Delta |\langle \Psi_4|x|\Psi_3 \rangle|^2 \approx 0.4\), at the \(E_4 \rightarrow E_3\) optical transition. There is only a small spontaneous emission rate, \(\gamma_{43} = 5 \times 10^{-5} \, \text{meV}\), at the mid-infrared frequency set by \(\Delta = 295 \, \text{meV}\). However, the significant waveguide confinement factor, \(\Phi \sim 0.5\), of the lasing mode intensity to the \(N_p = 25\) optically active superlattice ensures a significant peak effective gain \(\Phi g J_{th} \sim 45-78 \, \text{cm}^{-1}\). This value is larger than, but comparable to, the estimated total loss \(\alpha_I + \alpha_M \sim 25 \, \text{cm}^{-1}\) both due to the internal absorption, \(\alpha_I\), and due to the actual lasing emission rate, \(\alpha_M\), at the two end mirrors.
<table>
<thead>
<tr>
<th>Description</th>
<th>Symbol</th>
<th>Quantum Cascade Laser $^{†(‡)}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Subband separation (Lasing frequency)</td>
<td>$\Delta$</td>
<td>$= 295 \text{ meV}$</td>
</tr>
<tr>
<td>Optical matrix element $^{†}$</td>
<td>$\langle \Psi_4</td>
<td>x</td>
</tr>
<tr>
<td>Spontaneous emission rate $^{†}$</td>
<td>$\Gamma_{43}^{sp}$</td>
<td>$\sim 5 \times 10^{-5} \text{ meV}$</td>
</tr>
<tr>
<td>Active period width ($L_{QB} + L_{Inj}$)</td>
<td>$-$</td>
<td>$= 3.97 \times 10^{-2} \text{ µm}$</td>
</tr>
<tr>
<td>Total coupled active periods</td>
<td>$N_p$</td>
<td>$= 25$</td>
</tr>
<tr>
<td>Total width of active periods</td>
<td>$-$</td>
<td>$\approx 1.0 \text{ µm}$</td>
</tr>
<tr>
<td>Width of wave-guide core</td>
<td>$-$</td>
<td>$= 1.68 \text{ µm}$</td>
</tr>
<tr>
<td>Waveguide confinement factor $^{†(‡)}$</td>
<td>$\Phi$</td>
<td>$\approx 0.46 (0.5)$</td>
</tr>
<tr>
<td>Internal loss $^{†(‡)}$</td>
<td>$\alpha_I$</td>
<td>$\sim 9 (10) \text{ cm}^{-1}$</td>
</tr>
<tr>
<td>Threshold population inversion $^{†}$</td>
<td>$\Delta n_{th}$</td>
<td>$\approx 1.7 \times 10^{11} \text{ cm}^{-2}$</td>
</tr>
<tr>
<td>Normalized gain coefficient $^{†(‡)}$</td>
<td>$g$</td>
<td>$\sim 9 (29) \text{ cm/kA}$</td>
</tr>
<tr>
<td>Peak threshold material gain $^{†(‡)}$</td>
<td>$g J_{th}$</td>
<td>$\sim 99 (155) \text{ cm}^{-1}$</td>
</tr>
<tr>
<td>Peak effective threshold gain $^{†(‡)}$</td>
<td>$\Phi g J_{th}$</td>
<td>$\sim 45 (78) \text{ cm}^{-1}$</td>
</tr>
<tr>
<td>Length of cleaved mesa $^{†(‡)}$</td>
<td>$L_{mesa}$</td>
<td>$= 0.72 (1.2) \text{ mm}$</td>
</tr>
<tr>
<td>Mirror reflection coefficient $^{†}$</td>
<td>$R_M$</td>
<td>$\approx 0.27$</td>
</tr>
<tr>
<td>Mirror loss $^{†(‡)}$ ($-\ln(R_M)/L_{mesa}$)</td>
<td>$\alpha_M$</td>
<td>$\approx 18.5 (11) \text{ cm}^{-1}$</td>
</tr>
<tr>
<td>Total loss</td>
<td>$\alpha_I + \alpha_M$</td>
<td>$\sim 28 (21) \text{ cm}^{-1}$</td>
</tr>
</tbody>
</table>

$^{†(‡)}$ Reported in Ref. 1 (Ref. 3).
because the significant waveguide-confinement factor, $\Phi \sim 0.5$, both increases the effective gain and limits the internal loss $\alpha_I$.

However, to achieve threshold conditions, that is, the onset of stimulated emission and lasing, one must also ensure a containment in the in-plane direction of propagation of the lasing mode. Such a (longitudinal) containment is realized for the quantum cascade laser investigated in Ref. 1 (Ref. 3) by cleaving both ends of the 12 $\mu$m by 0.72 mm (14 $\mu$m by 1.2 mm) etched mesa structure.

The lasing threshold is characterized by a beginning build up of the radiation intensity inside the cavity formed by the cladding layers and by the two cleaved end mirrors. This concentration of the lasing mode is achieved when the net amplification during one passage of length $L_{\text{mesa}}$ (from one end mirror to the other) exactly compensate for the intensity emitted at the first mirror. Denoting the reflection coefficient (of the lasing mode) at the end mirrors by $R_M$, the threshold condition becomes

$$R_M \exp ([\Phi g J_{\text{th}} - \alpha_I] L_{\text{mesa}}) \equiv 1. \quad (46)$$

Introducing the so-called mirror loss,

$$\alpha_M \equiv -\ln (R_M)/L_{\text{mesa}}, \quad (47)$$

the above threshold condition, Eq. (46), can be reformulated simply as

$$\Phi g J_{\text{th}} = \alpha_I + \alpha_M. \quad (48)$$

That is, the lasing threshold obtains when the effective gain, $\Phi g J$, at current density $J$ overcomes both the internal reabsorption and the mirror loss.

For the mesa structure reported on in Ref. 1 (Ref. 3,) we have $L_{\text{mesa}} = 0.72$ mm ($L_{\text{mesa}} = 1.2$ mm) and using the estimate, $R_M = 0.27$, we obtain the estimate,
\( \alpha_M = 18.5 \pm 11 \text{ cm}^{-1} \), for the mirror loss. The estimated total radiation loss, 
\( \alpha_I + \alpha_M \approx 28 \pm 21 \text{ cm}^{-1} \), for the mesa structure investigated in Ref. 1 (Ref. 3) is thus smaller, but comparable to, the estimated peak effective gain, \( \Phi_{gJ_{th}} = 45 \pm 78 \text{ cm}^{-1} \).

We finally observe that \( \alpha_M \) dominates the total radiation losses. It should thus be possible to achieve a significant reduction of the threshold current by changing the geometry of the lasing cavity. For example, increasing the mesa length \( L_{\text{mesa}} \) obviously reduces \( \alpha_M \), see Eq. (47), and in particular results in a larger peak optical power (see Table 2.3) for the longer quantum-cascade-laser-mesa realization (investigated in Ref. 3.) Furthermore, a significant improvement should be possible by increasing the effective reflection coefficient of the cavity mirrors. Such an improvement may in particular be achieved within a so-called quantum-disk-mesa realization\(^{19,20}\) of a quantum cascade laser. In such quantum-disk lasers an effective potential for the radiation field confines also the in-plane extension of the lasing mode (in analogy with the confinement in the growth direction discussed in Section II.D.) This in-plane confinement potential causes the mirror loss to become extremely small because the lasing mode is not just reflected but must actually tunnel (through an effective potential barrier) out from the cavity.
REFERENCES


7. Dr. F. Capasso, private communication; the author thanks Dr. Capasso for detailed discussions of the waveguide design during several phone conversations.


9. A continuous-wave operation has been achieved in a later quantum-cascade-laser design; Dr. J. Faist, private communications.

10. Dr. F. Capasso, private communication.


CHAPTER III

A POSSIBLE FAR-INFRARED QUANTUM CASCADE LASER

In this chapter we describe in detail the possible far-infrared quantum-cascade-laser design with conduction-band potential illustrated in Figure 1.1. In particular, we introduce a possible chemical composition and discuss the resulting tunneling potential as a function of the voltage drop \( V \) applied across the central tunneling region. We furthermore determine the voltage-drop dependence of the quasi-bound resonant levels and find that the so-called quantum-confined Stark effect\(^1\) at \( V_{\text{sym}} \approx 23 \text{ mV} \) causes an avoided crossing, corresponding to the minimal value, \( D \geq D(V_{\text{sym}}) = 10.9 \text{ meV} \), of the subband separation. By design, this voltage drop \( V_{\text{sym}} \) is contained within the range, \( 12 \text{ mV} \lesssim V \lesssim 30 \text{ mV} \), of voltage drops that ensures both a strong current injection exclusively into the upper subband and a fast lower-level escape rate whose voltage-drop dependence we estimate.

We also consider the quantum-confined Stark effect on the quasi-bound wavefunction symmetry.\(^1,2\) Specifically we demonstrate that the special applied bias \( V_{\text{sym}} \) causing the avoided crossing at the same time also restores a near-exact \textit{wavefunction}-inversion symmetry in the still asymmetric potential. Moreover, we
introduce the center-of-charge separation (dipole matrix element) as a simple measurement of the wavefunction symmetry (overlap.) Finally we discuss the voltage-drop dependence of the wavefunction-inversion symmetry which we in Chapter IV find significantly affects the intersubband electron-electron scattering rates.

We furthermore describe the experimental determination\(^3\) of the intersubband decay rate in the corresponding *isolated* asymmetric quantum-well structure.\(^3,4\) This structure is formed by the same double-quantum-well potential which constitutes the core of the Figure 1.1 tunneling structure but surrounded instead by very thick (modulation-doped) Al\(_{0.3}\)Ga\(_{0.7}\)As barriers. The experimental observation\(^3\) of a very small intersubband decay rate, \(1/\tau \lesssim 0.03\) meV at \(T \lesssim 50\) K, observed at weak optical pumping of this quantum-well structure motivated our choice of the specific tunneling structure with potential shown in Figure 1.1.

The main focus of this dissertation is an estimate of the intersubband decay and resulting population inversion arising with a strong current injection into the Figure 1.1 tunneling structure. In this chapter we argue that the total *single*-particle decay, \(\Gamma_{sp}\), of the nonequilibrium current-injected upper-subband occupation remains approximately bounded by the experimental value, \(1/\tau \approx 0.03\) meV (at \(T \lesssim 50\) K) observed at a weak optical pumping.\(^3\) At the same time we emphasize that no such experimental bound applies to the *nonequilibrium* electron-electron intersubband scattering. This observation motivates our subsequent detailed study of the nonequilibrium electron-electron scattering reported in Chapter IV.
Figure 3.1 shows schematics of the asymmetric double-quantum-well tunneling structure for which we in this dissertation estimate the intersubband decay and resulting population inversion. Specifically, the top panel of Figure 3.1 shows a possible chemical composition with a central tunneling region (of extension $L_{QB} = 243 \, \text{Å}$) surrounded by n-doped digital Al$_{x}$Ga$_{1-x}$As alloy leads. The tunneling region is formed as a double-quantum-well structure surrounded by two $L_B = 30 \, \text{Å}$ Al$_{0.3}$Ga$_{0.7}$As tunneling barriers allowing final tunneling rates into and out from the lowest two quasi-bound resonant levels, $E_1$ and $E_2$.

The bottom panel of Figure 3.1 shows a schematics of the corresponding tunneling potential in equilibrium and in the absence of any electron charging effects.* The solid bars indicates the equilibrium positions of the quasi-bound resonant levels $E_1^0$ and $E_2^0$. Table 3.1 list the physical parameters characterizing this equilibrium potential with all energy positions listed relative to the equilibrium potential in the GaAs wells.

The choice of a digital Al$_{x}$Ga$_{1-x}$As alloy with an $x \approx 0.05$ Aluminum content raises both the emitter and collector band edge, $\phi_L^0 = \phi_R^0 = 36 \, \text{meV}$, relative to the GaAs quantum-well potential. The equilibrium positions of the emitter and collector chemical potentials, $\mu_{L/R}^0 = \phi_{L/R}^0 + 10 \, \text{meV}$, is given by the assumed $N_{3D} \sim 10^{17} \text{cm}^{-3}$ lead doping concentration. We assume that this doping concentration ensures a fixed thickness, $\mu_L - \phi_L = \mu_R - \phi_R = 10 \, \text{meV}$, of the emitter and collector Fermi sea also out of equilibrium. The raised positions of the emitter

* We shall neglect such self-consistent charging effects on the potential and level positions throughout the entire dissertation.
FIGURE 3.1 Schematics of hypothetical far-infrared quantum-cascade-laser design in equilibrium (schematics of tunneling potential at a finite voltage drop illustrated in Figure 1.1.) The top panel shows (a possible) chemical composition of the asymmetric double-quantum-well tunneling structure. In particular, the structure comprises the central tunneling region of total extension \( L_{QB} = 243 \, \text{Å} \) surrounded n-doped leads formed as digital \( \text{Al}_{x}\text{Ga}_{1-x}\text{As} \) alloys. The bottom panel shows a schematics of the resulting tunneling potential in equilibrium (and neglecting all electron-charging effects.) Table 3.1 list the physical parameters characterizing this tunneling potential and the equilibrium positions, \( E^0_1 \) and \( E^0_2 \), of the quasi-bound resonant levels (indicated by the solid bars. For the emitter ('\( L'\)) and collector ('\( R'\)) leads we assume a value \( x \approx 0.05 \) for the Al-content in the digital \( \text{Al}_{x}\text{Ga}_{1-x}\text{As} \) alloys. As illustrated, this choice raises the equilibrium positions of the lower emitter and collector band edge, \( \phi^0_L = \phi^0_R = 36 \, \text{meV} \), relative to the bottom of the GaAs quantum wells. An assumed \( N_{3D} \sim 10^{17} \, \text{cm}^{-3} \) lead doping concentration positions the emitter and collector chemical potentials at \( \mu^0_{L/R} = \phi^0_{L/R} + 10 \, \text{meV} \). We shall assume that the relation \( \mu_L - \phi_L = \mu_R - \phi_R = 10 \, \text{meV} \) also holds true in the presence of a finite voltage-drop \( V \) applied across the central tunneling region.
FIGURE 3.1
TABLE 3.1 Parameters characterizing the equilibrium tunneling potential, electron occupation, and position of quasi-bound resonant levels, $E_1^0$ and $E_2^0$, for specific tunneling structure with schematics shown in Figure 3.1. We neglect all electron charging effects and list the equilibrium tunneling-barrier heights ($\phi_B^0 = 214$ meV) and resonant-level energy positions ($E_1^0$ and $E_2^0$) relative to the equilibrium position of the GaAs quantum wells. The choice of digital Al$_x$Ga$_{1-x}$As ($x \approx 0.05$) leads raises the equilibrium positions of the emitter and collector lower band edges, $\phi_L^0 = \phi_R^0 = 36$ meV. The equilibrium positions, $\mu_L^{0/R} - \phi_L^{0/R} = 10$ meV, of the emitter and collector chemical potentials, $\mu_L$ and $\mu_R$, are given by the assumed lead doping concentration $N_{3D} \sim 10^{17}$ cm$^{-3}$. We emphasize that the raised positions of the emitter and collector band edges allow both a strong upper-subband current injection and a fast lower escape rate at just a moderate voltage drop, $12$ mV $\leq V \leq 30$ mV, see Table 3.2.
<table>
<thead>
<tr>
<th>Physical quantity</th>
<th>Symbol</th>
<th>Equilibrium value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total central region thickness</td>
<td>$L_{QB}$</td>
<td>243 Å</td>
</tr>
<tr>
<td>Barrier thickness</td>
<td>$L_B$</td>
<td>30 Å</td>
</tr>
<tr>
<td>Al$<em>{0.3}$Ga$</em>{0.7}$As-barrier potential</td>
<td>$\phi^0_B$</td>
<td>214 meV</td>
</tr>
<tr>
<td>Emitter/collector band edge</td>
<td>$\phi_{L/R}$</td>
<td>36 meV</td>
</tr>
<tr>
<td>Lead doping concentration</td>
<td>$N_{3D}$</td>
<td>$\sim 10^{17}\text{cm}^{-3}$</td>
</tr>
<tr>
<td>Equilibrium chemical potential</td>
<td>$\mu^0_L = \mu^0_R$</td>
<td>46 meV</td>
</tr>
<tr>
<td>Thickness of Fermi sea</td>
<td>$\mu^0_{L/R} - \phi^0_{L/R}$</td>
<td>10 meV</td>
</tr>
<tr>
<td>Upper resonant level</td>
<td>$E^0_2$</td>
<td>52.9 meV</td>
</tr>
<tr>
<td>Lower resonant level</td>
<td>$E^0_1$</td>
<td>38.3 meV</td>
</tr>
<tr>
<td>Subband separation</td>
<td>$\Delta^0 \equiv E^0_2 - E^0_1$</td>
<td>14.6 meV</td>
</tr>
</tbody>
</table>
and collector band edges implies in particular that only a moderate voltage drop \( V \) applied across the tunneling region results in an exclusive upper-subband current injection. Assuming also that the tunneling escape rate out to the collector can maintain a finite population inversion in spite of the intersubband decay, a net stimulated emission will then obtain at a frequency \( \omega_\Delta \) given by the far-infrared subband separation \( \Delta \equiv E_2 - E_1 \approx 11 \text{ meV} \).

### III.B The nonequilibrium current flow and optical response

In this section we describe for the Figure 3.1 tunneling structure both the nonequilibrium current flow and the regimes of the optical response. Specifically we estimate (a) the quantum-confined Stark effect\(^1\) on (i.e., the voltage-drop dependence of) the quasi-bound resonant levels, (b) the range of voltage drops that results in the so-called emission regime with both an exclusive upper-subband current injection (\( \Gamma_e \)) and a fast lower-level escape rate (\( \Gamma_{c1} \)) and finally (c) the voltage-dependence of the tunneling escape rates, \( \Gamma_{c1} \) and \( \Gamma_{c2} \), within this emission regime. Table 3.2 summarizes these estimates.

We shall as previously stated neglect all electron charging effects and thus assume, in the presence of a finite voltage drop \( V \), a constant internal field \( F_{de} = V/L_{QB} \) within the tunneling region. We assume in particular a simple variation of the emitter and collector lower band edges and chemical potentials,

\[
\phi_{L(R)} = \phi_0 + (-)eV/2, \\
\mu_{L(R)} = \mu_0 + (-)eV/2,
\]

relative to equilibrium values, \( \phi_{L(R)} = \phi_0 \), and \( \mu_{L(R)} = \mu_0 \).
We neglect electron-charging effects, that is, the self-consistent effects on the potential arising with a finite electron occupation. We assume in particular a constant internal field $F_{dc} = V/LQB$ within the tunneling region (as illustrated in Figure 1.1) in the presence of a finite voltage drop $V$ which raises/lowers the emitter/collector band edges, $\phi_{L/R} = \phi_{L/R}^{0} + / - eV/2$, and chemical potentials, $\mu_{L/R} = \phi_{L/R} + 10$ meV. We also neglect electron charging effects in estimating the voltage-drop dependence of the quasi-bound resonant levels (described further in Figure 3.3.) The so-called emission regime with both an exclusive upper-subband current injection ($\Gamma_{e}$) and a fast lower-subband tunneling escape ($\Gamma_{c1}$) requires both of the following conditions: $\mu_{L} > E_{2} > \phi_{L}$ and $\phi_{L} > E_{1} > \mu_{R}$. As indicated this regime with possible net stimulated intersubband emission results at voltage-drops $12$ mV $\ll V \ll 30$ mV. Within the limited range of voltage drops we find only a moderate variation of the current injection rate of the tunneling escape rates $\Gamma_{c1}$ and $\Gamma_{c2}$, see text. The table furthermore indicates the voltage drop dependence of the optical (dipole) transitions matrix element and center-of-charge separation, discussed further in Figs. 3.2 and 3.3. For completeness the table also list the assumed operating temperature, $T \leq 25$ K and $T \ll (\mu_{L} - E_{2})$. The first of these criteria ensures a vanishing value of the total single-electron decay, $\Gamma_{se} \leq 0.03$ meV, see text. The second conditions for the temperature, $T \ll (\mu_{L} - E_{2})$, arises because we in Chapter IV evaluate the nonequilibrium electron-electron scattering at zero temperature only.

### TABLE 3.2 Voltage-drop dependence of tunneling potential, the escape rates ($\Gamma_{c1}, \Gamma_{c2}$ and $\Gamma_{e}$) and of the quasi-bound resonant-level wavefunctions, $\Psi_{1}(x)$ and $\Psi_{2}(x)$, for the tunneling potential schematically illustrated in Figure 3.1.

<table>
<thead>
<tr>
<th>Voltage Drop (mV)</th>
<th>$\Gamma_{c1}$</th>
<th>$\Gamma_{c2}$</th>
<th>$\Gamma_{e}$</th>
<th>$\Psi_{1}(x)$</th>
<th>$\Psi_{2}(x)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.05</td>
<td>0.03</td>
<td>0.02</td>
<td>0.1</td>
<td>0.05</td>
</tr>
<tr>
<td>10</td>
<td>0.06</td>
<td>0.04</td>
<td>0.03</td>
<td>0.12</td>
<td>0.06</td>
</tr>
<tr>
<td>30</td>
<td>0.08</td>
<td>0.05</td>
<td>0.04</td>
<td>0.15</td>
<td>0.08</td>
</tr>
<tr>
<td>50</td>
<td>0.10</td>
<td>0.06</td>
<td>0.05</td>
<td>0.18</td>
<td>0.10</td>
</tr>
</tbody>
</table>
## TABLE 3.2

<table>
<thead>
<tr>
<th>Physical quantity</th>
<th>Symbol</th>
<th>Value in equilibrium</th>
<th>At finite applied bias $V$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Emitter/collector chemical potential</td>
<td>$\mu_{L/R}$</td>
<td>$\mu_{L/R}^0 = 46 \text{ meV}$</td>
<td>$\mu_{L/R} = \mu_{L/R}^0 + / - eV/2$</td>
</tr>
<tr>
<td>Emitter/collector band edge</td>
<td>$\phi_{L/R}$</td>
<td>$\phi_{L/R}^0 = 36 \text{ meV}$</td>
<td>$\phi_{L/R} = \phi_{L/R}^0 + / - eV/2$</td>
</tr>
<tr>
<td>Upper resonant level</td>
<td>$E_2$</td>
<td>$E_2^0 = 52.9 \text{ meV}$</td>
<td>$E_2(V) \geq 50.8 \text{ meV}^\dagger$</td>
</tr>
<tr>
<td>Lower resonant level</td>
<td>$E_1$</td>
<td>$E_1^0 = 38.3 \text{ meV}$</td>
<td>$E_1(V) \leq 39.8 \text{ meV}^\dagger$</td>
</tr>
<tr>
<td>Subband separation</td>
<td>$\Delta \equiv E_2 - E_1$</td>
<td>$\Delta^0 = 14.6 \text{ meV}$</td>
<td>$\Delta(V) \geq 10.9 \text{ meV}^\dagger$</td>
</tr>
<tr>
<td>Emission regime</td>
<td>—</td>
<td>—</td>
<td>12 meV $\lesssim eV \lesssim 30 \text{ meV}$</td>
</tr>
<tr>
<td>Lower-level escape rate</td>
<td>$\Gamma_{c1}$</td>
<td>—</td>
<td>0.4 meV $\lesssim \Gamma_{c1} \lesssim 0.6 \text{ meV}$</td>
</tr>
<tr>
<td>Upper-level escape rate</td>
<td>$\Gamma_{c2}$</td>
<td>—</td>
<td>0.9 meV $\lesssim \Gamma_{c2} \lesssim 1.1 \text{ meV}$</td>
</tr>
<tr>
<td>Emitter injection rate</td>
<td>$\Gamma_e$</td>
<td>—</td>
<td>$\Gamma_e \sim \Gamma_{c2}/2$</td>
</tr>
<tr>
<td>Optical transition matrix element</td>
<td>$\langle \Psi_2 \mid x \mid \Psi_1 \rangle$</td>
<td>38.8 Å</td>
<td>$\langle \Psi_2 \mid x \mid \Psi_1 \rangle(V) \leq 51.2 \text{ Å}^\dagger$</td>
</tr>
<tr>
<td>Center-of-charge separation</td>
<td>$\langle \Psi_2 \mid x \mid \Psi_2 \rangle$</td>
<td>67.2 Å</td>
<td>$</td>
</tr>
<tr>
<td>Assumed temperature</td>
<td>$T$</td>
<td>$T \leq 25 \text{ K}$ and $T \ll \mu_L - E_2(V)$</td>
<td></td>
</tr>
</tbody>
</table>

$\dagger$ See Figure 3.3  
$\dagger$ See Figure 3.5  
$\S$ Measured from $\langle \Psi_1 \mid x \mid \Psi_1 \rangle \equiv 0$
We estimate the resonant-level positions $E_1$ and $E_2$ (and corresponding quasi-bound wavefunctions $\Psi_1(x)$ and $\Psi_2(x)$) as given by the lowest two bound energy levels\textsuperscript{5} of the corresponding isolated double-quantum-well structure (investigated in Ref. 3,4) when subjected to the same internal field, $F_{dc} = V/L_{QB}$. Within this approximation we proceed to determine the quantum-confined Stark effect,\textsuperscript{1} that is, the voltage drop-dependence of the (quasi-bound) levels.

The top panel of Figure 3.2 shows schematics of tunneling potential, resonant level positions $E_1^0$ and $E_2^0$ (solid bars,) and corresponding wavefunctions $\Psi_1^0(x)$ and $\Psi_2^0(x)$ in equilibrium. Both the upper- and lower-level wavefunction extend throughout both quantum wells but more of the upper- (lower)-level wavefunction is concentrated in slightly narrower right (wider left) quantum well. There is thus in equilibrium a finite center-of-charge separation, $(\Psi_2^0|x|\Psi_2^0) - (\Psi_1^0|x|\Psi_1^0) \approx 67 \text{ Å}.$

Applying a finite voltage drop raises (lowers) the (bottom of) the left (right) quantum well relative to the quantum-well center and will eventually force the lower (upper) quasi-bound level into the narrower right (wider left) quantum well. This quantum-confined stark effect\textsuperscript{1} must in particular cause an avoided crossing of the (quasi-bound) level position at some intermediate voltage drop $V = V_{sym}$ with a minimal subband separation $\Delta^s = \Delta(V_{sym}) = 22.9 \text{ meV}$.

The bottom panel of Figure 3.2 shows the tunneling potential, energy levels (solid bars,) and wavefunctions $\Psi_{1,2}^s(x)$ at this avoided crossing $V_{sym}$. The set of dashed bars indicate the corresponding equilibrium positions of the resonant level positions and we observe that the quantum-confined Stark effect does result in a finite voltage-drop variation of the quasi-bound energy positions $E_1$ and $E_2$. 
FIGURE 3.2 Quantum-confined Stark effect\(^1\) on the quasi-bound resonant levels and on the corresponding wavefunction-inversion symmetry.\(^2\) Top panel shows the position of the (quasi-bound) resonant levels \(E_{1,2}^0\) (solid bars) and corresponding approximate wavefunctions \(\Psi_{1,2}^0(x)\) in equilibrium. Note that more of the upper- (lower-)level wavefunction is situated in the narrower rightmost (wider leftmost) quantum well and the equilibrium wavefunctions are characterized by a finite center-of-charge separation, \(\langle \Psi_2^0|x|\Psi_2^0 \rangle - \langle \Psi_1^0|x|\Psi_1^0 \rangle > 0\). Applying a finite voltage drop \(V\) thus initially lowers (raises) the upper (lower) resonant levels until, eventually (at \(V > V_{sym}\)) the center of charge is reversed and more of the upper- (lower-)level wavefunction is concentrated in the wider, but leftmost (narrower, but rightmost,) quantum well. At a finite voltage drop, \(V = V_{sym} = 22.9\) meV, this so-called quantum-confined Stark effect\(^1\) results in an avoided crossing of the level positions with a minimal sub-band separation, \(\Delta^s = \Delta(V_{sym}) = 10.9\) meV. The bottom panel illustrates the tunneling potential, resonant level positions, \(E_1\) and \(E_2\), and corresponding wavefunctions, \(\Psi_{1,2}^s(x)\), at this avoided crossing, \(V = V_{sym}\). For comparison the bottom panel also shows the equilibrium positions of the resonant levels (dashed bars.)
FIGURE 3.2
FIGURE 3.3 Avoided crossing of resonant-level positions and regimes of the nonequilibrium current flow and optical response. Top panel determines the quantum-confined Stark effect\textsuperscript{1} on the resonant levels and determines the minimum subband separation arising at the avoided crossing between $E_1(V)$ and $E_2(V)$. Bottom panel identifies the qualitative regimes of the far-infrared optical response of the tunneling structure based on the estimate level positions $E_{1,2}(V)$. Specifically, at voltage drop $V \ll 10$ mV, the upper- (lower-)resonant level is still located above (within) the emitter (collector) Fermi sea, $E_2 > \mu_L$ ($\mu_R > E_1$) and there is no an upper-subband current injection but a finite lower-subband occupation density. Radiation tuned to the subband separation thus results in a (resonantly enhanced) absorption. However, as indicated by the pair of downwards arrows, only a slightly increased voltage drop, $12$ mV $\ll V \ll 30$ mV, ensures both $\mu_L > E_2 > \phi_L$ and $\phi_L > E_1 > \mu_R$. Such moderate voltage drops thus provides an exclusive upper-subband current injection ($\Gamma_e$) — since $E_2$ but not $E_1$ is located within the emitter Fermi sea — and a fast lower-subband tunneling escape rate ($\Gamma_{c1}$) — because the lower level is situated above the collector Fermi surface and all final collector states are available for the tunneling-out process. Under these conditions the lower level is only populated by intersubband scattering and the current injection may thus provide a finite intersubband population inversion and a net stimulated emission as indicated by the pair of downward arrows.
FIGURE 3.3
Top panel of Figure 3.3 shows the voltage-drop variation of the level positions and also illustrates the avoided crossing. The panel also shows the variation of the subband separation, $\Delta(V) \equiv E_2 - E_1 > \Delta^e$.

The bottom panel of Figure 3.3 identifies the regimes of the nonequilibrium optical response in the tunneling structure. Specifically, the lower panel of Figure 3.3 compares the estimated variation of the resonant level positions with the assumed voltage-drop dependence of the emitter lower band edge, $\phi_L$, and with the emitter and collector chemical potential, $\mu_L$ and $\mu_R$ (see Eqs. (1) and (2)). The knowledge of the relative positions of $E_1$ and $E_2$ and of $\phi_L$, $\mu_L$, and $\mu_R$ allows a determination of the (nonequilibrium) optical regimes.

Consider first the situation at a small applied voltage drop, $V \approx 10$ mV. The upper level $E_2$ then remains located above the emitter chemical potential and there is only a vanishing upper-subband electron occupation. The lower level is on the other hand situated below the collector chemical potential and there will be a finite lower-subband occupation density. As a consequence, radiation with a frequency tuned to the subband separation will thus experience a resonantly enhanced intersubband absorption, as indicated by the upward arrow in the bottom panel of Figure 3.3.

However, as indicated by the pair of downward arrows in Figure 3.3, it takes only a moderate voltage drop

$$12 \text{ mV} \leq V \leq 30 \text{ mV},$$

(3)

to ensure both of the following conditions for a possible net intersubband stimulated emission

$$\phi_L \leq E_2 \leq \mu_L,$$

(4)
\[ \phi_L > E_1 > \mu_R. \]  

(5)

As a result of the condition Eq. (4) there will be a finite current injection \( \Gamma_e \) directly into the upper subband. In contrast, because the lower level \( E_1 \) is situated below \( \phi_L \), there will be no current injection directly into the lower subband. Moreover, because Eqs. (4) and (5) ensures \( E_2, E_1 > \mu_R \), there will be fast tunneling escape rates, \( \Gamma_{c2} \) and \( \Gamma_{c1} \), out from both resonant levels (as none of the finite collector states are thus occupied.)

Adapting the discussion in Section I.B we may estimate the tunneling escape rates as follows

\[ \Gamma_{cj=1,2} = \frac{v_j}{2L_{QB}} T_R(E_j) = \frac{\sqrt{2E_j/m^*_e}}{2L_{QB}} T_R(E_j). \]  

(6)

Here \( v_j = \sqrt{2E_j/m^*_e} \) denotes the velocity of resonant level \( E_j=1,2 \) and

\[ T_R(E_j) \approx 16\theta(E_j - \phi_R) \frac{\sqrt{E_j(E_j - \phi_R)}}{\phi_B - E_j} \exp(-2L_B \sqrt{2m^*_e(\phi_B - E_j)}), \]  

(7)

denotes the probability for tunneling through the \( L_B = 30 \, \text{Å} \) thick barriers for which we assume a constant potential height \( \phi_B = 214 \, \text{meV} \).

As listed in Table 3.2, within the range, Eq. (3), of voltage drops allowing the potential realization of a net stimulated emission, we predict from Eqs. (6) and (7) only a moderate voltage-drop dependence of the escape rates

\[ 0.40 \, \text{meV} \ll \Gamma_{c1} \ll 0.56 \, \text{meV}, \]  

(8)

\[ 0.93 \, \text{meV} \ll \Gamma_{c2} \ll 1.09 \, \text{meV}. \]  

(9)

Such a moderate variation with the voltage drop (as well as the possible electron-charging effects on these tunneling rates) can (if desired) be negated by a small
charge in the width of the tunneling barriers \( L_B \) which dramatically modifies the tunneling probability, see Eq. (7).

III.C The wavefunction-symmetry variation

Figure 3.2 above also illustrate the significant quantum-confined Stark effect\(^1\) on the symmetry of the quasi-bound levels.\(^2\) In particular, it is clear from the bottom panel of Figure 3.2 that the voltage drop restores an approximate wavefunction-inversion symmetry at the avoided crossing, \( V = V_{\text{sym}} \). In this section we (a) demonstrate this inversion-symmetry is almost exact, (b) introduce the center-of-charge separation \( \langle \Psi_2 | x | \Psi_2 \rangle - \langle \Psi_1 | x | \Psi_1 \rangle \) (dipole matrix element \( \langle \Psi_2 | x | \Psi_1 \rangle \)) as a qualitative measure of the wavefunction asymmetry (overlap,) and (c) determine the wavefunction symmetry and overlap as function of the voltage drop \( V \).

The vanishing center-of-charge separation,

\[
\langle \Psi_2^\delta | x | \Psi_2^\delta \rangle - \langle \Psi_1^\delta | x | \Psi_1^\delta \rangle \equiv 0, \tag{10}
\]

characterizing the avoided crossing at \( V_{\text{sym}} \) automatically ensures an approximate inversion symmetry of the corresponding wavefunctions. However, for the Figure 3.1 tunneling structure we find an almost exact symmetry because there is only a small difference in the widths of the individual quantum wells.

Figure 3.4 verifies that the wavefunction-inversion symmetry is almost exact at the avoided crossing, \( V = V_{\text{sym}} \). Specifically, the top and bottom panels of Figure 3.4 test the expected anti-symmetry and symmetry,

\[
-\Psi_2^\delta(x_0 - x) = \Psi_2^\delta(x - x_0), \tag{11}
\]

\[
\Psi_1^\delta(x_0 - x) = \Psi_1^\delta(x - x_0), \tag{12}
\]
FIGURE 3.4 Test of the restored near-exact wavefunction-inversion symmetry at avoided crossing, \( V = V_{\text{sym}} = 22.9 \) mV. The set of vertical dashed lines indicates the positions of both the central quantum-well barrier and of the external tunneling barriers confining the wavefunctions, \( \Psi_{1,2}^{\phi}(x) \). The quantum-confined Stark effect\(^1\) causes at \( V = V_{\text{sym}} \) an avoided crossing in the resonant level positions, see Figure 3.3. By symmetry the center-of-charge separation must vanish at this avoided crossing, \( \langle \Psi_{2}^{\phi}|x|\Psi_{2}^{\phi} \rangle - \langle \Psi_{1}^{\phi}|x|\Psi_{1}^{\phi} \rangle \equiv 0 \), (see also Figure 3.5) and the quantum-confined Stark effect must thus in addition restore an approximate inversion-symmetry of the corresponding wavefunctions,\(^2\) \( \Psi_{1,2}^{\phi}(x) \). For the specific far-infrared tunneling structure (with schematics shown in Figure 3.1) this wavefunction-inversion symmetry is very accurate. Specifically, the top panel demonstrates that the upper-resonant-level wavefunction which vanishes at \( x = x_0 \) (indicated by vertical dotted line) is almost completely anti-symmetric, \( \Psi_{2}^{\phi}(x - x_0) = -\Psi_{2}^{\phi}(x_0 - x) \). The bottom panel correspondingly demonstrates that the lower-resonant-level wavefunction is symmetric, \( \Psi_{1}^{\phi}(x - x_0) = \Psi_{1}^{\phi}(x_0 - x) \), also around \( x = x_0 \).
FIGURE 3.4

Applied bias

$V_{sym}=22.9 \text{ mV}$

$\Psi_2^s(x)$

$E_2$

$\Psi_1^s(x)$

$E_1$

$x_0-L_{QB}/2 \quad x_0 \quad x_0+L_{QB}/2$

$x \quad [\text{Å}]$
of upper- and lower-level wavefunction $\Psi_2^\delta(x)$ and $\Psi_1^\delta(x)$ assuming the node $x_0$ of
$\Psi_2^\delta(x)$ forms the inversion point. The excellent agreement between the left- and
right-hand-side expressions of Eqs. (11) and (12) verifies the near-exact wavefunc-
tion-inversion symmetry restored at $V_{sym}$ in the still asymmetric potential (see
bottom panel of Figure 3.2.)

This near-exact correspondence between the vanishing center-of-charge sepa-
ration, Eq. (10), and a restored inversion symmetry, Eqs. (11) and (12), suggest
$\langle \Psi_2 | x | \Psi_2 \rangle - \langle \Psi_1 | x | \Psi_1 \rangle$ as a qualitative measure of the wavefunction asymmetry at
$V \neq V_{sym}$. We also introduce the dipole matrix element $\langle \Psi_2 | x | \Psi_1 \rangle$ as a qualitative
measure of the wavefunction overlap.

To motivate these qualitative measures of the wavefunction characteristics we
consider a simple two-level model and assume we can expand the upper- and lower-
level wavefunctions at voltage drop $V$,

$$
\Psi_2^{(V)}(x) = \cos(\chi(V - V_{sym})) \Psi_2^\delta(x) - \sin(\chi(V - V_{sym})) \Psi_1^\delta(x), \quad (13)
$$

$$
\Psi_1^{(V)}(x) = \sin(\chi(V - V_{sym})) \Psi_2^\delta(x) + \cos(\chi(V - V_{sym})) \Psi_1^\delta(x), \quad (14)
$$

exclusively in terms of $\Psi_{1,2}^\delta(x)$. We furthermore assume these $V = V_{sym}$ wavefunc-
tions has an exact inversion symmetry

$$
\langle \Psi_2^\delta | x | \Psi_2^\delta \rangle \equiv \langle \Psi_1^\delta | x | \Psi_1^\delta \rangle \equiv x_0, \quad (15)
$$

around the node $x_0$ of $\Psi_2^\delta(x)$.

At $V = V_{sym}$ we assume the unitary angle $\chi$ in Eqs. (13) and (14) take the
value, $\chi(V = V_{sym}) \equiv 0$. To determine the voltage drop dependence of the unitary
angle in general $\chi(V - V_{sym})$, we expand the Hamiltonian $H_V$ for the electron
motion in the confinement potential into \( H_s \) (corresponding to \( V = V\text{sym} \)) and a correction term \( H_1 \),

\[
H_V = H_s + H_1,
\]

\[
H_1 = -e(V - V\text{sym}) \frac{(x - x_0)}{L_{QB}}.
\]

At a general value of \( \chi \) the Hamiltonian \( H_V \) has the off-diagonal matrix elements

\[
\langle \psi_2^{(V)} | H_V | \psi_1^{(V)} \rangle = \langle \psi_2^{(V)} | H_s | \psi_1^{(V)} \rangle + \langle \psi_2^{(V)} | H_1 | \psi_1^{(V)} \rangle,
\]

\[
\langle \psi_2^{(V)} | H_s | \psi_1^{(V)} \rangle = \frac{\Delta_s}{2} \sin(2\chi(V - V\text{sym}))
\]

\[
\langle \psi_2^{(V)} | H_1 | \psi_1^{(V)} \rangle = -\frac{e(V - V\text{sym})}{L_{QB}} \cos(2\chi(V - V\text{sym})) \langle \psi_2^s | x | \psi_1^s \rangle,
\]

where \( \Delta_s \) denotes the subband separation at \( V = V\text{sym} \). The combined off-diagonal matrix element, Eq. (18), must vanish for the correct value of \( \chi(V - V\text{sym}) \). Hence we obtain the condition

\[
\tan(2\chi(V - V\text{sym})) = \frac{\langle \psi_2^s | x | \psi_1^s \rangle}{\Delta_s} \frac{2e}{L_{QB}} (V - V\text{sym}).
\]

We note that in the limit \( V \rightarrow \pm \infty \) we obtain the value \( \chi(V \rightarrow \pm \infty) = \pm \pi/4 \) and that in particular the \( V \rightarrow \infty \) limit results in upper- and lower-level wavefunctions

\[
\psi_2^{(\infty)}(x) = \psi_L(x) \equiv [\psi_2^s(x) - \psi_1^s(x)] / \sqrt{2},
\]

\[
\psi_1^{(\infty)}(x) = \psi_R(x) \equiv [\psi_2^s(x) + \psi_1^s(x)] / \sqrt{2},
\]

concentrated (although not completely localized) in the right and left quantum well, respectively. Within our two-level description these wavefunctions represent the largest possible wavefunction asymmetry and the variation \(-\pi/4 < \chi(V - V\text{sym}) < \pi/4 \) of the unitary angle present itself as a qualitative measure of this asymmetry.
FIGURE 3.5 Voltage-drop variation of the center-of-charge separation, \( \langle \Psi_2 | x | \Psi_2 \rangle - \langle \Psi_1 | x | \Psi_1 \rangle \) and of the dipole-matrix element \( \langle \Psi_2 | x | \Psi_1 \rangle \) (top panel) around avoided crossing, \( V = V_{sym} \), identified in bottom panel. Solid curve in top panel shows dramatic variation around \( V = V_{sym} \) of the center-of-charge separation introduced (see text) as a simple measure of the wavefunction symmetry. In Chapter IV we demonstrate this symmetry-variation causes a dramatic voltage-drop variation of the nonequilibrium electron-electron scattering rate \( \Gamma_{22 \rightarrow 21} \) (involving two upper-subband electrons of which only one decays to subband \( E_1 \).) The double-dashed-dotted curve in top panel shows a moderate voltage-drop variation (also related to the wavefunction symmetry, see text) of the dipole-matrix element — a simple measure of the wavefunction overlap. In Chapter IV we find this moderate variation of \( \langle \Psi_2 | x | \Psi_1 \rangle \) causes a significant variation also of the nonequilibrium electron-electron scattering rate \( \Gamma \equiv \Gamma_{22 \rightarrow 11} \) (involving two upper-subband electrons which both decay to two subband \( E_1 \).) We emphasize that the avoided crossing, \( V = V_{sym} \), results (by design) within the range of voltage drops — identified in the lower panel — which ensures an exclusive upper-subband current injection. We have arranged this so that our predictions for a dramatic symmetry/voltage-drop dependence of the nonequilibrium electron-electron scattering rate is relevant for the range of possible current injections. This choice does not, however, ensures the maximum possible intersubband population inversion as explained in Chapter IV.
FIGURE 3.5
Moreover, the variation of this unitary angle $\chi(V - V_{sym})$ is directly reflected in the center-of-charge separation

$$\langle \Psi_2^{(V)} | x | \Psi_2^{(V)} \rangle - \langle \Psi_1^{(V)} | x | \Psi_1^{(V)} \rangle = -2 \sin(2\chi(V - V_{sym})) \langle \Psi_2^s | x | \Psi_1^s \rangle, \quad (24)$$

and in the dipole matrix element

$$\langle \Psi_2^{(V)} | x | \Psi_1^{(V)} \rangle = \cos(2\chi(V - V_{sym})) \langle \Psi_2^s | x | \Psi_1^s \rangle. \quad (25)$$

We shall assume these relations also holds approximately for the actual potential problem for which the eigenvalues and wavefunctions must of course be determined not through Eq. (21) but using a Schrödinger-solver code. This assumption finally motivates the introduction of the center-of-charge separation, $\langle \Psi_2^s | x | \Psi_2^s \rangle - \langle \Psi_1^s | x | \Psi_1^s \rangle$, as a qualitative measure of the wavefunction asymmetry.

To motivate our use of the dipole matrix element, $\langle \Psi_2 | x | \Psi_1 \rangle$, as a qualitative measure of the wavefunction overlap we mention that Eq. (24) is consistent with an expected maximum (minimal) overlap at $V = V_{sym}$ ($V \to \pm \infty$).

The top panel of Figure 3.5 shows the calculated voltage-drop dependence of both the dipole matrix element, solid curve, and the center-of-charge separation, dashed curve. The center-of-charge separation (measure of wavefunction asymmetry) exhibits a significant voltage-drop dependence. The charge-separation vanishes at $V = V_{sym}$ but the magnitude quickly rises and begins to saturate (essentially at the inter-quantum-well separation $\sim 90 \text{ Å}$) at $|V - V_{sym}| \gtrsim V_{sym}$. The observed strong quantum-confined Stark effect on the wavefunction asymmetry causes a dramatic variation on the nonequilibrium electron-electron scattering, see Chapter IV.

* The beginning saturation at $V = 0$ is also evident in the top panel of Figure 3.2 where the upper- (lower)-level charge-density is found concentrated mostly in the narrower right (wider left) quantum-well.
Finally we observe that there is in contrast only a moderate variation of the dipole matrix element (measure of the wavefunction overlap,) although this variation is of course still given by the wavefunction asymmetry, see Eq. (24). The largest value obtains at the avoided crossing, \( V = V_{\text{sym}} \), but the dipole matrix element (and hence the optical transition rate) remains significant within the entire (potential) emission regime identified in the bottom panel.

### III.D Experimental determination of intersubband decay

Our choice of the specific tunneling structure shown in Figure 3.1 is motivated by the observed small intersubband decay rate, \( 1/\tau \ll 0.03 \text{ meV} \) arising at temperatures \( T \ll 50 \text{ K} \) under weak optical pumping of the corresponding isolated quantum-well structure.\(^3\)\(^4\) We shall argue in Section III.E below that the value \( 1/\tau = 0.03 \text{ meV} \) constitute a strict experimental bound on the impurity, interface-defect and on the acoustic-phonon scattering. Since we furthermore find that the thermally activated phonon emission can be ignored at temperatures \( T \leq 25 \text{ K} \) we feel justified in assuming that \( \Gamma_{\text{sp}} = 0.03 \text{ meV} \) constitutes at \( T \leq 25 \text{ K} \) an experimental bound on the total single-electron decay (\( \Gamma_{\text{se}} \)) arising with the nonequilibrium current injection.

The experimental determination of the intersubband decay rate by Dr. J. Heyman et al., at the Free Electron Laser lab at U. C. Santa Barbara used a photovoltage measurement to determine the net optical excitation. By furthermore balancing the net intersubband absorption with the intersubband decay they obtained an estimate for the net decay.
The investigated structure\textsuperscript{3,4} comprises the same central asymmetric double-quantum-well structure as in our Figure 3.1 tunneling structure but surrounded instead by two 5200 Å digital Al\textsubscript{0.3}Ga\textsubscript{0.7}As-alloy barrier layers. A pair of delta-doped Si layers more than 700 Å away provides a finite quantum-well sheet density \(N_s \sim 10^{11} \text{ cm}^{-2}\) without introducing a large ionized-impurity scattering within the double-quantum-well potential. An ohmic contact is formed to this sheet-density of quantum-well electrons which together with a top gate evaporated onto the heterostructure surface \(d \approx 5000\) Å above the double-quantum-well potential forms a dielectric capacitor.

The experimental measurements are undertaken in the presence of a finite bias, \(V_G = -0.8\) V, applied between the top gate and the quantum-well electrons. This result\textsuperscript{6} in an estimated sheet-density of \(N_s = 1.18 \times 10^{11} \text{ cm}^{-2}\) sufficient to ensure a strong optical response (absorption.) The capacitance charge, \(eN_s\), remains essentially constant during the short (\(\sim 1\) µs) pulses of the optical pumping with the Free Electron Laser radiation.

The dashed curve in the bottom panel of Figure 3.6 shows the equilibrium chemical potential\textsuperscript{*} \(\mu_0\) as a function of the temperature \(T\). The equilibrium distribution is at low temperature, \(T \ll 25\) K, characterized as a lower-subband Fermi sea, i.e., with a near-constant chemical potential (Fermi surface) and with the sheet-density \(N_s = 1.18 \times 10^{11} \text{ cm}^{-2}\) located almost exclusively in the lower subband. However, at temperatures \(T \gtrsim 25\) K there is a dramatic drop in the chemical potential \(\mu_0\) and the system can at \(T \gtrsim 50\) K essentially be described by a Boltzmann distribution. There is in particular a finite upper-subband occupation which within this

\* We shall in the following discussion of the optical pumping experiment define the energy zero-point by \(E_1 \equiv 0\).
FIGURE 3.6 Comparison of measured net intersubband decay rate $1/\tau$ (triangles) and theory estimate of optical-phonon induced decay rates $\Gamma_{LO}^{op}/\Gamma_{LO}^{ci}$ (top panel) for the optical-pumped/current-injected distribution described by chemical potential $\mu_0/\mu_2$ (given in bottom panel.) At temperatures $T \ll 25$ K, our theory estimate $\Gamma_{LO}^{op}$ is in reasonable agreement with the measured intersubband decay rates which can be described by thermal activation energy $\Omega_{LO} - \Delta \approx 24$ meV. The measured value, $1/\tau = 0.03$ meV constitute a strict bound on the total impurity, interface-defect, and acoustic-phonon scattering also in the presence of a strong upper-subband current injection. Our theory estimate, $\Gamma_{LO}^{ci}$, of the corresponding optical-phonon induced decay is evaluated for the maximum possible upper-subband current injection below $\mu_L \equiv \mu_2 + E_2$. This rate $\Gamma_{LO}^{ci}$ does exceed the decay rate $\Gamma_{LO}^{op}$ for the weakly optically pumped distribution. However, even with the current-injected distribution the optical-phonon induced decay rate $\Gamma_{LO}^{ci}$ is still thermally activated and can essentially be ignored at temperatures $T \leq 25$ K. We feel, as a consequence, ourselves justified in assuming that also the total single-electron decay rate, $\Gamma_{se}$, at $T \leq 25$ K remains bounded by the experimental value $1/\tau = 0.03$ meV.
FIGURE 3.6
Boltzmann description is estimated at
\[
\frac{n_2^0}{N_s} \bigg|_B = \frac{\exp(-\Delta/T)}{1 + \exp(-\Delta/T)} \approx 0.07N_s \quad \text{at } T = 50 \text{ K},
\]
while the actual (Fermi-Dirac) distribution yields \(n_2^0(50 \text{ K}) \approx 0.1N_s\).

Under such equilibrium conditions, i.e., in the absence of any optical pumping we gave of course a balance between the intersubband transitions,
\[
\frac{n_2^0}{\tau_{2\rightarrow 1}} \equiv \frac{n_1^0}{\tau_{1\rightarrow 2}},
\]
where \(1/\tau_{2\rightarrow 1} \ (1/\tau_{1\rightarrow 2})\) denotes the transition rate from subband \(E_2 \ (E_1)\) to \(E_1 \ (E_2)\) — averaged over the equilibrium electron-distribution.

The optical pumping by the Free Electron Laser radiation excites an intersubband plasmon and increases the upper-subband occupation to \(n_2\). At strong optical pumping intensities and/or with very slow plasmon relaxation by intra- and intersubband scattering it may be necessary\(^7\) to include coherent effects in a discussion of the correspondingly increased resulting intersubband decay. However, we believe that it is appropriate to neglect such coherent effects at weak optical pumping and at \(T \sim 50 \text{ K}\) where the approximate Boltzmann electron distribution ensures\(^8\) a fast (pico-second) electron-electron scattering and in particular plasmon decay, see for example Ref. 9. We assume one may also neglect plasmon effects at the intermediate temperatures, \(25 \text{ K} \lesssim T \lesssim 50 \text{ K}\) and shall describe the effects of the weak optical pumping simply in terms of a change in the upper-subband single-particle distribution function.

Specifically, with a weak optical excitation \(\delta n_2 \equiv n_2 - n_2^0\) we expect a linear increase (decrease) of the intersubband scattering from subband \(E_2 \ (E_1)\) to \(E_1 \ (E_2)\).
(E_2) resulting in a net decay:

$$\frac{\delta n_2}{\tau} = \delta n_2 \left( \frac{1}{\tau_{2 \rightarrow 1}} + \frac{1}{\tau_{1 \rightarrow 2}} \right).$$  \hspace{1cm} (28)$$

Moreover, we assume that the transition rates $1/\tau_{2 \rightarrow 1}$ and $1/\tau_{1 \rightarrow 2}$ in Eq. (28) obtains as a simple averaging over the weakly optically excited distribution and shall neglect the change $1/\tau_{1 \rightarrow 2}$ with optical pumping. On the other hand, in the resulting approximation,

$$\frac{1}{\tau} \approx \frac{1}{\tau_{2 \rightarrow 1}} + \frac{n_2^0}{n_1^0} \frac{1}{\tau_{2 \rightarrow 1}}.$$  \hspace{1cm} (29)$$

for the net intersubband decay we note that the optically excited rate, $1/\tau_{2 \rightarrow 1}$, exceeds the equilibrium rate $1/\tau_{2 \rightarrow 1}^0$ because the optically excited distribution results in a stronger optical-phonon emission.*

The increased (net) intersubband decay, $\delta n_2/\tau$, must be balanced by the net absorption. Assuming a pump frequency $\omega$ (tuned to the intersubband optical transitions) and intensity $S_{FEL}(\omega)$ we have,

$$\frac{\delta n_2}{\tau} = \frac{S_{FEL}(\omega)}{\omega} \sigma_{ab}(\omega)(n_2 - n_1),$$  \hspace{1cm} (30)$$

where we have introduced the lower-subband occupation density $n_1 = N_s - n_2$, and the absorption cross section $\sigma_{ab}(\omega)$.

The key idea in the experimental determination involves using an estimate for the center-of-charge separation to determine the total number $\delta n_2 \equiv (n_2 - n_2^0)$ of optically excited electrons from a measurement of the photovoltage. To make this connection we reiterate that the top contact and the $N_s$ quantum-well electrons

* The thermal activation energy for optical-phonon emission in the equilibrium distribution is given by the phonon frequency, $\Omega_{LO}$, itself. However, the thermal activation energy in the (weakly) optically excited distribution is reduced to $\Omega_{LO} - \Delta$, see Section III.E.
together forms a dielectric capacitor. The total charge, $eN_s$, bound on this capacitor remains constant during the short pulses of the pumping radiation. The effective charge-separation in equilibrium is denoted $d$ and following Ref. 3 we observe that the optical excitation $\delta n_2$ increases this separation by

$$\delta d = \delta n_2 \times [\langle \Psi_2|x|\Psi_2 \rangle - \langle \Psi_1|x|\Psi_1 \rangle], \quad (31)$$
due to the finite center-of-charge separation. This increase, Eq. (31), in the effective capacitor separation is reflected in the gate-bias,

$$\frac{\Delta V_G}{V_G} = -\frac{\delta d}{d} = [\langle \Psi_2|x|\Psi_2 \rangle - \langle \Psi_1|x|\Psi_1 \rangle] \times \left( \frac{\delta n_2}{N_{2D}} \right). \quad (32)$$

Finally, inserting the expression for the photo-voltage, Eq. (32), into Eq. (30) finally yields an expression for the decay rate,

$$\frac{1}{\tau} = \frac{S_{FEL}(\omega)}{\omega} \sigma_{ab}(\omega) \left\{ 2 - (1 + 2n_2^0) \left[ \frac{\langle \Psi_2|x|\Psi_2 \rangle - \langle \Psi_1|x|\Psi_1 \rangle}{d\Delta V_G} \right] V_G \right\}. \quad (33)$$

Given measurements of (a) the photo-voltage, $\Delta V_G$, (b) the absorption cross section, $\sigma_{ab}(\omega)$ at lasing frequency $\omega$, and (c) the Free Electron Laser pump intensity $S_{FEL}(\omega)$, and a theory estimate of the center-of-charge separation, Eq. (33) finally allows the experimental determination reported in Ref. 3.

The set of triangles in Figure 3.6 shows, as a function of inverse temperature, these the experimentally determined net decay rates obtained at weak optical pumping, $S_{FEL} \approx 10$ mW/cm². We observe in particular that the weak-optical pumping decay rate remains bounded at $1/\tau \approx 0.03$ meV at temperatures $T < 50$ K but shows a significant temperature dependence which in Ref. 3 was fit to two thermal activation energies. For the higher-temperature regime, $25$ K $\approx T \approx 50$ K,

* Heyman et al. used instead an equivalent determination of the radiation transmission coefficient, see Ref. 3.
they found the thermal activation energy $24 \pm 3$ meV which corresponds well to the difference $\Omega_{LO} - \Delta \approx 25$ meVs between the optical-phonon frequency $\Omega_{LO}$ and the subband separation.\textsuperscript{3} For the low-temperature regime ($T \lesssim 25$ K, however, the experimental data is fit to a thermal activation energy ($\sim 3$ meV) of unknown origin.\textsuperscript{3}

III.E Single-electron decay in tunneling structure

In this final section we consider the total single-electron decay arising with the exclusive upper-subband current injection. A central issue is whether these single-electron decay processes are faster than in the presence of a weak optical pumping of the corresponding quantum-well structure.

Formal estimates for the impurity, interface-defect, and acoustic-phonon scattering are described in Ref. 11. However, rather than providing a detailed estimate for these rates we argue below that the weak-optical-pumping experimental\textsuperscript{3} value, $1/\tau \approx 0.03$ meV, constitute an experimental bound for the impurity, interface-defect, and acoustic-phonon scattering also with a current-injected upper-subband electron distribution (at temperatures $T \lesssim 50$ K.)

In contrast, we do find that the decay due to the thermally activated optical-phonon scattering, increases with the current injection. However, we still predict a vanishing rate, $\Gamma_{LO}^{cf} \leq 10^{-3}$ meV at temperatures $T \leq 25$ K. We consequently fell justified in assuming also the total single-electron decay rate $\Gamma_{se}$ bounded by $1/\tau = 0.03$ meV at temperatures $T \leq 25$ K.
Consider first the decay due to impurity and interface-defect scattering. These intersubband decay processes are obviously elastic and are thus not effected by any Pauli exclusion even for the weakly optically pumped electron distribution. Although the current-injection may result in a wider range of possible in-plane momentum transfer, see lower left panel in Fig. I.4, the average momentum transfer is still going to be the characteristic intersubband momentum

\[ q_\Delta \equiv \sqrt{2m_e^* \Delta}. \]  

We thus expect the impurity and interface defect scattering to be almost unchanged from the weak-optical-pumping distribution and to the nonequilibrium distribution resulting from the current injection.

Consider next the decay due to the acoustic-phonon scattering. Using the formal estimates provided in Ref. 11, it follows directly (from the combined conservation of in-plane momentum and energy) that also these scattering processes are essentially elastic.* Specifically, for an electron phonon located at the bottom of the upper subband, we estimate the electron-phonon transfer at just 0.5 meV. We expect no difference between the acoustic-phonon decay rate for the weakly optically pumped distribution and the current-injected distribution arising from neither (i) the Pauli exclusion principle, of (ii) a difference in the average matrix element.

To complete our discussion of the total single-electron decay we need only consider the decay due to the optical-phonon emission. These spontaneous emission processes are of course at all experimental temperatures partially inhibited because the optical-phonon frequency \( \Omega_{LO} \approx 36 \text{ meV} \) exceeds the subband separation \( \Delta \approx 11 \text{ meV} \). Adapting the formal treatment in Ref. 11 we have estimated

* The electron-acoustic-phonon scattering illustrated by the dashed arrow in the lower left panel of Fig. I.4 is shown with a strongly exaggerated energy transfer
the thermally activated intersubband decay rates resulting from optical-phonon-emission processes both for the optically-pumped distribution ($\Gamma_{LO}^{op}$) and for the current injected distribution ($\Gamma_{LO}^{ci}$). The solid (dashed) curve in the top panel of Figure 3.6 shows our Fermi-golden-rule estimate for decay rate $\Gamma_{LO}^{ci}$ ($\Gamma_{LO}^{op}$).

In estimating the rate $\Gamma_{LO}^{op}$ we have assumed that the optical pumping results in an increased upper-subband occupation density $\delta n_2$ distributed according to

$$f_{2}^{op}(\overline{k}) = \frac{\delta n_2}{n_1^0} \frac{1}{1 + \exp(E_1(k) - \mu)}, \quad (35)$$

where $n_1^0$ denoted the equilibrium lower-subband occupation. We have furthermore neglected all effects of the Pauli exclusion principle although there is at $T \sim 50$ K a finite occupation $> 0.5$ of the bottom of the lowest subband.

Although we have thus overestimated the actual decay due to the optical-phonon scattering we find a reasonable agreement between the estimated rate, $\Gamma_{LO}^{ci}$ (dashed curve in top panel of Figure 3.6) and the experimentally observed values of $1/\tau$. In particular, there is a reasonable agreement with the reported thermal activation energy

$$E_{act} = \Omega_{LO} - \Delta \approx 24 \pm 3 \text{ meV}, \quad (36)$$

at intermediate temperatures, $25 \text{ K} \lesssim T \lesssim 50 \text{ K}$.

Consider finally the decay rate $\Gamma_{LO}^{ci}$ arising from the optical-phonon emission processes with a current injected distribution. In providing this estimate we neglect again the Pauli exclusion within the lower subband and have assumed the maximum possible upper-subband occupation given by a choice of $\phi_L = E_2$ and a complete subband occupation between $E_2$ and $\mu_L$. This occupation is described by
the distribution function
\[ f_2^c(k) = f_\mu_2(E_{||}(\vec{k})) = \frac{1}{1 + \exp(E_{||}(k) - \mu_2)} \]  

(37)

with effective upper-subband chemical potential,
\[ \mu_2 \equiv \mu_L - E_2 = \mu_L - \phi_L. \]  

(38)

The solid curve in the bottom panel of Figure 3.6 shows the temperature variation of this chemical potential. Nevertheless, as is clear in the top panel of Figure 3.6, the rate \( \Gamma_L^{ci} \) still remains thermally activated and eventually becomes negligible. In particular, we find that the rate can be ignored, \( \Gamma_L^{ci} \ll 10^{-3} \text{ meV}, \) at temperatures \( T \leq 25 \text{ K}. \)

In summary we have obtained an experimental bound on the total single-electron decay in the presence of the current injection,
\[ \Gamma_{sp} \ll 0.03 \text{ meV}, \quad \text{at} \quad T \leq 25 \text{ K}. \]  

(39)

This estimate results because we can (a) assume the impurity, interface-defect, and acoustic-phonon scattering strictly bounded by the experimental value, \( 1/\tau = 0.03 \text{ meV}, \) and (b) because the thermally activated optical-phonon emission can be completely ignored at temperatures \( T \leq 25 \text{ K}. \)

Finally, we emphasize that no such experimental bound applies to the nonequilibrium electron-electron scattering even though Ref. 3 also reports measurements of the net decay rate at a strong optical pumping with a finite upper-subband occupation density \( n_2 \gtrsim N_s/4. \) This follows because the strong optical pumping (a) could make coherent effects very important, \( 7 \) and (b) results in a different nonequilibrium upper-subband occupation than with a strong current injection into the
Figure 3.1 structure. The second observation is important because the electron-electron scattering depends on the actual nonequilibrium distribution.

A detailed modeling and discussion of the intersubband decay in the presence of a strong optical pumping is beyond the scope of this dissertation. However, we can determine the nonequilibrium electron-electron intersubband scattering arising with the current injection into the Figure 3.1 tunneling structure and thus determine also the total intersubband decay and resulting population inversion. This motivates the study of the nonequilibrium intersubband electron-electron scattering reported on in Chapter IV.
REFERENCES


5. We thank Dr. Galdrikian, UCSB for kind permission to use his Schrödinger-solver code in determining the (quasi-bound) energy levels and corresponding wavefunctions.

6. Professor James Heyman, MacAlester College; private communications.

7. Professor W. Kohn, UCSB; private communications.


10. Dr. Bryan Galdrikian, UCSB; private communications.

CHAPTER IV

THE NONEQUILIBRIUM
ELECTRON-ELECTRON SCATTERING

In this chapter we study the nonequilibrium intersubband electron-electron scattering in detail. Specifically we evaluate for a complete upper-subband occupation below emitter chemical potential, $\mu_L \equiv \mu_2 + E_2$, the total scattering rate $\Gamma \equiv \Gamma_{22\rightarrow11} (\Gamma_{22\rightarrow21})$ between two upper-subband electrons which both decay to the lower subband (of which only one decays to subband $E_1$) and estimate the resulting population inversion in the (hypothetical) Figure 1.1-tunneling structure.

We found in the previous Chapter III that the total single-electron intersubband decay, $\Gamma_{se}$, arising with the nonequilibrium current injection is at temperatures $T \approx 0.03 \text{ meV}$ bounded by decay rate, $1/\tau \approx 0.03 \text{ meV}$, measured\textsuperscript{1,2} at weak optical pumping of the corresponding isolated double-quantum-well structure.\textsuperscript{3} If the total intersubband decay rate $\Gamma_{nr}$, where restricted to $\Gamma_{se} \approx 0.03 \text{ meV}$, it would be straightforward to maintain the intersubband population inversion.

We find, however, a very significant nonequilibrium electron-electron scattering (\(\Gamma\)) whose strength can be deduced from measurements\textsuperscript{1,2} of the equilibrium depolarization shift, $\Delta^\ast$, that is, the shift of the equilibrium absorption peak, $\Delta^\ast$, from
the subband separation, $\Delta$. We furthermore find that the nonequilibrium scattering $\Gamma$ is never significantly reduced by screening and, unlike the near-equilibrium electron-electron scattering, is not inhibited by the Pauli exclusion principle (as we can assume population inversion.)

We consequently: (1) identify a simple scaling of the nonequilibrium electron-electron scattering $\Gamma$ with the upper-subband occupation, (2) explain why the Pauli exclusion within the (assumed completely filled) upper subband prevents such a scaling for the other nonequilibrium electron-electron scattering rate $\Gamma_{22\rightarrow21}$, (3) identify a dramatic voltage-drop dependence of both nonequilibrium electron-electron scattering rates, $\Gamma$ and $\Gamma_{22\rightarrow21}$, associated with the quantum-confined Stark effect on the wavefunction inversion symmetry, (4) document that this wavefunction-symmetry variation in particular allows a significant reduction of also the combined electron-electron intersubband decay, $\sim 2\Gamma + \Gamma_{22\rightarrow21}$, (5) predict a very strong decay rate $\sim 2\Gamma \approx 1$ meV for an upper-subband sheet-density $N_L \approx 10^{11}$ cm$^{-2}$ comparable to that in the mid-infrared quantum cascade laser, and finally (6) demonstrate that a smaller population inversion density ($\sim 0.2 \times 10^{11}$ cm$^{-2}$) can be maintained at a moderate tunneling current density.

The detailed outline of this chapter is as follows. In Section IV.A we introduce the intersubband Coulomb matrix element $U(q)$ which describes the $(2, 2) \rightarrow (1, 1)$ scattering $\Gamma$. We discuss both the unscreened and effectively screened interaction and explain how the strength of this interaction can be extracted from an experimental determination of the depolarization shift. In Section IV.B we demonstrate and explain an approximate scaling with electron occupation, $\mu_2/\Delta$, of the intersubband scattering rate $\Gamma$. In particular, we find the unscreened scattering
rate is well approximated by a linear-in-$\mu_2$ scaling result whereas, for the effective screened interaction, we find some deviation. The effective screened causes, however, at most a factor-of-two reduction.

In Section IV.C we consider the other nonequilibrium intersubband electron-electron scattering $(2,2) \to (2,1)$. We evaluate the scattering rate $\Gamma_{22\to21}$ assuming a complete upper-subband electron occupation below $\mu_L = \mu_2 + E_2$ and we consequently include only the scattering events in which the final upper-subband state is located above $\mu_L$ and is thus available. For comparison we also evaluate the unscreened rate $\Gamma^*_{22\to21}$ in which this Pauli exclusion effect is ignored. For the unscreened rate $\Gamma^*_{22\to21}$ we find again an almost exact linear-in-$\mu_2$ scaling result. However, for the scattering rate $\Gamma_{22\to21}$ we find that the restrictions on the scattering phase space imposed by the Pauli exclusion principle prevents such a simple scaling even for the unscreened interaction.

In Section IV.D we predict a dramatic voltage-drop dependence of both $\Gamma$ and $\Gamma_{22\to21}$ which we explain based on the so-called quantum-confined Stark effect on the wavefunction symmetry. We show that the combined intersubband electron-electron decay rate ($\propto 2\Gamma + \Gamma_{22\to21}$) enhances to a maximum at the avoided crossing, $V = V_{sym}$. Finally, in Section IV.E we provide a simple estimate for the resulting intersubband population inversion also at this avoided crossing. We demonstrate in particular, that a finite intersubband population inversion can be maintained in the Figure 1.1-tunneling structure in spite of the very strong nonequilibrium electron-electron scattering.
IV.A The effective intersubband Coulomb interaction

The intersubband scattering $(2, 2) \rightarrow (1, 1)$ involves, as illustrates in the top panel of Figure 1.1, two upper-subband electrons which both decay to lower subband $E_1$. For this intersubband electron-electron scattering, $(2, 2) \rightarrow (1, 1)$, the subband separation $\Delta$ defines a characteristic in-plane momentum transfer

\[ q_\Delta = \sqrt{2m^*_e \Delta}, \]  

in the intersubband electron-electron scattering rate $\Gamma \equiv \Gamma_{22-11}$. Together with the zero-frequency background dielectric constant $\epsilon_0$, this characteristic momentum transfer provides a natural scaling of the effective Coulomb interaction,

\[ V_{21,21}(q) \equiv \frac{e^2}{\epsilon_0 q_\Delta} U(q), \]  

which describe an intersubband scattering event, $(2, 2) \rightarrow (1, 1)$, with in-plane momentum transfer $q$.

The effectively screened dimensionless matrix element $U(q)$ in Eq. (2) is defined

\[ U(q) \equiv U_{21,21}(q) = 2\pi \int dx_2 \int dx_1 \Psi_2(x_2)\Psi_1(x_2) \times \]
\[ q_\Delta \exp \left( -\sqrt{q^2 + q_{TF}^2} |x_2 - x_1| \right) / \sqrt{q^2 + q_{TF}^2} \Psi_2(x_1)\Psi_1(x_1), \]  

in terms of the resonant-level wavefunctions\textsuperscript{14} and Thomas-Fermi wave vector $q_{TF}$ introduced below. The corresponding unscreened interaction matrix element $U^0(q)$ is given by the $q_{TF} \rightarrow 0$ limit of Eq. (3).

We observe that (even) the unscreened interaction matrix element, $U^0(q)$, is finite at $q = 0$. For the effectively screened ($U(q)$) and unscreened ($U^0(q)$) dimensionless matrix elements we furthermore find (a) a moderate $q$ variation, (b) a
correspondingly moderate dependence on the Thomas-Fermi screening wave vector 
$q_{TF} < q_{\Delta}$, and (c) a numerical value of $U^0(q = 0)$ that can be estimated from experiments.$^2$

The moderate variation of $U^0(q)$ (point (a),) namely,

$$U^0(q_{\Delta}) \approx U^0(0)/4,$$  \hspace{1cm} (4)

can be deduced analytically for a square quantum well with infinite barriers. Choosing the width, $L_0 \equiv \sqrt{3}\pi/q_{\Delta}$, of the quantum well to provide the actual subband separation $\Delta$ the unscreened dimensionless matrix element becomes

$$U_{sqw}^0(q) = 2\pi^2\sqrt{3}[A_1(qL_0) + A_1(qL_0)$$

$$- 2qL_0(1 - e^{-qL_0})(A_1(qL_0) - A_3(qL_0))^2],$$  \hspace{1cm} (5)

where

$$A_j(qL_0) = \frac{1}{(qL_0)^2 + (j\pi)^2}.\hspace{1cm} (6)$$

The value at $q = 0$ is $U_{sqw}^0(0) \approx 4$ whereas at $q = q_{\Delta}$ the unscreened matrix element reduces to $U_{sqw}^0(q_{\Delta}) \approx 1$.

Screening of the nonequilibrium electron-electron interaction, Eq. (3), is for simplicity treated within in an effective Thomas-Fermi approach defined by a corresponding heated equilibrium three-dimensional electron distribution. Specifically, the electron distribution within the tunneling region (having upper- and lower-subband occupation densities, $n_1$ and $n_2$, respectively) is described by an isotropic three-dimensional electron gas of density $n_{3D} = (n_1 + n_2)/LQB$ at an elevated effective temperature, $1/\beta_{eff} = \Delta$. As an effective treatment of screening in the intersubband Coulomb interaction we use Eq. (3) the wave vector, $q_{TF}$, defined by
this three-dimensional gas,

\[ q_{TF}^2 = \left( \frac{4\pi e^2}{\epsilon_0 L Q B \Delta} \right) (n_1 + n_2). \tag{7} \]

As illustrated in top panel of Figure 1.1, a complete current-injected upper-
subband electron occupation below the emitter chemical potential, \( \mu_L \), naturally
defines a quasi-Fermi level

\[ \mu_2 \equiv \mu_L - E_2, \tag{8} \]

and a corresponding wave vector

\[ k_{\mu_2} \equiv \sqrt{2m^*} \mu_2. \tag{9} \]

This wave vector identifies the in-plane momentum of the most energetic of the
current-injected states in the upper subband. The maximum upper-subband occu-
pation density,

\[ N_L = \frac{k_{\mu_2}^2}{2\pi} \propto \mu_2, \tag{10} \]

result with a complete occupation below this wave vector \( k_{\mu_2} \). Neglecting the
lower-subband occupation \( (n_1 = 0,) \) and assuming such a maximum upper-subband
occupation, \( n_2 = N_L \), we obtain the Thomas-Fermi wave vector

\[ q_{TF} = 2 \left( \frac{R y^* a^*}{\Delta L Q B} \right)^{1/2} k_{\mu_2} \]

\[ \approx 0.9 k_{\mu_2}, \tag{11} \]

used in the effectively screened matrix element, Eq. (3).

Note that the Thomas-Fermi screening wave vector remains smaller than the
characteristic momentum transfer, \( q_{TF} < k_{\mu_2} \leq q_\Delta \) at \( \mu_2 \leq \Delta \), even at \( \mu_2 = \Delta \). That this effective Thomas-Fermi screening is ineffective (observation (b)) in
modulating the nonequilibrium electron-electron scattering thus follows directly from the observation
\[ U(q) = U^0(\sqrt{q^2 + q_{TF}^2}), \]  
for (12)

since we expect (observation (a)) only a moderate \( q \)-variation of \( U^0(q) \) around \( q = q_\Delta \).

Finally, the strength of the effective nonequilibrium electron-electron interaction, Eq. (2), is evident (point (c)) from the observed\(^1,2\) large equilibrium depolarization shift\(^4,5,6,7\) \( \Delta^* - \Delta \approx 2 \) meV of the absorption peak, \( \Delta^* \), from the far-infrared subband separation \( \Delta \approx 11 \) meV at sheet-density \( N_s \approx 10^{11} \) cm\(^{-2}\). In particular, neglecting the coupling to other quantum levels and assuming an inversion symmetry of the wavefunctions we have\(^6\)

\[ (\Delta^*)^2 - \Delta^2 = 2\Delta N_s(e^2/\epsilon_0 q_\Delta)U^0(q = 0). \]  
for (13)

For a finite occupation density \( n_2 \propto N_L \sim N_s \approx 10^{11} \) cm\(^{-2}\) we thus expect the strong interaction \( N_L(e^2/\epsilon_0 q_\Delta)U^0(0) \ll 2 \) meV.

To motivate the relation, Eq. (13), we follow the discussion in Ref. 4 and consider the dynamic screening response of the double-quantum-well structure. Specifically, we describe the response of a sheet density \( N_s \) of electrons — initially located in lower level \( E_1 \) of quantum-well potential \( \phi_{dc}(x) \) and described by wavefunction \( \Psi_1(x) \) — to an external ac-field\(^*\) \( E_{ext} \exp(-i\omega t) \). This electric field results in a time-dependent potential \( \phi_{ac}(x) \exp(-i\omega t) \). An approximate treatment of the dynamic screening results by assuming that \( \phi_{dc}(x) \exp(-i\omega t) \) includes the self-consistent field arising from the electrons.

\* Polarized in the \( \hat{x} \)- or growth-direction.
The time-dependent Schrödinger equation,

\[-i \frac{\partial}{\partial t} \Psi(x,t) = - \frac{1}{2m_e^*} \frac{\partial^2}{\partial x^2} \Psi(x,t) + e [\phi_{dc}(x) + \phi_1(x) \exp(-i\omega t)] \Psi(x,t), \quad (14)\]

for the electron wavefunction, \( \Psi(x,t) \), is formally solved to linear order in the potential \( \phi_{ac}(x) \). Inserting this formal result in the Poisson equation,

\[ \frac{\partial^2}{\partial x^2} \phi_{ac}(x) \exp(-i\omega t) = \frac{4\pi N_s e^2}{\epsilon_0} \left[ |\Psi_1(x)|^2 - |\Psi(x,t)|^2 \right], \quad (15)\]

allows an analytical determination\(^4\) of \( \phi_{ac}(x) \) for a two level system.

Following Ref. 4 we introducing an effective length,

\[ S_{22} = \int_{-\infty}^{\infty} dx \left( \int_{-\infty}^{x} dx' \Psi_2(x')\Psi_1(x') \right)^2, \quad (16)\]

assume an effective absorption line-width, \( \Gamma_\phi \), and define the intersubband plasmon frequency \( \omega_{ip} \) by

\[ \omega_{ip}^2 = \frac{8\pi N_s e^2}{\epsilon_0} \Delta S_{22}. \quad (17)\]

The power dissipated within the entire quantum-well region can then be written\(^4\)

\[ P(\omega) = N_s e^2 |\langle \Psi_2 |x| \Psi_1 \rangle|^2 |E_{ext}|^2 \frac{\omega^2 \Delta \Gamma_\phi}{(\omega^2 - \Delta^2 - \omega_{ip}^2)^2 + (\omega \Gamma_\phi)^2}. \quad (18)\]

This power dissipation describes in particular the frequency-dependent absorption from level \( E_1 \) to level \( E_2 \) which is peaked at a frequency

\[ \Delta^* = \sqrt{\Delta^2 + \omega_{ip}^2} \approx \Delta + \frac{4\pi N_s e^2 S_{22}}{\epsilon_0}. \quad (19)\]

This dynamical-screening effect results in the quantum-well structure investigated in Ref. 1,2 in the significant depolarization shift, \( \Delta^* - \Delta \approx 2 \text{ meV} \).

To establish the connection with the intersubband Coulomb interaction, expressed above in Eq. (13), we interpret the depolarization-shifted absorption peak,
Eq. (19), as a collective node identified as a node of an effective dielectric constant. Specifically, while the actual self-consistent field does exhibit a spatial variation within the double-quantum-well potential (as a result of the dynamic screening\textsuperscript{4}) we can define an effective dielectric function through

\[
\langle \Psi_2 | \Phi_{ac} | \Psi_1 \rangle \equiv -\frac{E_{ext}}{\epsilon_{eff}(\omega)} \langle \Psi_2 | x | \Psi_1 \rangle.
\]  
(20)

Using the results for a two-level system (listed in in Ref. 4) we then have

\[\epsilon_{eff}(\omega) = 1 - \frac{4\pi e^2}{\epsilon_0} \chi_{12}^{0R}(\omega) S_{22},\]  
(21)

\[\chi_{12}^{0R}(\omega) = \frac{2\Delta}{\omega^2 - \Delta^2 + 2i\delta\omega}.
\]  
(22)

Inserting this expression for \(\epsilon_{eff}(\omega)\) in Eq. (18) we obtain

\[P(\omega) = N_s e^2 |\langle \Psi_2 | x | \Psi_1 \rangle|^2 \frac{|E_{ext}|^2}{\left|1 - \frac{4\pi e^2 S_{22}}{\epsilon_0} \chi_{12}^{0R}(\omega)\right|}
\]  
(23)

and the absorption peak, Eq. (19), coincides with the nodes of \(\epsilon_{eff}(\omega)\).

We next observe that — for a symmetric potential (only) — the effective dielectric constant, \(\epsilon_{eff}(\omega)\), is identical with the standard intersubband RPA-result\textsuperscript{6}

\[\epsilon_{RPA}\text{Inter}(\omega) = 1 - \left(\frac{e^2}{\epsilon_0 q\Delta}\right) U^0(q \to 0) \chi_{12}^{0R}(\omega).
\]  
(24)

The equivalence between Eqs. (21) and (24) (for symmetric wavefunctions) can be expressed simply through the condition

\[4\pi q\Delta S_{22} = U^0(q \to 0).
\]  
(25)

To verify the identity, Eq. (25), we observe that

\[\lim_{q \to 0} U^0(q) = -q\Delta 2\pi \int_{-\infty}^{\infty} dx_2 \int_{-\infty}^{\infty} dx_1 \Psi_2(x_2) \Psi_1(x_2) |x_2 - x_1| \Psi_2(x_1) \Psi_1(x_1).
\]  
(26)
We furthermore rewrite the length, Eq. (16), according to

\[ 2S_{22} = -2 \int_{-\infty}^{\infty} dx_1 \Psi_2(x_1) \Psi_1(x_1) \times \]
\[ \int_{-\infty}^{\infty} dx_2 \Theta(x_1 - x_2)(x_1 - x_2) \Psi_2(x_2) \Psi_1(x_2). \] (27)

For a symmetric potential the identity Eq. (25) then follows simply by the inversion \((x_j=1,2 \rightarrow -x_j=1,2)\) within one of the two double-integrations in Eq. (27).

The equivalence between \(e_{\text{eff}}(\omega)\) and the intersubband RPA-result \(e_{\text{Inter}}^{RPA}(\omega)\), finally established the connection, Eq. (13), between the measured\(^1\)\(^2\) equilibrium depolarization shift, \(\Delta^* - \Delta\), and the intersubband Coulomb matrix element \(U^0(q \rightarrow 0)\). Specifically, since the nodes of \(e_{\text{Inter}}(\omega)\) are given by

\[ (\omega^2 - \Delta^2) = \frac{e^2}{\epsilon_0 q \Delta} U^0(q \rightarrow 0) 2N_s \Delta, \] (28)

we obtain the following approximate expression for the depolarization shift

\[ \Delta^* - \Delta \approx N_s \frac{e^2}{\epsilon_0 q \Delta} U^0(q \rightarrow 0). \] (29)

As previously stated, the large equilibrium depolarization shift, \(\Delta^* - \Delta \approx 2 \text{ meV}\) observed\(^1\)\(^2\) for a \(N_s \approx 10^{11} \text{ cm}^{-2}\) electron sheet density thus indicates a very significant nonequilibrium intersubband scattering \(\Gamma\).

IV.B Scaling of nonequilibrium scattering \(\Gamma\)

The nonequilibrium current injection results, as illustrated in Figure 1.1, in a finite upper-subband electron occupation between \(E_2\) and the emitter chemical potential \(\mu_L\). In contrast, the lower subband is only populated through intersubband decay processes. We shall here, using the Fermi golden rule, estimate the
opposite-spin scattering rate$^{15}$ $\Gamma \equiv \Gamma_{22\rightarrow11}$ assuming (a) a complete upper-subband occupation given by the quasi-Fermi level, $\mu_2$, introduced in Eq. (8), and (b) a completely empty lower-subband. The second assumption (b) allows us to ignore the Pauli exclusion principle in our estimate of $\Gamma$ since all final lower-subband states are available.

The scattering rate $\Gamma$ arises from opposite-spin $(2, 2) \rightarrow (1, 1)$ scattering events with a finite in-plane momentum transfer $q$. The transition rate is given by the intersubband Coulomb matrix element, Eq. (2). Based on the formal derivation in Appendix A we obtain at zero temperature the following Fermi-golden-rule estimate$^{15}$

$$\Gamma = \frac{\text{Ry}^* (\mu_2)}{\pi^2} \left( \frac{\mu_2}{\Delta} \right) \int \frac{dq}{k_{\mu_2}} |U(q)|^2 \left[ \left( \frac{q}{k_{\mu_2}} \right) P(q) \right].$$

(30)

Here, $P(q)$, denotes a dimensionless phase-space contribution given by

$$N_L^2 \mu_2^{-1} P(q) = \frac{1}{2} \left( \frac{2}{A} \right)^2 \sum_{\vec{k}, \vec{k}'} \Theta(\mu_2 - E_{\|}(k)) \Theta(\mu_2 - E_{\|}(k')) 2\pi \delta(E_f - E_i),$$

(31)

where $A$ denotes the in-plane area of the structure and where the implied energy conservation reads

$$E_f - E_i = 2E_{\|}(q) + q \cdot (\vec{k} - \vec{k}')/m_e^* - 2\Delta.$$

(32)

The conservation of both in-plane momentum and energy, expressed in Eqs. (31) and (32), restricts the range of possible in-plane momentum transfers,

$$-1 \leq q/k_{\mu_2} - \sqrt{1 + (q\Delta/k_{\mu_2})^2} \leq 1.$$

(33)

The domain, Eq. (33), of finite phase-space contributions, $P(q)$, also specifies the integration range in the estimate, Eq. (30). We observe in particular that the intersubband scattering always occurs at a finite in-plane momentum transfer $q > 0$. 
The displayed factor one-half in the phase-space contribution Eq. (31) arises because we in this dissertation only consider the direct scattering between opposite-spin electrons. In addition to the opposite-spin scattering $\Gamma$ there is of course also a same-spin scattering which comprises both a direct contribution ($\equiv \Gamma$) and an exchange contribution. However, we demonstrate in Appendix A that the direct and exchange contributions to the same-spin scattering exactly cancel if the interaction matrix element $(U(q))$ is independent of $q$. Because we expect just a moderate $q$-variation of the interaction matrix element (see Section IV.A) we restrict ourselves to evaluating alone the (dominant) opposite-spin direct scattering $\Gamma$.

The dashed-single-dotted curve in Figure 4.1 shows the (opposite-spin) scattering rate $\Gamma$ evaluated from Eqs. (30), (31), and (32) using unscreened matrix element $U^0(q)$. The dashed-double-dotted curve in Figure 4.1 shows the scattering rate $\Gamma$ evaluated using the effectively screened interaction matrix element $U(q) = U^0(\sqrt{q^2 + q^2_{TF}})$ defined by the effective Thomas-Fermi screening wave vector $q_{TF}$ introduced in Section IV.A. We find that screening causes at most a factor-of-two reduction even at $\mu_2 = \Delta$.

The solid curve in Figure 4.1 demonstrates a linear-in-$\mu_2$ scaling of the scattering rate $\Gamma$. This approximate scaling can be expressed

$$\Gamma \approx \frac{\text{Ry}^*}{\pi^2} \left( \frac{\mu_2}{\Delta} \right) |U(q_\Delta)|^2 I_P(\mu_2/\Delta), \quad (34)$$

where

$$I_P(\mu_2/\Delta) \equiv \int \frac{dq}{k_{\mu_2}} \frac{q}{k_{\mu_2}} P(q) \approx I_P(0) = 0.785 \quad (35)$$

represent a dimensionless integrated phase-space measure essentially independent of $\mu_2/\Delta$. For the unscreened interaction (dashed-single-dotted curve) the linear
FIGURE 4.1 Approximate linear-in-µ2 scaling, solid curve, of nonequilibrium scattering rate Γ estimated for a complete (current-injected) upper-subband occupation (between E2 and emitter chemical potential µL = E2 + µ2.) The dashed-single(double)-dotted curve shows the scattering rate Γ evaluated for the unscreened (effectively screened) intersubband Coulomb interaction matrix element U0(q) (U(q) = U0(√q2 + qTF2)) defined by the screening wave vector qTF < qΔ introduced in Section IV.A) In Figure 4.2 we justify the scaling approximation, Γ ≈ (Ry*/π2)(µ2/Δ)U(qΔ)|2IP(0), given by the interaction matrix element evaluated at the characteristic momentum transfer, q Δ = √2m*Δ, and an almost constant dimensionless integrated phase-space measure, IP(µ2/Δ) ≈ IP(0). The solid curve shows this scaling approximation evaluated for the unscreened interaction, i.e., using U0(qΔ). Comparing with the unscreened rate Γ (dashed-single-dotted curve) we find the predicted linear-in-µ2 scaling is almost exact. For the effectively screened interaction (dashed-double-dotted curve) there is some deviation arising with the increased value of the Thomas-Fermi wave vector (qTF 2 ≈ µ2.) At most this screening causes a factor-of-two reduction even at µ2 = Δ.
\[ \Gamma = \Gamma_{22,11} [\text{meV}] \]

\[ \left( \frac{\text{Ry}^*}{\pi^2} \right) \left( \frac{\mu_2}{\Delta} \right) |U^0(q_\Delta)|^2 I_P(0) \]

- \( V = 27.0 \text{ mV} \)
- \( \Delta = 11.1 \text{ meV} \)

\( q_{TF} = 0 \)

\( q_{TF}/k_{\mu_2} = 0.9 \)

**FIGURE 4.1**
scaling, Eqs. (34) and (35), is nearly exact. For the screened interaction there is some deviation arising from the decreasing value of the squared characteristic matrix element $|U(q_\Delta)|^2 = |U^0(\sqrt{q^2 + q^2_\Delta})|^2$ with the enhanced Thomas-Fermi screening wave vector, $q_{TF} \propto k_{\mu_2}$, at higher electron occupation, $\mu_2/\Delta$.

The middle panel of Figure 4.2 demonstrates scaling of weighted dimensionless phase-space contribution, $(q/k_{\mu_2})P(q)$, and explains the result Eq. (35). In particular, we find this weighted phase-space measure, $(q/k_{\mu_2})P(q)$, (a) is restricted to a domain (Eq. (33)) with a $\mu_2/\Delta$-independent extension, (b) is always strongly peaked at the characteristic momentum transfer $q_\Delta$ resulting in the constant maximum value $(q_\Delta/k_{\mu_2})P(q_\Delta) = 8/(3\pi)$, and consequently (c) result in an almost $\mu_2/\Delta$-independent integrated phase-space measure, $I_P(\mu_2/\Delta) \approx I_P(0)$.

The key observation is (b) which follows from the assumed quadratic subband dispersion, $E_\parallel(k)$. Specifically, the delta-function argument, Eq. (32), reduces at the characteristic momentum transfer, $q = q_\Delta$ (only,) to

$$E_f - E_i = q_\Delta(k_y - k'_y)/m^*_e,$$

where we have chosen the $y$-direction to be parallel to the in-plane momentum transfer $\hat{q}$. The phase-space contribution, given by Eq. (31), then scales as

$$N^2_L k_{\mu_2}^{-1} P(q_\Delta) = 4m^*_e k_{\mu_2}^3 / 2\pi^3 q_\Delta,$$

and (upon extracting $N^2_L k_{\mu_2}^{-1} = m^*_e k_{\mu_2}^2 / 2\pi^2$) we arrive at the predicted constant maximum value

$$(q_\Delta/k_{\mu_2})P(q_\Delta) = 8/(3\pi).$$

The observations (a)-(c) taken together justifies the central scaling approximation, Eqs. (34) and (37), assuming that the interaction matrix element $U(q)$ only
FIGURE 4.2 [Proof that no many-body theorist are needed here, or] Scaling with electron occupation, \(\mu_2/\Delta\), of weighted phase-space contribution, middle panel, and unscreened (effectively screened) squared interaction matrix element, top (bottom) panel, describing the scattering rate \(\Gamma\). The middle panel shows the weighted phase-space contribution, \((q/k\mu_2)P(q)\) (defined by \(k_\mu^2 = 2m^*\mu_2\)) at different electron occupations. We find in the text (a) a constant extension of the scattering domain, \(-1 \leq 1/k\mu_2 - \sqrt{1 + (q_\Delta/k\mu_2)^2} \leq 1\), (b) a constant maximum value, \((q_\Delta/k\mu_2)P(q_\Delta) = 8/(3\pi)\) (indicated by horizontal dotted line,) at the characteristic momentum transfer \(q_\Delta = \sqrt{2m^*_e\Delta}\), and consequently (c) an almost constant integrated dimensionless phase-space measure, \(I_P(\mu_2/\Delta) \approx I_P(0) \sim 1\). The top (bottom) panel demonstrates that the \((q/k\mu_2)\)-variation of the squared unscreened interaction matrix element remains moderate at all \(\mu_2/\Delta\). Because, furthermore, the weighted phase-space contribution is peaked at \(q = q_\Delta\) we can approximate \(\Gamma\) using \(|U^0(q)|^2 \approx |U^0(q_\Delta)|^2\) (\(|U(q)|^2 \approx |U(q_\Delta)|^2\) for the unscreened (effective screened) interaction. This finally justifies the scaling approximation introduced in Figure 4.1.
$\Gamma = \Gamma_{22 \rightarrow 11}$

$V = 27.0 \text{ mV}$
$q_{TF}/k_{\mu_2} = 0.0$

$|U^0(q_\Delta)|^2$

$|U(q)|^2$

$(q/k_{\mu_2})P(q)$

$I_P(\mu_2/\Delta) \sim I_P(0) \sim 1$

$V = 27.0 \text{ mV}$

$\mu_2/\Delta = 1/4$
$q_{TF}/k_{\mu_2} = 0.9$

$\mu_2/\Delta = 1/2$

$\mu_2/\Delta = 3/4$

$(q - q_\Delta)/k_{\mu_2}$

FIGURE 4.2
exhibits a moderate $q$-variation. In particular, since the scattering phase space is peaked at $q = q_\Delta$ we may then introduce the approximation $U(q) \approx U(q_\Delta)$ and obtain Eqs. (34) and (35).

The top panel in Figure 4.2 demonstrates that the $q/k\mu_2$-variation of squared unscreened matrix element $|U^0(q)|$ remains — at all electron occupations, $\mu_2/\Delta$ — small within the domain of the phase-space contribution, $(q/k\mu_2)P(q)$. It also illustrates that the characteristic value, $|U^0(q_\Delta)|^2$, is a a good (weighted) average value of actual squared unscreened matrix element $|U^0(q)|^2$. The characteristic value, $U^0(q_\Delta)$, of the unscreened interaction is of course independent of the electron occupation, $\mu_2/\Delta$, which explains the almost exact agreement between the scaling result, Eq. (34), and the numerically evaluated estimate, Eq. (30), for the unscreened case — compare solid and dashed-single-dotted curves in Figure 4.1.

Similarly, the bottom panel of Figure 4.2 demonstrates that the $q/k\mu_2$-variation of squared, effective screened, interaction matrix element $|U(q)|^2$ remains small and can be approximated by $|U(q_\Delta)|^2$. This again motivates the approximation approximation Eqs. (34) and (35) also for the screened interaction — provided we use the effectively screened characteristic matrix element, $U(q_\Delta) = U^0(\sqrt{q_\Delta^2 + q_{TF}^2})$ (this approximation is not, however, evaluated in Figure 4.1.) That is, the deviation from a linear-in-$\mu_2$ scaling for the interacting rate is primarily due to the increased screening of $|U(q_\Delta)|^2$ given by $q_{TF}^2 \propto \mu_2$.

IV.C The nonequilibrium scattering $\Gamma_{22\to21}$

In addition to the scattering $\Gamma$, the nonequilibrium upper-subband current injection also results in a finite scattering $(2, 2) \to (2, 1)$ involving two upper-subband
electrons of which only one decays to subband $E_1$. In this section we evaluate a Fermi-golden-rule estimate for the nonequilibrium electron-electron scattering rate $\Gamma_{22\rightarrow 21}$ assuming again (a) a complete upper-subband electron occupation (of density $N_L$) below $\mu_L \equiv \mu_2 + E_2$, and (b) an empty lower subband $E_1$.

Because of the assumption (a) we must respect the Pauli exclusion principle within the upper subband. That is, in evaluating the rate $\Gamma_{22\rightarrow 21}$ it is necessary to ensure that contributing scattering event has the final upper-subband state positioned above the emitter chemical potential $\mu_L = \mu_2 + E_2$. For comparison we also evaluate the scattering rate $\Gamma_{22\rightarrow 21}$ in which we do not thus restrict the scattering phase-space.

The contribution to $\Gamma_{22\rightarrow 21}$ from a scattering event $(2, 2) \rightarrow (2, 1)$ with in-plane momentum transfer $q$ is described by the effective Coulomb interaction

$$V_{22,21}(q) = \left( \frac{e^2}{\epsilon_0 q \Delta} \right) U_{12,22}(q)$$

(39)

In analogy with Section IV.A we have again introduced a scaling by $q\Delta \equiv \sqrt{2m_e \Delta}$ and have thus define the dimensionless matrix element

$$U_{22,21}(q) = 2\pi \int dx_2 \int dx_1 \Psi_2(x_2)\Psi_2(x_2) \times \frac{q\Delta \exp\left(-\sqrt{q^2 + q_{TF}^2}|x_2 - x_1|\right)}{\sqrt{q^2 + q_{TF}^2}} \Psi_2(x_1)\Psi_1(x_1).$$

(40)

We assume the same effective screening as for the matrix element $U_{21,21}(q)$. That is, we use in Eq. (40) the Thomas-Fermi wave vector $q_{TF}$ introduced in Section IV.A. Again the unscreened interaction matrix element, $U_{22,21}^0(q)$, results in the $q_{TF} \rightarrow 0$ limit of Eq. (40).
Based on a formal derivation provided in Appendix A we estimate the opposite-spin scattering at zero temperature using the following Fermi-golden-rule estimate

\[ \Gamma_{22\rightarrow21} = \frac{\text{Ry}^*}{\pi^2} \left( \frac{\mu_2}{\Delta} \right) \int \frac{dq}{k_{\mu_2}} |U_{22,21}(q)|^2 \left[ \frac{(q/k_{\mu_2})P_{22\rightarrow21}(q)}{E_{f1} - E_{i1}} \right]. \]  

In analogy with the discussion in Section IV.B we have in Eq. (41) introduced a dimensionless phase-space contribution, \( P_{22\rightarrow21}(q) \), defined by

\[ N_L^2 \mu_2^{-1} P_{22\rightarrow21}(q) = \frac{4 \Theta(\mu_2 - E_{\parallel}(k)) \times}{A^2} \sum_{k,k'} \left[ \Theta(\mu_2 - E_{\parallel}(k')) \Theta(E_{\parallel}(k' - q) - \mu_2) \right] 2\pi\delta(E_f - E_i), \]  

where again \( A \) denotes the in-plane area of the tunneling structure.

In contrast to the discussion in Section IV.B, however, the condition for energy conservation in Eq. (42) now reads

\[ E_f - E_i = 2E_{\parallel}(q) + \vec{q} \cdot (\vec{k} - \vec{k'})/m_e^* - \Delta, \]  

as only one electron decays to subband \( E_1 \). Also, the additional term, \( \Theta(E_{\parallel}(k' - q) - \mu_2) \), Eq. (42), restricts the final upper-subband state to be located above \( \mu_L \) in accordance with the Pauli exclusion principle.*

The different condition, Eq. (43), for energy conservation and the restriction imposed by the Pauli exclusion principle modifies the scattering phase-space. We find that

\[ q_{\Delta/2} \equiv \sqrt{2m_e^*(\Delta/2)} = q_{\Delta}/\sqrt{2}, \]  

and not \( q_{\Delta} \) itself, constitute the actual characteristic in-plane momentum transfer for \( \Gamma_{22\rightarrow21} \). Also, the phase-space domain, i.e., the range of possible in-plane

* The Pauli exclusion principle does not of course affect the rate \( \Gamma \equiv \Gamma_{22\rightarrow11} \) as all lower-subband states are assumed empty.
FIGURE 4.3 Electron-occupation dependence of nonequilibrium electron-electron scattering rate $\Gamma_{22\rightarrow21}$ estimated for a complete (current-injected) upper-subband occupation (between $E_2$ and emitter chemical potential $\mu_L \equiv E_2 + \mu_2$). In estimating $\Gamma_{22\rightarrow21}$ we respect the Pauli exclusion within the upper-subband (only) and include only the scattering events in which the final upper-subband state is located above $\mu_L$. The dashed-dotted curve shows the resulting estimate evaluated using the unscreened interaction described by intersubband Coulomb matrix element, $U_{22,21}(q)$. The solid curve shows the scattering rate estimated for the screened interaction, $U_{22\rightarrow21}(q) = U_{22,21}^0(\sqrt{q^2 + q_{TF}^2})$, where $q_{TF}$ denotes the effective Thomas-Fermi screened wave vector introduced in Section IV.A. We observe that this effective screening (given by $q_{TF}^2 \propto \mu_2$) again causes only a factor-of-two reduction even at $\mu_2 = \Delta$. In contrast to the scattering rate $\Gamma \equiv \Gamma_{22\rightarrow11}$, however, we find that the Pauli exclusion within the upper-subband prohibits a linear-in-$\mu_2$ scaling of even the unscreened scattering $\Gamma_{22\rightarrow21}$. To illustrate this point the figure also shows the corresponding (unscreened) rate, $\Gamma_{22\rightarrow21}^0$ (dotted curve,) in which we assume all final upper-subband states are available. Comparing unscreened scattering rates, $\Gamma_{22\rightarrow21}^0$ and $\Gamma_{22\rightarrow21}$, we observe that the Pauli exclusion within the upper-subband eventually causes a factor-of-two reduction of the scattering phase-space at $\mu_2 \approx \Delta$. 

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FIGURE 4.3
momentum transfers, is here restricted to
\[-1 \leq q/k_{\mu_2} - \sqrt{1 + (q_{\Delta/2}/k_{\mu_2})^2} \leq 1. \tag{45}\]

We observe that the phase-space contribution, Eq. (42), contains a displayed factor one half since we again only consider the opposite-spin scattering rate $\Gamma_{22\rightarrow21}$. To justify the neglect of the same-scattering we note that although the unscreened interaction matrix element, $U_{22,21}^0(q)$, will generally* diverge in the limit $q \rightarrow 0$, we find below a very moderate $q$-variation with the actual phase-space domain, Eq. (45), of possible in-plane momentum transfers $q$. Again we thus expect the exchange and the direct contribution to the same-spin scattering to almost cancel.

The solid curve in Figure 4.3 shows the estimated opposite-spin scattering rate, $\Gamma_{22\rightarrow21}$, evaluated for the effectively screened interaction defined by $U_{22,21}(q) = U_{22,21}^0(\sqrt{q^2 + q_T^2})$. For comparison the dashed-single-dotted curve shows the estimate rate $\Gamma_{22\rightarrow21}$ evaluated using the unscreened interaction. We note that the screening defined by the effective Thomas-Fermi wavevector, $q_{TF} \propto k_{\mu_2}$, causes at most a factor-of-two reduction also of this other nonequilibrium electron-electron scattering rate $\Gamma_{22\rightarrow21}$.

The top (bottom) panel of Figure 4.4 demonstrates that the variation with scaled momentum transfer, $q/k_{\mu_2}$, of squared unscreened (effectively screened) matrix element, $|U_{22,21}^0(q)|^2$ ($|U_{22,21}(q)|^2 = |U_{22,21}^0(\sqrt{q^2 + q_T^2})|^2$) remains small at all electron occupations, $\mu_2/\Delta$. The matrix element may as a consequence be approximated by the characteristic value, $U(q_{\Delta/2} \equiv q_{\Delta}/\sqrt{2})$.

The middle panel of Figure 4.4 shows $q/k_{\mu_2}$-variation of the weighted phase-space contribution, $(q/k_{\mu_2})P_{22\rightarrow21}(q)$. We first observe that since this contribution

* Except for strictly symmetric wavefunctions $\Psi_{1,2}(x)$. 
FIGURE 4.4 Electron-occupation dependence of weighted phase-space contribution \((q/k_{\mu_2})P_{22-21}(q)\), middle panel, and the unscreened (effectively screened) squared interaction matrix element, top (bottom) panel, defining scattering rate \(\Gamma_{22\rightarrow21}\). The middle panel shows the weighted phase-space contribution, \((q/k_{\mu_2})P_{22-21}(q)\) at different electron occupations. We find that \(q_{\Delta/2} \equiv q_{\Delta}/\sqrt{2}\) (identified by vertical dotted line) constitute a characteristic in-plane momentum transfer in the scattering \(\Gamma_{22\rightarrow21}\). We also find a \(\mu_2/\Delta\)-independent extension of the scattering domain, \(-1 \leq 1/k_{\mu_2} - \sqrt{1 + (q_{\Delta/2}/k_{\mu_2})^2} \leq 1\) for \(\Gamma_{22\rightarrow21}\). In contrast to the scattering \(\Gamma \equiv \Gamma_{22\rightarrow11}\), however, we find that the Pauli exclusion within the upper-subband reduces the scattering phase-space by as much as a factor of two at \(\mu_2 \approx \Delta\). To illustrate this point, the dotted curve shows the corresponding weighted phase-space measure, \((q/k_{\mu_2})P^*_{22\rightarrow21}(q)\), evaluated at \(\mu_2/\Delta = 1/2\). The top (bottom) panel demonstrates that the \(q/k_{\mu_2}\)-variation of squared unscreened (effective screened) interaction matrix element \(|U^0_{22,21}(q)|^2\) remains moderate at all electron occupations, \(\mu_2/\Delta\), and may be approximated by the characteristic value, \(|U^0_{22,21}(q_{\Delta/2})|^2\) \(\equiv |U^0_{22,21}(\sqrt{q_{\Delta/2}^2 + q_{TF}^2})|^2\). However, as is evident in Figure 4.3, there is no approximate linear-in-\(\mu_2\) scaling of even unscreened scattering rate \(\Gamma_{22\rightarrow21}\) because the integrated dimensionless phase-space measure, \(I_{22-21}(\mu_L/\Delta)\), decreases with \(\mu_2/\Delta\).
\[ \Gamma_{22\rightarrow 21} \]
\[ q_{\Delta/2} \]
\[ |U_{22,21}(q_{\Delta/2})|^2 \]
\[ P^*_{22\rightarrow 21}(q) \]
\[ I_{22\rightarrow 21}(\mu_2/\Delta) \]
\[ |U_{22,11}(q)|^2 \]
\[ (q/\mu_2)P_{22\rightarrow 21}(q) \]

**FIGURE 4.4**

- \( V = 27.0 \text{ mV} \)
- \( q_{TF}/k\mu_2 = 0.0 \)
- \( q_{TF}/k\mu_2 = 0.9 \)
- \( \mu_2/\Delta = 1/4 \)
- \( \mu_2/\Delta = 1/2 \)
- \( \mu_2/\Delta = 3/4 \)
(at relevant electron occupations, $\mu_2/\Delta < 1$,) remains peaked at the characteristic momentum transfer, Eq. (44), we may again approximate

$$\Gamma_{22\rightarrow21} \approx \frac{R_y^*}{\pi^2} \left( \frac{\mu_2}{\Delta} \right) |U_{22,21}(q\Delta)|^2 I_{22\rightarrow21}(\mu_2/\Delta),$$

with integrated phase-space measure

$$I_{22\rightarrow21}(\mu_2/\Delta) \equiv \int \frac{dq}{k_{\mu_2}} \frac{q}{k_{\mu_2}} P_{22\rightarrow21}(q).$$

However, the middle panel of Figure 4.4 also demonstrates a significant dependence on electron occupation, $\mu_2/\Delta$, of the weighted phase-space contribution, $(q/k_{\mu_2})P_{22\rightarrow21}(q)$, and thus of the integrated phase-space measure, Eq. (47). This reduction of the phase-space measure, Eq. (42), and in particular of the integrated measure, $I_{22\rightarrow21}(\mu_2/\Delta)$, prevents a linear-in-$\mu_2$ scaling of even the unscreened scattering rate $\Gamma_{22\rightarrow21}$.

We emphasize that this reduction of $I_{22\rightarrow21}(\mu_2/\Delta)$ results from Pauli exclusion within the upper-subband, see definition of scattering phase-space Eq. (42). To illustrate this point we also consider the scattering rate

$$\Gamma_{22\rightarrow21}^* = \frac{R_y^*}{\pi^2} \left( \frac{\mu_2}{\Delta} \right) \int \frac{dq}{k_{\mu_2}} |U_{22,21}(q)|^2 \left[ (q/k_{\mu_2})P_{22\rightarrow21}^*(q) \right],$$

with dimensionless phase-space contribution $P_{22\rightarrow21}^*(q)$, defined by

$$N_L^2 \mu_2^{-1} P_{22\rightarrow21}^*(q) = \frac{1}{2} \left( \frac{2}{A} \right)^2 \sum_{\vec{k},\vec{k}'} \Theta(\mu_2 - E_{||}(k)) \Theta(\mu_2 - E_{||}(k')) 2\pi \delta(E_f - E_i), \quad (49)$$

and Eq. (43). In this modified phase-space contribution, $P_{22\rightarrow21}^*(q)$, we do not require the final upper-subband state to be above $\mu_L$ unlike in Eq. (42).

The dotted curve in the middle panel of Figure 4.4 shows the weighted dimensionless phase-space measure, $(q/k_{\mu_2})P_{22\rightarrow21}^*(q)$ at $\mu_2/\Delta = 1/2$. In complete
analogy with the discussion in Section IV.B we find that weighted measure (a) is restricted to the same domain, Eq. (45), as \((q/k\mu_2)P_{22-21}(q)\), (b) is always strongly peaked at the characteristic momentum transfer, \(q_{\Delta/2} \equiv q_\Delta/\sqrt{2}\), with constant peak value, \((q_{\Delta/2}/k\mu_2)P(q_{\Delta/2}) = 8/(3\pi)\), and consequently (c) result in an almost \(\mu_2/\Delta\)-independent integrated phase-space measure, \(I_{22-21}(\mu_2/\Delta) \sim I_P(0)\), given by Eq. (35). We find as a consequence, an almost linear-in-\(\mu_2\) scaling of the scattering rate \(\Gamma^*_{22-21}\) when evaluated for the unscreed interaction, (dotted curve in Figure 4.4.)

Finally, comparing in Figure 4.4 the \(\mu_2/\Delta\)-variation of unscreened scattering rate \(\Gamma^*_{22-21}\) (dotted curve) and the corresponding variation of unscreened rate, \(\Gamma_{22-21}\) (dashed-single-dotted curve,) we identify the integrated effect of the Pauli exclusion within the upper-subband. Specifically, it is clear from Figure 4.4 that the upper-subband Pauli-exclusion at \(\mu_2/\Delta = 1\) causes an approximate factor-of-two reduction of the scattering rate, \(\Gamma_{22-21}\).

IV.D The wavefunction-symmetry dependence

The bottom panel of Figure 4.5 shows the quantum-confined Stark effect\(^9\) on the subband separation and on the wavefunction overlap and symmetry,\(^10\) discussed in Section III.C. The minimal subband separation occurs at voltage drop \(V_{sym}\) (vertical dotted line,) i.e., at the avoided crossing between levels \(E_1\) and \(E_2\). The dipole matrix element, \(\langle\Psi_2|x|\Psi_1\rangle\) (solid curve,) enhances only slightly with the increased wavefunction overlap at \(V_{sym}\). In contrast, the center-of-charge separation, \(\langle\Psi_2|x|\Psi_2\rangle - \langle\Psi_1|x|\Psi_1\rangle\) (dashed curve) vanishes at \(V_{sym}\) but rapidly changes with \(V - V_{sym}\). This variation of the center-of-charge separation reflects, as ex-
plained in Section III.C, the loss of wavefunction-inversion symmetry.

The top panel of Figure 4.5 shows the corresponding dramatic voltage-drop dependence of both scattering rate $\Gamma$ (solid curve) and of $\Gamma_{22\rightarrow21}$ (dashed curve). This voltage-drop variation — evaluated for an assumed constant ratio $\mu_{2}/\Delta = 1/2$ — reflects the wavefunction-symmetry dependence of the characteristic intersubband Coulomb matrix elements $U(q_\Delta)$ ($U_{22,21}(q_\Delta/2)$) which through the approximation Eq. (34) (Eq. (46)) determines $\Gamma$ ($\Gamma_{22\rightarrow21}$.) In particular, the characteristic matrix element $U(q_\Delta)$ contains an even number of upper-subband wavefunctions, can never be zero, and enhances significantly around $V \approx V_{sym}$ with the increased wavefunction overlap (as measured by the dipole matrix element.) In contrast, the characteristic matrix element $U_{22,21}(q_\Delta/\sqrt{2})$ contains three upper-subband wavefunctions and vanishes at $V \approx V_{sym}$ due to the restored approximate wavefunction-inversion symmetry (identified by the zero center-of-charge separation.)

In our discussion of this voltage-drop variation we first express the the general intersubband matrix element as

$$U_{ij,kl}(q) = 2\pi \int_{-\infty}^{\infty} dx_{1} \int_{-\infty}^{x_{1}} dx_{2} \frac{q_\Delta \exp(-\sqrt{q^2 + q_{TF}^2(x_{1} - x_{2})})}{\sqrt{q^2 + q_{TF}^2}} \times$$

$$[\Psi_{i}(x_{1})\Psi_{j}(x_{1})\Psi_{l}(x_{2})\Psi_{k}(x_{2}) + \Psi_{i}(x_{1})\Psi_{j}(x_{1})\Psi_{l}(x_{2})\Psi_{k}(x_{2})].$$

For symmetric wavefunctions it follows that the only finite intersubband matrix elements, Eq. (50), contains an even number of upper- and lower-level wavefunctions.\(^6\) Within the simple two-level description introduced in Section III.C we can then explicitly relate the variation of characteristic matrix element $U(q_\Delta)$ ($U_{22,21}(q_\Delta/2 = q_\Delta/\sqrt{2})$) to the corresponding voltage-drop variation in the dipole matrix element (center-of-charge separation.)
FIGURE 4.5 Dramatic voltage-drop dependence (top panel) of nonequilibrium electron-electron scattering rates, $\Gamma$ and $\Gamma_{22,21}$, explained (bottom panel) by the quantum-confined Stark effect on the wavefunction overlap and symmetry. Bottom panel identifies $V_{\text{sym}}$ (vertical dotted line) as the voltage drop with minimal subband separation (dashed-dotted curve). Observe that the dipole matrix element (solid curve) is nearly constant whereas the center-of-charge separation (dashed curve) vanishes at $V_{\text{sym}}$. The bias dependence of $\Gamma$ and $\Gamma_{22\rightarrow21}$ reflects the wavefunction-symmetry dependence of the characteristic matrix element $|U^2(q_\Delta)|^2$ and $|U^2_{22,21}(q_\Delta/2 = q_\Delta/\sqrt{2})|^2$, respectively. In particular, the matrix element $U(q_\Delta)$ and thus $\Gamma$ enhances at $V_{\text{sym}}$ because of the increased wavefunction overlap. In contrast, the matrix element $U_{22,21}(q_\Delta/2q_\Delta/\sqrt{2})$ and thus $\Gamma_{22\rightarrow21}$ are strongly reduced close to $V_{\text{sym}}$ but increases dramatically when, for $V \neq V_{\text{sym}}$, the wavefunction symmetry is lost. Finally, the alternating-long-short dashed curve in the top panel shows the combined electron-electron decay, $2\Gamma + \Gamma_{22\rightarrow21}$. We emphasize the strong voltage-drop variation of also this combined decay rate which enhances to a maximum at $V = V_{\text{sym}}$ but is significantly reduced at $V \neq V_{\text{sym}}$. 

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FIGURE 4.5
In this two-level model we assume the wavefunctions at a general voltage drop \( V \) can be expanded,

\[
\Psi_2^{(V)}(x) = \cos(\chi(V - V_{\text{sym}})) \Psi_2^s(x) - \sin(\chi(V - V_{\text{sym}})) \Psi_1^s(x),
\]

\[
\Psi_1^{(V)}(x) = \sin(\chi(V - V_{\text{sym}})) \Psi_2^s(x) + \cos(\chi(V - V_{\text{sym}})) \Psi_1^s(x).
\]

in terms of the assumed symmetric wavefunctions \( \Psi_{1,2}^s(x) \) characterizing the avoided crossing, \( V = V_{\text{sym}} \). The rotation angle, \( \chi \) in this unitary transformation is given by

\[
\tan(2\chi(V - V_{\text{sym}})) = \frac{\langle \Psi_2^s | x | \Psi_1^s \rangle}{E_{Q_B} - \Delta s} (V - V_{\text{sym}}),
\]

and varies between \(-\pi/4\) (at \( V \to -\infty \)) over 0 (at \( V = V_{\text{sym}} \)) and to \(+\pi/\) (in the limit \( V \to \infty \)), see Section III.C. The corresponding assumed variation of the dipole matrix element and center-of-charge separation is described by

\[
\langle \Psi_2^{(V)} | x | \Psi_1^{(V)} \rangle = \cos(2\chi(V - V_{\text{sym}})) \langle \Psi_2^s | x | \Psi_1^s \rangle,
\]

and

\[
\langle \Psi_2^{(V)} | x | \Psi_2^{(V)} \rangle - \langle \Psi_1^{(V)} | x | \Psi_1^{(V)} \rangle = -2\sin(2\chi(V - V_{\text{sym}})) \langle \Psi_2^s | x | \Psi_1^s \rangle.
\]

Consider first the significant variation of characteristic intersubband matrix element \( U(q) \). We assume that the wavefunctions \( \Psi_{1,2}^s(x) \) at \( V = V_{\text{sym}} \) are exactly symmetric and denote by \( U_{21,21}^s(q) \) the value of the matrix element \( U(q) \) at \( V = V_{\text{sym}} \). We approximate the matrix element at a general voltage drop \( V \) by inserting the two-level wavefunctions \( \Psi_{1,2}^{(V)}(x) \) in for \( \Psi_{i=k=2/j=l=1}(x) \) in Eq. (50).

Within the approximate two-level description the limit \( V \to \infty \) is described by upper- (lower)-level wavefunction \( \Psi_L(x) \) (\( \Psi_R(x) \)) concentrated in the left (right)
quantum well and given by

\[ \psi_{2}^{(\infty)}(x) = \psi_L(x) \equiv \left[ \psi_{2}^{s}(x) - \psi_{1}^{s}(x) \right] / \sqrt{2}, \tag{56} \]

\[ \psi_{1}^{(\infty)}(x) = \psi_R(x) \equiv \left[ \psi_{2}^{s}(x) + \psi_{1}^{s}(x) \right] / \sqrt{2}. \tag{57} \]

These wavefunction does have a small but finite wavefunction overlap resulting in a non-zero matrix element

\[ U_{12,12}^{(\infty)}(q) = U_{LR,LR}(q), \tag{58} \]

given by inserting the wavefunctions \( \psi_{R,L}(x) \) for \( i = k = 1, j = l = 2 \) in Eq. (50). At a general voltage-drop \( V \) the approximate matrix element can now be expressed

\[ U_{12,12}^{(V)}(q) = \cos^2(2\chi(V - V_{sym}))U_{12,12}^{s}(q) + \sin^2(2\chi(V - V_{sym}))U_{LR,LR}(q), \tag{59} \]

\[ = U_{LR,LR}(q) + \cos^2(2\chi(V - V_{sym}))(U_{12,12}^{s}(q) - U_{LR,LR}(q)). \]

The assumed behavior, \( U_{12,12}^{(V)}(q) \rightarrow U_{LR,LR}(q) \) in the limit \( V \rightarrow \infty \) must be considered an artifact of the two-level description. However, we expect Eq. (59) to provide the correct voltage-drop dependence around around \( V = V_{sym} \), and note that the value \( U_{LR,LR} \) can instead be expresses directly in terms of the actual matrix elements at \( V = V_{sym} \):

\[ U_{LR,LR}(q) = \left[ U_{22,22}^{s}(q) + U_{11,11}^{s}(q) - 2U_{11,22}^{s}(q) \right] / 4. \tag{60} \]

In particular, we conclude based on Eq. (59), that the significant voltage-drop variation of characteristic matrix element \( U(q_{\Delta}) \) evident in Figure 4.5 results directly from the moderate variation of the dipole matrix element, Eq. (54).

For the intersubband matrix element \( U_{12,22}^{(V)}(q) \) (similarly given by inserting the two-level wavefunctions \( \psi_{1,2}^{(V)}(x) \) in Eq. (50)) it clear that

\[ U_{22,21}^{s}(q) = 0, \tag{61} \]
because of the assumed symmetry at $V_{\text{sym}}$. For a general voltage drop $V$ we expand the two-level wavefunctions $\Psi_{1,2}^{(V)}(x)$ in terms of $\Psi_{1,2}^{\pm}(x)$ and obtain an approximate matrix element,

$$U_{22,21}^{(V)}(q) \propto \sin(2\chi(V - V_{\text{sym}})), \tag{62}$$

proportional to the center-of-charge separation. It follows in particular that the actual characteristic intersubband matrix element, $U_{22,21}(q = q_{\Delta}/2 = q_{\Delta}/\sqrt{2})$, must vanish at a bias $V = V'_{\text{sym}} \approx V_{\text{sym}}$. Although the condition, $U_{22,21}(q = q_{\Delta}/2) = 0$, does not of course ensure that the general matrix element, $U_{22,21}(q)$, vanishes at $V = V'_{\text{sym}}$, the quantum-confined Stark effect\cite{9} on the wavefunction symmetry\cite{10} in $U_{22,21}(q)$ does cause a more than six orders of magnitude of scattering rate $\Gamma_{22-21}$ around $V = V_{\text{sym}}$.

Finally, we observe that the dramatic voltage-drop/wavefunction-symmetry variation of the intersubband Coulomb matrix elements $U(q)$ and $U_{12,22}(q)$ also causes an strong variation in the total nonequilibrium electron-electron intersubband decay. This follows because a scattering event (unlike $\Gamma_{22-21}$) removes both upper-subband electrons to the lower subband and the total decay is thus given by $2\Gamma + \Gamma_{22-21}$. The alternating-long-short-dashed curve in the top panel of Figure 4.5 shows the variation of this combined decay rate, $2\Gamma + \Gamma_{22-21}$, which enhances to a maximum at $V = V_{\text{sym}}$ but is significantly reduced at $V \neq V_{\text{sym}}$.

IV.E The finite intersubband population inversion

Thanks to the above study of the nonequilibrium electron-electron scattering we are now able to estimate the total intersubband decay and resulting population
inversion, the main focus of this dissertation. We provide this estimate at the
avoided crossing, \( V = V_{sym} \), where the combined electron-electron decay, \( \sim 2\Gamma + \Gamma_{22\rightarrow 21} \), enhances to a maximum as demonstrated in Figure 4.5.

We denote the upper- and lower-subband occupation density by \( n_2 \) and \( n_1 \), respectively. Using the two-level rate equation introduced in Section I.D:

\[
\frac{dn_2}{dt} = (N_L - n_2)\Gamma_e - n_2\Gamma_{c2} - n_2\Gamma_{nr}(n_2),
\]

\[
\frac{dn_1}{dt} = n_2\Gamma_{nr}(n_2) - n_1\Gamma_{c1},
\]

and a simple assumption,

\[
\Gamma_{nr}(n_2) = \Gamma_{sp} + 2\left(\frac{n_2}{N_L}\right)\text{Ry}^*\left(\frac{\mu_2}{\Delta}\right)|U^0(q\Delta)|^2I_P(0),
\]

for the total intersubband decay rate we furthermore determine the resulting inter-
subband population inversion, \( n_2 - n_1 \), and current densities, \( J = e\Gamma_e(N_L - n_2) \).

These estimates for the population inversion and current densities are shown in the
bottom panel of Figure 4.6, left and right axis, respectively.

The rate equation, Eq. (63), involves tunneling the tunneling rates \( \Gamma_e \), \( \Gamma_{c1} \) and
\( \Gamma_{c2} \) illustrated in Figure 1.1 and estimated in Section III.D. We may assume\(^{17}\) the
total single-electron decay rate \( \Gamma_{se} \) experimentally bounded by the value, \( 1/\tau \approx 0.03 \text{ meV} \), measured\(^2\) at weak optical pumping and at temperatures \( T \lesssim 50 \text{ K} \).

The top panel of Figure 4.6 shows the \( \mu_2/\Delta \)-dependence at \( V = V_{sym} \) of the
electron-electron scattering rates — evaluated for a complete upper-subband oc-
cupation below the emitter chemical potential, \( \mu_L \equiv E_2 + \mu_2 \). The estimate,
\( \Gamma_{nr}(n_2) - \Gamma_{se} \), for the total decay due to the electron-electron scattering at \( V = V_{sym} \) and a partial current-injected upper-subband occupation, \( n_2 \leq N_L \), results as follows. The scattering \( \Gamma_{22\rightarrow 12} \) (shown by dotted curve in top panel) can be
FIGURE 4.6 Top panel shows the approximate scaling, solid curve, with electron occupation, $\mu_2/\Delta$, of unscreened (screened) nonequilibrium scattering rate $\Gamma$, dashed-single(double)-dotted curve. Screening causes at most a factor of two reduction of $\Gamma$ even at $\mu_2 = \Delta$. The interaction matrix elements are evaluated at $V_{sym}$ where the rate $\Gamma_{22 \rightarrow 21}$, dotted curve, essentially vanishes. Bottom panel demonstrates that a finite population inversion (left axis) $n_2 - n_1 \sim 0.17 \times 10^{11}$ cm$^{-2}$ can be maintained at a moderate current density (right axis) $J = e\Gamma e(N_L - n_2)$ in spite of the strong intersubband scattering. Note, however, that the population inversion quickly saturates and eventually decreases whereas the current density $J = eN_L(1 - n_2/N_L)$ shows a faster-than-linear increase with $\mu_2/\Delta$. 
\( \left( \frac{Ry^*}{\pi^2} \right) \left( \frac{\mu_2}{\Delta} \right) |U^0(q_\Delta)|^2 I_p(0) \)

\( V_{\text{sym}} = 22.9 \text{ mV} \)
\( \Delta = 10.9 \text{ meV} \)
\( q_{TF} = 0 \)
\( q_{TF} / k_{\mu_2} = 0.9 \)
\( \Gamma_{22-21} \)
\( \Gamma_{se} = 0.03 \text{ meV} \)
\( \Gamma_{c1} = 0.51 \text{ meV} \)
\( \Gamma_{c2} = 1.01 \text{ meV} \)
\( \Gamma_e = \Gamma_{c2} / 4 \)

**FIGURE 4.6**
neglected at $V_{sym}$ due to the restored wavefunction-inversion symmetry (Section IV.D.) The scattering $\Gamma$ does remove two electrons at a time but is reduced by the partial upper-subband occupation, $n_2 \leq N_L$. For simplicity we assume this partial upper-subband occupation is distributed according to

$$f_2(k) \equiv \left(\frac{n_2}{N_L}\right) \times \Theta(\mu_2 - E_\| (k)).$$

Finally, we approximate the resulting electron-electron decay $2(n_2/N_L)\Gamma$ using the scaling approximation (solid curve in top panel) for the unscreened rate $\Gamma$.

The current-injection in the mid-infrared quantum cascade laser$^{11,12,13}$ maintains a population inversion $n_2 - n_2 \approx n_2 \approx N_L \sim 10^{11}$ cm$^{-2}$ which requires $\mu_2 \approx 5$ meV and $\Gamma_e \gg \Gamma_{c2}$. In the present far-infrared structure, however, the resulting strong scattering, $\Gamma \approx 0.5$ meV, will eliminate such a population inversion. Nevertheless, the estimates reported in the bottom panel of Figure 4.6 demonstrates that a smaller population inversion, $n_2 - n_1 \approx 0.17 \times 10^{11}$ cm$^{-2}$ can be maintained at current densities comparable those in the mid-infrared quantum cascade laser.$^{11,12,13}$

These estimates are given by the steady-state solutions of the rate equation, Eq. (63). Specifically estimate at the avoided crossing, $V = V_{sym}$ the upper-subband population density at

$$\frac{n_2}{N_L} = \frac{(\Gamma_e + \Gamma_{c2} + \Gamma_{se})}{4\Gamma} \left[ \sqrt{1 + \frac{8\Gamma_e}{(\Gamma_e + \Gamma_{c2} + \Gamma_{se})^2}} - 1 \right],$$

which in particular determines the current density

$$J = e\Gamma_e N_L (1 - \frac{n_2}{N_L}).$$
For the resulting population inversion we find

\[
\frac{n_2 - n_1}{N_L} = -\frac{\Gamma_e}{\Gamma_{c1}} + \frac{(\Gamma_e + \Gamma_{c2} + \Gamma_{c1})(\Gamma_e + \Gamma_{c2} + \Gamma_{se})}{4\Gamma_{c1}} \times \left[ \sqrt{1 + \frac{\Gamma\Gamma_e}{(\Gamma_e + \Gamma_{c2} + \Gamma_{se})^2}} - 1 \right].
\]

(68)

The bottom panel of Figure 4.6 shows these estimate for the population inversion density and current density evaluated at the specified tunneling rates.

We emphasize that this estimated population inversion, \( n_2 - n_1 \), as shown in Figure 4.6, quickly saturates and eventually decreases whereas the current density, \( J = e\Gamma_e N_L (1 - n_2/N_L) \), shows a faster-than-linear increase with \( \mu_2/\Delta \). A choice of \( \Gamma_e \sim \Gamma_{c2} \approx 1.0 \text{ meV} \) (not shown) does not increase the maximum population inversion and causes a strongly nonlinear rise of the current with \( \mu_2/\Delta \). Hence, the electron-electron scattering forces a nontrivial optimization of \( \Gamma_e/\Gamma_{c2} \) and \( \mu_2/\Delta \).

Finally, we reiterate that we have above estimated the resulting intersubband population inversion at the avoided crossing \( V = V_{sym} \) and using the scaling result for the unscreened rate \( \Gamma \). At this avoided crossing the combined electron-electron decay (given by \( 2\Gamma + \Gamma_{22\rightarrow 21} \)) enhances to a maximum as shown in the top panel of Figure 4.5. Hence, we have above overestimated the effect the intersubband electron-electron scattering. It should thus be possible to increase the population inversion (beyond the value \( n_2 - n_1 \approx 0.17 \times 10^{11} \text{ cm}^{-2} \), reported in Figure 4.6) by ensuring a strong upper-subband current injection at a voltage drop \( V \neq V_{sym} \) where the wavefunction-inversion symmetry is lost and the combined electron-electron decay is significantly reduced.
REFERENCES


3. Reference 2 also report a moderate decay rate \(1/\tau \approx 0.05\) meV at \(T = 10\) K under a strong optical pumping. A comparison requires, however, a detailed modeling of the optically excited electron gas and is not presently undertaken.


14. We thank Dr. B. Galdrikian for kind permission to use his Schrödinger-solver code.

15. The rate $\Gamma$ is defined as the total rate of scattering between two upper-subband electrons which both decay to subband $E_1$ — per upper-subband electron assuming a complete upper-subband occupation, i.e., $n_2 = N_L$. For an area $A$ the total number of upper-subband electrons is thus $AN_L$ and we have $\{AN_L\} \Gamma \equiv \sum_q (e^2/\epsilon_0 q \Delta)^2 |U(q)|^2 N_L^2 \mu_2^{-1} P(q)$ with phase-space contribution $N_L^2 \mu_2^{-1} P(q)$ listed in Eq. (31).

16. The rate $\Gamma_{22 \rightarrow 21}$ is defined as the total rate of scattering between two upper-subband electrons of which only one decays to subband $E_1$ — again per upper-subband electron assuming a complete upper-subband occupation, i.e., $n_2 = N_L$, and respecting the Pauli exclusion within the upper-subband. For an area $A$ the total number of upper-subband electrons is again $AN_L$ and we have $\{AN_L\} \Gamma_{22 \rightarrow 21} \equiv \sum_q (e^2/\epsilon_0 q \Delta)^2 |U_{22,21}(q)|^2 N_L^2 \mu_2^{-1} P_{22 \rightarrow 21}(q)$ with phase-space contribution $N_L^2 \mu_2^{-1} P_{22 \rightarrow 21}(q)$ listed in Eq. (42).

17. The intersubband decay due to impurity, interface defect and acoustic phonon scattering remains at temperatures $T \leq 50$ K strictly bounded by the experimental value $1/\tau = 0.03$ meV. We estimate the decay due to thermally activated optical-phonon emission bounded at $10^{-3}$ meV for $T \leq 25$ K.

18. We take in this evaluation $\Gamma_{c1}(e2) = 0.51(1.01)$ meV (estimated in Section I.D at the avoided crossing $V = V_{sym}$) and use $\Gamma_e = \Gamma_{c2}/4$. 
CHAPTER V

CONCLUSIONS AND OPEN QUESTIONS

In this dissertation we have investigated the possible intersubband stimulated emission in a hypothetical far-infrared quantum-cascade-laser design. In particular we have, for the asymmetric double-quantum-well tunneling structure with schematics shown in Figure 1.1 and resonant-level separation $\Delta \approx 11$ meV, investigated the intersubband decay and resulting population inversion.

In this concluding chapter we first summarize the results of our investigations and then discuss a set of open questions beyond the scope of this dissertation. We stress in particular that while we have demonstrated that a finite intersubband population inversion can be maintained that not does ensure that actual far-infrared (or Tera-Hertz) intersubband lasing will result.

V.A Summary of dissertation results

In the quantum-cascade-laser design a strong nonequilibrium current injection exclusively into the upper subband provides a finite intersubband population inversion if the lower-level tunneling escape rate $\Gamma_{c1}$ exceeds the intersubband de-
cay rate $\Gamma_{nr}$. An intersubband population inversion density $\Delta n \sim 10^{11} \text{ cm}^{-2}$ as in the existing mid-infrared quantum cascade laser\textsuperscript{1,2,3} will provide a significant net stimulated emission because the intersubband transitions are concentrated at a single frequency $\omega_{\Delta}$ given by the subband separation, $\Delta$, and because the optical transitions are characterized by very large dipole matrix elements.

Our choice of specific tunneling structure was motivated by the recent experimental determination\textsuperscript{5} of a very small intersubband decay rate $1/\tau \leq 0.03 \text{ meV}$ at temperatures $T \leq 50 \text{ K}$ — measured at weak optical pumping of the corresponding isolated double-quantum-well structure.\textsuperscript{5,6} Such a small intersubband decay rate is possible because the optical-phonon frequency, $\Omega_{LO} \approx 36 \text{ meV}$, exceeds the subband separation $\Delta \approx 11 \text{ meV}$. Optical-phonon emission processes are thus inhibited at temperatures below the thermal activation energy, $\Omega_{LO} - \Delta \approx 25 \text{ meV}$.

We can, as a consequence, assume the total single-electron decay bounded, $\Gamma_{se} \leq 0.03 \text{ meV}$ at $T \leq 25 \text{ K}$, also in the presence of the nonequilibrium current injection. This single-electron decay, i.e., containing interface-defect, impurity, and electron-acoustic/optical-phonon scattering, is in particular much smaller that the lower-level tunneling escape rate, $\Gamma_{e1} \approx 0.5 \text{ meV}$, that we have estimated for the tunneling structure.

We have found, however, that the exclusive upper-subband current injection results in a very strong nonequilibrium electron-electron scattering which we have evaluated assuming a complete upper-subband occupation below the emitter chemical potential, $\mu_L = E_2 + \mu_2$. We have in particular estimated the nonequilibrium scattering $\Gamma$ ($\Gamma_{22 \rightarrow 21}$) which involves two upper-subband electrons which both decay (of which only one decays) to subband $E_1$ and have found that neither scattering
rate is significantly affected by screening. Also, the dominant scattering rate \( \Gamma \) is not affected by the Pauli exclusion principle since we have assumed population inversion. Moreover, we have found that measured large \( \Delta^* - \Delta \approx 2 \text{ meV} \), of the equilibrium absorption peak, \( \Delta^* \), directly indicates a very strong nonequilibrium scattering (\( \Gamma \)).

We have consequently provided a detailed study of the nonequilibrium electron-electron intersubband scattering within the Figure 1.1-tunneling structure and have (1) identified a simple scaling of nonequilibrium electron-electron scattering rate \( \Gamma \) with the electron occupation \( \mu_2 \), (2) explained how the Pauli exclusion within the upper-subband prevents such a scaling for the scattering rate \( \Gamma_{22 \rightarrow 21} \), (3) identified a dramatic voltage-drop dependence of both nonequilibrium electron-electron scattering rates, \( \Gamma \) and \( \Gamma_{22 \rightarrow 21} \), associated with the quantum-confined Stark effect \( \text{11} \) on the wavefunction inversion symmetry, \( \text{12} \) (4) documented that this wavefunction-symmetry variation in particular allows a significant reduction of also the combined electron-electron intersubband decay, \( \sim 2\Gamma + \Gamma_{22 \rightarrow 21} \), (5) predicted a very strong decay rate, \( \sim 2\Gamma \approx 1 \text{ meV} \), for an upper-subband sheet-density, \( n_2 \approx 10^{11} \text{ cm}^{-2} \), comparable to that in the mid-infrared quantum cascade laser, \( \text{1,2,3} \) and finally (6) demonstrated that a smaller population inversion density (\( \sim 0.2 \times 10^{11} \text{ cm}^{-2} \) can be maintained at a moderate tunneling current density.

V.B Open questions

We have in this dissertation demonstrated that an intersubband population inversion can be maintained thanks to the nonequilibrium current injection. The predicted population inversion is smaller than the intersubband inversion in the
existing mid-infrared quantum cascade laser\textsuperscript{1,2,3} and it reasonable to question if a comparable net stimulated emission can be obtained. Specifically, it is relevant to ask: (a) is it possible to achieve a peak material gain comparable to that in the mid-infrared quantum cascade laser? and (b) if so, is it possible to achieve a good waveguide confinement of the resulting radiation and hence achieve actual lasing?

A definite answer to either of these questions is beyond the scope of this dissertation. Below we include only a brief discussion and emphasize (in addressing point (b)) that although a net stimulated far-infrared emission may appear possible that does not ensure the realization of actual lasing.

(a) The peak material gain.

The peak material gain is introduced in Section II.C as the amplification of the (potentially) lasing mode (of frequency $\omega_A$) when traveling entirely within a superlattice of back-to-back optically active tunneling structures and interjacent injector layers serving as emitter and collector leads.

The optical transitions between subbands $E_i$ and $E_j$ is described by the oscillator strength

$$f_{ij} \equiv 2m^*_e \Delta |\langle \Psi_i | x | \Psi_j \rangle|^2, \quad (1)$$

through which we can in particular express the total spontaneous emission rate

$$\Gamma_{ij}^{sp} \propto f_{ij} \Delta^2. \quad (2)$$

The peak material gain depends in turn on both this total spontaneous emission rate, Eq. (2), the line width, $\Gamma_\phi$, of this spontaneous emission, and on the intersub-
band population-inversion density

\[ \gamma_{\text{mat}}(\omega_{\Delta}) \propto (\Delta n / \Gamma_{\phi}) \left( \frac{f_{ij}^{\text{sp}}}{\omega_{\Delta}^2} \right). \]  

(3)

However, both the mid-infrared quantum cascade laser\(^1,3\) and the Figure 1.1 tunneling structure is characterized by very large oscillator strengths, \( f_{ij} \sim 1 \). Thus it is clear that the discussion of the resulting peak material gain reduces to a comparison of the ratio \( \Delta n / \Gamma_{\phi} \), for the two quantum-well tunneling structures.

On the one hand we have in Section IV.E (at the avoided crossing \( V = V_{\text{sym}} \)) estimated a population inversion density,

\[ \Delta n \lesssim 0.17 \times 10^{11} \text{ cm}^{-2}, \]  

(4)

significantly smaller than the value, \( \gtrsim 10^{11} \text{ cm}^{-2} \), reported\(^3\) for the mid-infrared quantum cascade laser.

On the other hand, however, the mid-infrared quantum cascade laser is characterized by a wide spontaneous emission peak with a full-width-at-half-maximum value,\(^3\) \( 2\Gamma_{\phi}^{\text{el}} \approx 22 \text{ meV} \). This wide emission peak results in part from the significant interface-scattering in the very narrow (8 Å) upper-resonant-level quantum well. One can thus hope that the wider quantum wells of the hypothetical Figure 1.1 tunneling structure will result in significantly smaller values for \( \Gamma_{\phi} \).*

* It is in particular encouraging that the measured (equilibrium) absorption peak for the corresponding isolated double-quantum-well structure\(^5,6\) appears limited by the temperature\(^13\) \( T \) even at \( T \sim 10 \text{ K} \). This measured absorption line width tend to predict a narrow spontaneous emission peak (described by \( 2\Gamma_{\phi} \sim 1 \text{ meV} \)) in the Figure 1.1-tunneling structure. On the other hand, the increased scattering under the nonequilibrium conditions (i.e., current injection) may cause a finite increase in the value \( \Gamma_{\phi} \).
(b) The waveguide confinement

In addition to a large peak material gain, the realization of actual intersubband lasing also requires the design\textsuperscript{1,2,3} of a good waveguide confinement. Specifically, because of the finite extension of the optically active superlattice such a waveguide is, as discussed in Section II.D, essential to (i) concentrate the lasing mode which can then stimulate further transitions, and (ii) prevent reabsorption in the (heavily) doped outside regions.

In discussing the problems involved in achieving such a waveguide confinement for a far-infrared (potentially lasing) mode we assume that the optically active superlattice (comprising tunneling regions and interjacent leads) is surrounded by a set of waveguide cladding layers with a lower effective index of refraction. We furthermore assume these cladding layers are doped to $N_{3D} \geq 1.5 \times 10^{17}$ cm$^{-3}$ (as in the mid-infrared quantum cascade laser) which should prevent a large plasmon re-absorption of the far-infrared radiation emitted at $\omega_\Delta \approx \Delta \approx 11$ meV. Specifically, the choice of $N_{3D} \geq 1.5 \times 10^{17}$ cm$^{-3}$, results in plasmon frequencies,

$$\omega_{pl} = 4Ry^* \sqrt{N_{3D} \pi (a^*)^3} \geq 16 \text{ meV}. \quad (5)$$

To discuss the resulting waveguide confinement we follow the discussion in Section II.D. In particular we denote by $n_{\text{mode}}$ ($n_{\text{clad}}$) the effective index of refraction of the far-infrared mode (the background index of refraction of the cladding layers) and obtain the estimate,

$$\frac{1}{\kappa_{pl}} \sim \frac{1}{2\pi} \frac{\lambda_\Delta}{\sqrt{n_{\text{mode}}^2 - n_{\text{clad}}^2 + (\omega_{pl}/\omega_\Delta)^2}}, \quad (6)$$
for the decay length of the mode into the cladding layers. Note that, in contrast to
the discussion in Section II.D, we have in Eq. (6) kept the plasmon contribution,
$(\Omega_{pl}/\omega_{\Delta})^2$, to the cladding-layer effective dielectric constant because $\omega_{\Delta}$ is now
smaller than this plasmon frequency, $\Omega_{pl}$.

It follows from Eq. (6) that the waveguide confinement may thus be aided by a
large plasmon frequency in the cladding layers. It is in particular possible that the
waveguide confinement can be improved by increasing the doping concentration in
the cladding layers. However, because such an increase of the doping concentration
will also result in an increased impurity-aided single-electron reabsorption$^{14}$ it is
uncertain if this will provide an actual increase in the net effective gain.

It is in any case clear from Eq. (6) that the long wavelength, $\lambda \sim 100$ µm, of
the far-infrared radiation will make a good waveguide confinement very difficult.
Specifically, it appears necessary to grow waveguide cladding layers significantly
thicker than in the mid-infrared quantum cascade laser$^{1,2,3}$ to achieve a similar
waveguide confinement of the far-infrared radiation.

Finally we observe, as a consequence, that even a significant material gain does
not ensure that actual lasing can be realized in the far-infrared regime. On the
other hand, a far-infrared quantum-cascade-laser design might still be able to serve
as an amplifier of such radiation generated by other means. It may in particular
be possible to amplify the (pulsed) coherent radiation arising from quantum
beats or Bloch oscillations$^{15,16}$ in the asymmetric double-quantum-well tunneling
region with a femto-second interband optical excitation. The build-in advantage
of amplifying such quantum-beats radiation would be that the radiation pulse is
automatically tuned at (or close to) the peak material gain at frequency $\omega_{\Delta} \sim \Delta$. 
REFERENCES


13. Professor M. S. Sherwin, University of California; private communications.


APPENDIX A

THE OPPOSITE- AND SAME-SPIN ELECTRON-ELECTRON INTERACTION

In this appendix we derive formal Fermi-golden-rule estimates for both the opposite- and same-spin intersubband scattering rates. The opposite-spin scattering \((\alpha_{i1}, \alpha_{i2}) \rightarrow (\alpha_{f1}, \alpha_{f2})\) is given alone by a so-called direct contribution. In contrast the same-spin scattering comprises both a direct and an exchange contribution.

For the opposite-spin scattering we derive the formal Fermi-golden-rule estimate evaluated in Chapter IV. In particular, we express the opposite-spin direct contribution as a \(q\)-sum over dimensionless Coulomb interaction matrix element \(U_{\alpha_{i1}, \alpha_{i2}; \alpha_{f1}, \alpha_{f2}}(q)\) weighted by the dimensionless measure, \(P_{\alpha_{i1}, \alpha_{i2} \rightarrow \alpha_{f1}, \alpha_{f2}}(q)\), of the scattering phase-space at in-plane momentum transfer \(q\).

For the same-spin scattering we demonstrate that the exchange and direct contribution will exactly cancel if the \(q\)-variation of the dimensionless matrix element \(U_{\alpha_{i1}, \alpha_{i2}; \alpha_{f1}, \alpha_{f2}}(q)\) can be ignored. This motivates our focus on the opposite-spin scattering in Chapter IV.
Section A.1 The intersubband Coulomb interaction

We describe the Coulomb interaction between an electron at \( \vec{R}_1 \) and one at \( \vec{R}_2 \) in terms of the Hamiltonian

\[
H_{e-e}(\vec{R}_1, \vec{R}_2) = \left( \frac{e^2}{\epsilon_0} \right) \frac{\exp(-k_s \sqrt{(x_1 - x_2)^2 + (\vec{r}_1 - \vec{r}_2)^2})}{\sqrt{(x_1 - x_2)^2 + (\vec{r}_1 - \vec{r}_2)^2}},
\]

(1)

where \( \vec{r} \) denoted the position in the in-plane directions. The wave vector \( k_s \) in Eq. (1) represents a convergence factor and the unscreened interaction results in the limit \( k_s \to 0 \).

A scattering event in which two electrons — initially in the subband states \( |\alpha_1, k_1, s_1\rangle \) and \( |\alpha_2, k_2, s_2\rangle \) — scatters to states in the final subbands, \( \alpha_3 \) and \( \alpha_4 \), with an in-plane momentum transfer \( \vec{q} \) is described by the matrix element

\[
V^0_{\alpha_2\alpha_4, \alpha_1\alpha_3}(\vec{q}) \equiv A(\alpha_4, \vec{k}_2 + \vec{q}, s_2; \alpha_3, \vec{k}_1 - \vec{q}, s_1|H_{e-e}|\alpha_2, \vec{k}_2, s_2; \alpha_1, \vec{k}_1, s_1),
\]

(2)

where \( A \) denotes the in-plane area. Following the discussion in Section IV.A we scale this matrix element by the characteristic intersubband momentum transfer \( q_\Delta \equiv \sqrt{2m_e^*\Delta} \),

\[
V^0_{\alpha_2\alpha_4, \alpha_1\alpha_3}(q) = \left( \frac{e^2}{\epsilon_0 q_\Delta} \right) U_{\alpha_4\alpha_2, \alpha_3\alpha_1}(q),
\]

(3)

and thus introduce the dimensionless interaction matrix element

\[
U_{\alpha_2\alpha_4, \alpha_1\alpha_3}(q) = 2\pi \int dx_1 \int dx_2 \Psi^*_\alpha_4(x_2)\Psi_{\alpha_2}(x_2) \times \frac{q_\Delta \exp(-\sqrt{k_s^2 + q^2} |x_1 - x_2|)}{\sqrt{k_s^2 + q^2}} \Psi^*_\alpha_3(x_1)\Psi_{\alpha_1}(x_1).
\]

(4)

Again the unscreened interaction results in the limit \( k_s \to 0 \).
Section A.2 Direct and exchange scattering

In this section we discuss the rate of scattering \( \gamma_{\alpha_1, \alpha_2}^{s_{i_1}, s_{i_2}}(\overrightarrow{k}_{i_1}, \overrightarrow{k}_{i_2}) \) out from a pair of specified initially occupied states, \( |\alpha_{i_1, i_2}, \overrightarrow{k}_{i_1, i_2}, s_{i_1, i_2} \rangle \) and into available final states in subbands \( \alpha_{f_1, f_2} \). The opposite-spin scattering results alone in a so-called direct term whereas the same-spin scattering comprises both a direct and an exchange contribution. We demonstrate, however, that the exchange and direct contributions will exactly cancel in the same-spin scattering if the momentum dependence of the intersubband Coulomb matrix element, Eq. (4), can be ignored.

The electron occupation at in-plane momentum \( \overrightarrow{k} \) within subband \( \alpha \) is described by the generally nonequilibrium distribution function \( f_{\alpha}^{<}(\overrightarrow{k}) \) which we assume independent of both the spin and of the direction of \( \overrightarrow{k} \) (i.e., \( f_{\alpha}^{<}(\overrightarrow{k}) = f_{\alpha}^{<}(k = |\overrightarrow{k}|) \).) To simplify the formal expressions below we also introduce the distribution \( f_{\alpha}^{>}(\overrightarrow{k}) \) of available, i.e., empty, subband-\( \alpha \) states.

The Fermi-golden-rule estimate of \( \gamma_{\alpha_1, \alpha_2}^{s_{i_1}, s_{i_2}}(\overrightarrow{k}_{i_1}, \overrightarrow{k}_{i_2}) \) is given directly by the squared transition matrix elements, of the Hamiltonian, Eq. (1), evaluated between the anti-symmetric pair-states which describe the initial and final electron configuration. Specifically, we describe the pair of initially occupied states using

\[
|\alpha_{i_1}, \overrightarrow{k}_{i_1}, s_{i_1}; \alpha_{i_2}, \overrightarrow{k}_{i_2}, s_{i_2} \rangle_A = \frac{1}{\sqrt{2}} \left\{ |\alpha_{i_1}, \overrightarrow{k}_{i_1}, s_{i_1} \rangle |\alpha_{i_2}, \overrightarrow{k}_{i_2}, s_{i_2} \rangle - |\alpha_{i_2}, \overrightarrow{k}_{i_2}, s_{i_2} \rangle |\alpha_{i_1}, \overrightarrow{k}_{i_1}, s_{i_1} \rangle \right\}
\]

and use a similar pair state to describe the set of possible final pair-states within subbands \( \alpha_{f_1, f_2} \). The intersubband scattering rate resulting from the Coulomb in-
teraction, Eq. (1), is then given by

$$\gamma_{(\alpha_1, \alpha_2) \rightarrow (\alpha_f, \alpha_f)}(\vec{k}_{i_1}, \vec{k}_{i_2}) = \frac{1}{2} \sum_{\alpha_3, \vec{k}_3, s_3} f_{\alpha_3}^{>}(\vec{k}_3) \sum_{\alpha_4, \vec{k}_4, s_4} f_{\alpha_4}^{>}(\vec{k}_4) \times \left[ \delta_{\alpha_4, \alpha_f} \delta_{\alpha_3, \alpha_{f1}} + \delta_{\alpha_4, \alpha_f} \delta_{\alpha_3, \alpha_{f2}} \right] \times$$

$$|\langle \alpha_3, \vec{k}_3, s_3; \alpha_4, \vec{k}_4, s_4 \mid H_{e-e} \mid \alpha_{i_1}, \vec{k}_{i_1}, s_{i_1}; \alpha_{i_2}, \vec{k}_{i_2}, s_{i_2} \rangle|^2 \times$$

$$2\pi \delta \left( |E_{\alpha_{i_1}} - E_{\alpha_3} + E_{||}(\vec{k}_{i_1}) - E_{||}(\vec{k}_3)| \right)$$

$$+ |E_{\alpha_{i_2}} - E_{\alpha_4} + E_{||}(\vec{k}_{i_2}) - E_{||}(\vec{k}_4)| \right),$$

where the projection (second line) restricts all possible final states to available states actually in subbands $\alpha_{f1,2}$. The expression within the delta-function in Eq. (6) is just the energy difference between the final and initial pair states.

The interaction matrix elements in Eq. (6) is given by

$$\sum_{s_3, s_4} |\langle \alpha_4, \vec{k}_4, s_4; \alpha_3, \vec{k}_3, s_3 \mid H_{e-e} \mid \alpha_1, \vec{k}_1, s_1; \alpha_2, \vec{k}_2, s_2 \rangle_A|^2 =$$

$$\frac{1}{A^2} \sum_{q_a, q_b} \delta_{\vec{q}_a, \vec{k}_4 - \vec{k}_2} \delta_{\vec{q}_b, \vec{k}_3 - \vec{k}_2} \left( \frac{e^2}{\epsilon_0 q_\Delta} \right)^2 \left[ |U_{a_4a_2, a_3a_1}(q_a)|^2 + |U_{a_3a_2, a_4a_1}(q_b)|^2 \right.$$

$$\left. - \delta_{s_1, s_2} 2 \text{Re} \left\{ U_{a_4a_2, a_3a_1}(q_a) U_{a_3a_2, a_4a_1}(q_b)^* \right\} \right],$$

where we have included the trivial sum over the final electron spin configuration.

Note that the in-plane momentum is conserved in the scattering events since the specified condition, $\vec{q}_a + \vec{q}_b = \vec{k}_1 - \vec{k}_2$, along with the definitions, $\vec{q}_a \equiv \vec{k}_4 - \vec{k}_2$ and $\vec{q}_b \equiv \vec{k}_3 - \vec{k}_2$, is equivalent to the conservation rule $\vec{k}_3 + \vec{k}_4 = \vec{k}_1 + \vec{k}_2$.

If the two scattering electrons in the initial pair-state Eq. (5) has opposite spins the scattering is given alone by the so-called direct contribution. The formal
expression for this opposite-spin direct scattering is
\[ \gamma^{\uparrow\downarrow}_{(\alpha_{i_1}, \alpha_{i_2})} \rightarrow (\alpha_{f_1}, \alpha_{f_2}) (\vec{k}_{i_1}, \vec{k}_{i_2}) \equiv \gamma^{D}_{(\alpha_{i_1}, \alpha_{i_2})} \rightarrow (\alpha_{f_1}, \alpha_{f_2}) (\vec{k}_{i_1}, \vec{k}_{i_2}) = \left( \frac{e^2}{\epsilon_0 q \Delta} \right)^2 \frac{1}{A^2} \sum_{\vec{q}} f_{\alpha_{f_1}}^{>}(\vec{k}_{i_1} - \vec{q}) f_{\alpha_{f_2}}^{>}(\vec{k}_{i_2} + \vec{q}) \{ 2 |U_{\alpha_{f_2} \alpha_{i_2}, \alpha_{f_1} \alpha_{i_1}}(q)|^2 \} \]
\[ 2\pi \delta \left[ E_{\alpha_{i_1}} - E_{\alpha_{f_1}} + E_{||}(\vec{k}_{i_1}) - E_{||}(\vec{k}_{i_1} - \vec{q}) \right] \]
\[ + [E_{\alpha_{i_2}} - E_{\alpha_{f_2}} + E_{||}(\vec{k}_{i_2}) - E_{||}(\vec{k}_{i_2} + \vec{q})] \right). \]

In contrast, if the spins of the scattering electrons are identical we obtain again the direct contribution \( \gamma^{D}_{(\alpha_{i_1}, \alpha_{i_2})} \rightarrow (\alpha_{f_1}, \alpha_{f_2}) (\vec{k}_{i_1}, \vec{k}_{i_2}) \) and a so-called exchange contribution corresponding to the last term in Eq. (7). That is, the same-spin scattering rate is given by
\[ \gamma^{\uparrow\downarrow}_{(\alpha_{i_1}, \alpha_{i_2})} \rightarrow (\alpha_{f_1}, \alpha_{f_2}) (\vec{k}_{i_1}, \vec{k}_{i_2}) = \gamma^{D}_{(\alpha_{i_1}, \alpha_{i_2})} \rightarrow (\alpha_{f_1}, \alpha_{f_2}) (\vec{k}_{i_1}, \vec{k}_{i_2}) - \gamma^{Ex}_{(\alpha_{i_1}, \alpha_{i_2})} \rightarrow (\alpha_{f_1}, \alpha_{f_2}) (\vec{k}_{i_1}, \vec{k}_{i_2}), \]
with the exchange contribution defined as
\[ \gamma^{Ex}_{(\alpha_{i_1}, \alpha_{i_2})} \rightarrow (\alpha_{f_1}, \alpha_{f_2}) (\vec{k}_{i_1}, \vec{k}_{i_2}) = \left( \frac{e^2}{\epsilon_0 q \Delta} \right)^2 \frac{1}{A} \sum_{a} \sum_{\vec{q}_a} \sum_{\vec{q}_b} \delta_{\vec{q}_a + \vec{q}_b = \vec{k}_{i_1} - \vec{k}_{i_2}} f_{\alpha_{f_1}}^{>}(\vec{k}_{i_1} - \vec{q}_a) f_{\alpha_{f_2}}^{>}(\vec{k}_{i_2} + \vec{q}_a) \times \]
\[ 2\text{Re}\{U_{\alpha_{f_2} \alpha_{i_2}, \alpha_{f_1} \alpha_{i_1}}(\vec{q}_a)U_{\alpha_{f_1} \alpha_{i_1}, \alpha_{f_2} \alpha_{i_2}}(\vec{q}_b)^{*}\} \times \]
\[ 2\pi \delta \left[ E_{\alpha_{i_1}} - E_{\alpha_{f_1}} + E_{||}(\vec{k}_{i_1}) - E_{||}(\vec{k}_{i_1} - \vec{q}_a) \right] \]
\[ + [E_{\alpha_{i_2}} - E_{\alpha_{f_2}} + E_{||}(\vec{k}_{i_2}) - E_{||}(\vec{k}_{i_2} + \vec{q}_b)] \right). \]

There are three intersubband scattering processes with a net decay to the lower subband, namely (a) the near-equilibrium scattering \((2, 1) \rightarrow (1, 1)\) of a single upper-subband electron by an equilibrium lower-subband Fermi sea, (b) the nonequilibrium scattering \((2, 2) \rightarrow (1, 1)\) in which two upper-subband electrons both decays to the lower subband, and (c) the nonequilibrium scattering
\((2, 2) \rightarrow (2, 1)\) in which two upper-subband electrons scatters but only one decays to subband \(E_1\) whereas the other electron scatters within subband \(E_2\). In all three cases we have

\[
U_{\alpha f_2, \alpha i_2, \alpha f_1, \alpha i_1}(q) = U_{\alpha f_1, \alpha i_2, \alpha f_2, \alpha i_1}(q),
\]

and there will be no same-spin scattering if the interaction matrix element be approximated as constant: The exchange contribution, Eq. (10), then cancels exactly the direct contribution, Eq. (9).

Provided still that the \(q\)-variation of the Coulomb matrix elements can be ignored, the exact cancellations holds of course also for the total same-spin scattering, given by summing the results, Eqs. (9) and (10), over all initially occupied pair-states (in subbands \(\alpha_{i1,2}\)).

Of course, the actual intersubband Coulomb matrix elements exhibits some variation, and for example the unscreened matrix element \(U^{9}_{22,21}(q)\) will diverge in the limit \(q \rightarrow 0\). However, within the domain of possible in-plane momentum transfers \(q\) we find in Chapter IV only a very moderate \(q\)-variation of the Coulomb matrix elements. For that reason we expect a significant cancellation in the same-spin scattering and have, as a consequence, in this dissertation only evaluated the (dominant) opposite-spin direct scattering.

A.3 The total opposite-spin scattering

The total rate of opposite-spin scattering \((\alpha_{i1}, \alpha_{i2}) \rightarrow (\alpha_{f1}, \alpha_{f2})\) is given by summing the direct contribution, Eq. (8) over all initially occupied (opposite-spin)
pair-states in subbands $\alpha_{i_1,2}$:

$$\gamma_{\alpha_{i_1},\alpha_{i_2}\rightarrow\alpha_{f_1}\alpha_{f_2}} = \frac{1}{2} \sum_{\alpha_{1,2},\kappa_{1,2},s_{1,2}} \sum_{\delta_{\alpha_{i_1},\alpha_{1,2}},\delta_{\alpha_{i_2},\alpha_{2,2}}} \left[ \delta_{\alpha_{i_1},\alpha_{1,2}} \delta_{\alpha_{i_2},\alpha_{2,2}} + \delta_{\alpha_{i_1},\alpha_{2,2}} \delta_{\alpha_{i_2},\alpha_{1,2}} \right] \times$$

$$f_{\alpha_{i_1}}(\kappa_{1}) f_{\alpha_{i_2}}(\kappa_{2}) \gamma(\alpha_{i_1,2}) \rightarrow (\alpha_{f_1,2})(\kappa_{1},\kappa_{2}).$$

In terms of the dimensionless Coulomb matrix element, Eq. (3), the formal result Eq. (12) reads

$$\gamma_{\alpha_{i_1},\alpha_{i_2}\rightarrow\alpha_{f_1}\alpha_{f_2}} = \left( \frac{e^2}{\epsilon_0 q_{\Delta}} \right)^2 \sum_{\alpha_{i_2}} \left| U_{\alpha_{f_2}\alpha_{i_2},\alpha_{i_1}\alpha_{i_1}}(q) \right|^2 F_{\alpha_{i_1},\alpha_{i_2}\rightarrow\alpha_{f_1}\alpha_{f_2}}(q),$$

where we have introduced the phase-space contribution

$$F_{\alpha_{i_1},\alpha_{i_2}\rightarrow\alpha_{f_1}\alpha_{f_2}}(q) = \frac{1}{2} \left( \frac{2}{A} \sum_{\kappa_{1}} f_{\alpha_{i_1}}(\kappa_{1}) f_{\alpha_{f_1}}(\kappa_{1} - q) \right) \times$$

$$\left( \frac{2}{A} \sum_{\kappa_{2}} f_{\alpha_{i_2}}(\kappa_{2}) f_{\alpha_{f_2}}(\kappa_{2} + q) \right) \times$$

$$2\pi \delta \left[ |E_{\alpha_{i_1}} - E_{\alpha_{f_1}} + E_{||}(\kappa_{1}) - E_{||}(\kappa_{1} - q)| \right]$$

$$+ \left[ |E_{\alpha_{i_2}} - E_{\alpha_{f_2}} + E_{||}(\kappa_{2}) - E_{||}(\kappa_{2} + q)| \right].$$

Both the squared transition matrix elements and the phase-space factor, Eq. (14), depends as indicated only on the length, $q \equiv |\vec{q}|$ of the in-plane momentum transfer.

We emphasize that the formal result, Eq. (13), constitute an estimate for the total opposite-spin scattering within the in-plane area $A$ (containing a total of $A_{n_2}/1$ upper/lower-subband electrons.) In contrast the rates $\Gamma$ and $\Gamma_{22\rightarrow21}$ evaluated in Chapter IV represent the total scattering rate per upper-subband electron, $A_{n_2}$.

Specifically, in estimating the rates, $\Gamma$ and $\Gamma_{22\rightarrow21}$, we assume a complete upper-subband occupation below emitter chemical potential $\mu_L$, which then naturally
defines an upper-subband quasi-Fermi level

$$\mu_2 \equiv \mu_L - E_2,$$  \hspace{1cm} (15)

and a corresponding wave vector

$$k_{\mu_2} \equiv \sqrt{2m^*_e \mu_2}.$$  \hspace{1cm} (16)

The total upper-subband occupation density is

$$n_2 = N_L = \frac{k_{\mu_2}^2}{2\pi} \propto \mu_2.$$  \hspace{1cm} (17)

We furthermore assume that the lower subband is empty and obtain a formal estimate for scattering rate \( \Gamma \equiv \Gamma_{22 \rightarrow 11} \) defined through

$$\{ AN_L \} \Gamma = \sum_{\bar{q}} \left( \frac{e^2}{\epsilon_0 q \Delta} \right) |U_{21,21}(q)|^2 F_{22 \rightarrow 11}^D(q),$$  \hspace{1cm} (18)

where the phase-space contribution, Eq. (14), reduces to

$$F_{22 \rightarrow 11}^D(q) = N_L^2 \mu_2^2 P(q)$$

$$\equiv \frac{1}{2} \left( \frac{2}{A} \right)^2 \sum_{k,k'} \Theta(\mu_2 - E_{\|}(k)) \Theta(\mu_2 - E_{\|}(k')) 2\pi \delta(E_f - E_i).$$  \hspace{1cm} (19)

The delta-function argument in Eq. (19) is specified by the conservation of energy,

$$E_f - E_i = 2E_{\|}(q) + \bar{q} \cdot (\vec{k} - \vec{k}')/m^*_e - 2\Delta.$$  \hspace{1cm} (20)

Similarly, for the scattering rate \( \Gamma_{22 \rightarrow 21} \) we have

$$\{ AN_L \} \Gamma_{22 \rightarrow 21} = \sum_{\bar{q}} \left( \frac{e^2}{\epsilon_0 q \Delta} \right) |U_{22,21}(q)|^2 F_{22 \rightarrow 21}^D(q),$$  \hspace{1cm} (21)

given by the phase-space contribution,

$$F_{22 \rightarrow 21}^D(q) = N_L^2 \mu_2^2 P_{22 \rightarrow 21}(q)$$

$$\equiv \frac{1}{2} \left( \frac{2}{A} \right)^2 \sum_{k,k'} \Theta(\mu_2 - E_{\|}(k)) \times$$

$$\left[ \Theta(\mu_2 - E_{\|}(k')) \Theta+E_{\|}(\vec{k}' - \bar{q}) - \mu_2 \right] 2\pi \delta(E_f - E_i),$$  \hspace{1cm} (22)
for which the criteria of energy conservation is expressed in

\[ E_f - E_i = 2E_{||}(q) + \bar{q} \cdot (\vec{k} - \vec{k}')/m_e^* - \Delta. \]  

(23)


A. Imamoglu and R. J. Ram, University of California, Santa Barbara, *preprint*.


