Fundamental of QCL: active regions

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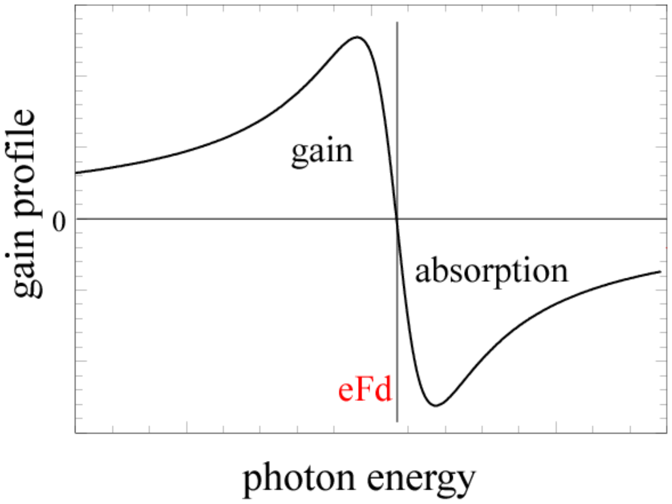
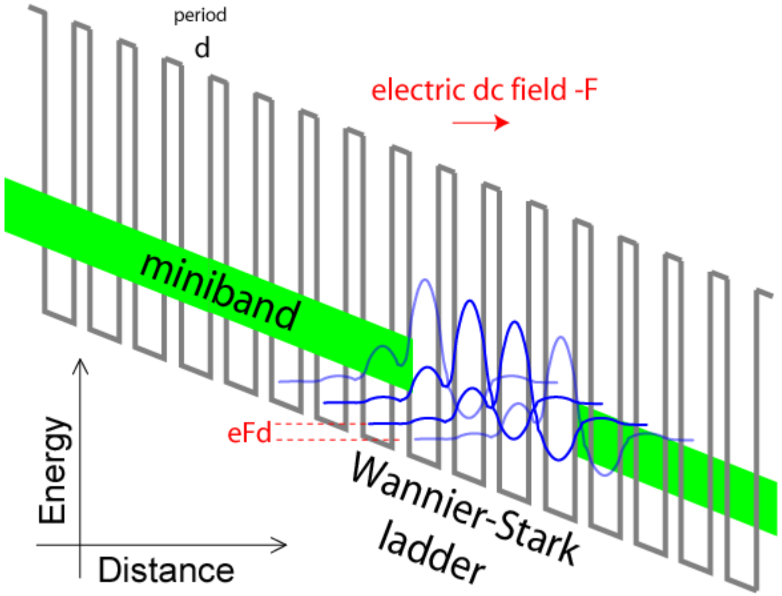
Outline

- QCL as an example of quantum engineering
    - A small look at history of the key ideas
    - Computing energy states
    - Rate equations and the parameters
    - Active region optimization
    - Resonant tunneling in QCLs

Superlattice – Bloch oscillator





- Original proposal
  - Esaki and Tsu, IBM JRD **14**, 61 (1970)
- Gain predicted in the semiclassical model
  - Ktitorov *et al.,* Fiz.tverd.Tela., **13**, 2230, (1971), Ignatov and Romanov, Phys. Stat. Sol. B**73**, 327, (1976)

Resonant/non-resonant tunneling

1971: R. Kazarinov and R. Suris propose using intersubband transitions in a biased superlattice for light amplification

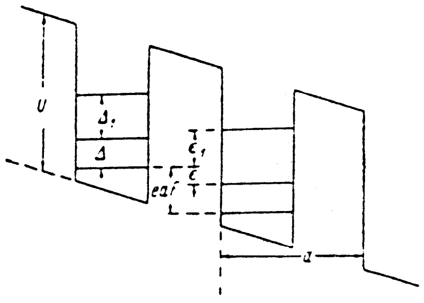


Fig. 1. Schematic representation of the superlattice potential and of the electron levels.

R. F. Kazarinov, R.A. Suris, Sov. Phys. Semicond. **5**, 707 (1971)

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1986-93: Proposals for QCL's using resonant tunneling in superlattices:

F. Capasso et al, JQE (1986)

H. C. Liu et al, JAP (1988)

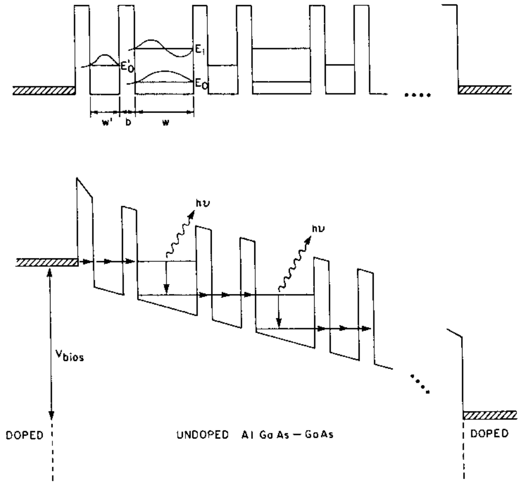
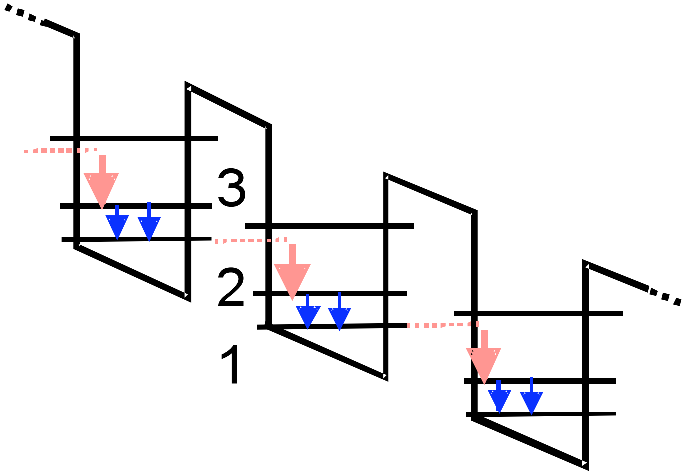


FIG. 1. Upper part: conduction-band edge profile of the proposed device under no bias. Lower part: biased device in operation. Heavily doped contact layers at either ends of the structure are hatched to show the Fermi seas. Photon ($h\nu$) emission processes occur in the wide wells.

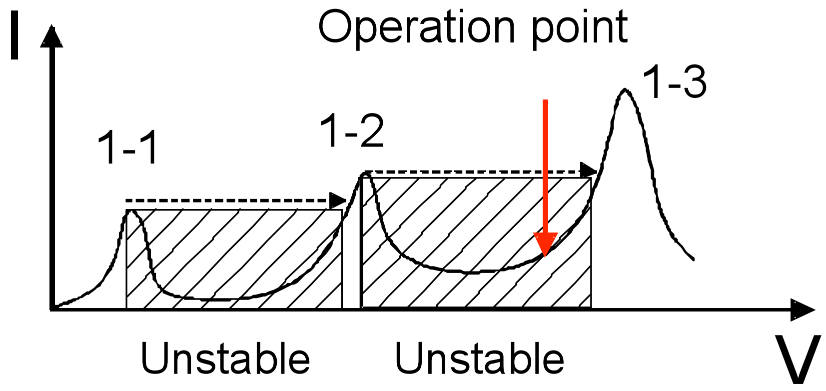
New ideas:

- Energy states by quantum confinement
- Lifetime engineering by tunneling
- Electrical injection
- Missing:
    - electrical stability
    - Better extraction
    - Waveguides

Electrical stability



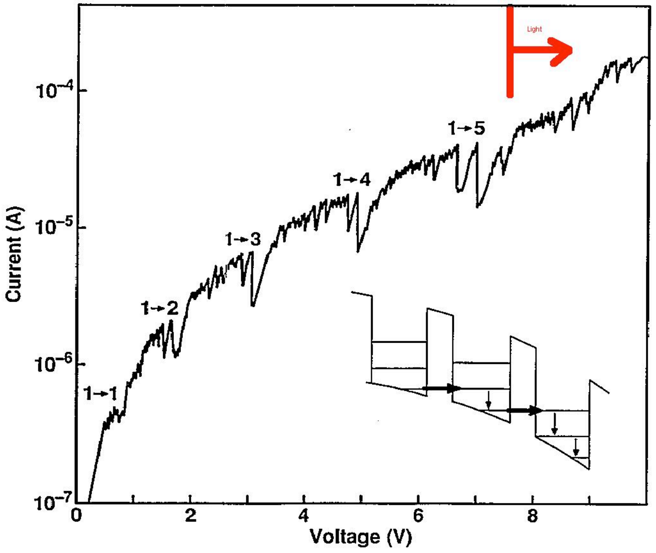
Schematic I-V curve:

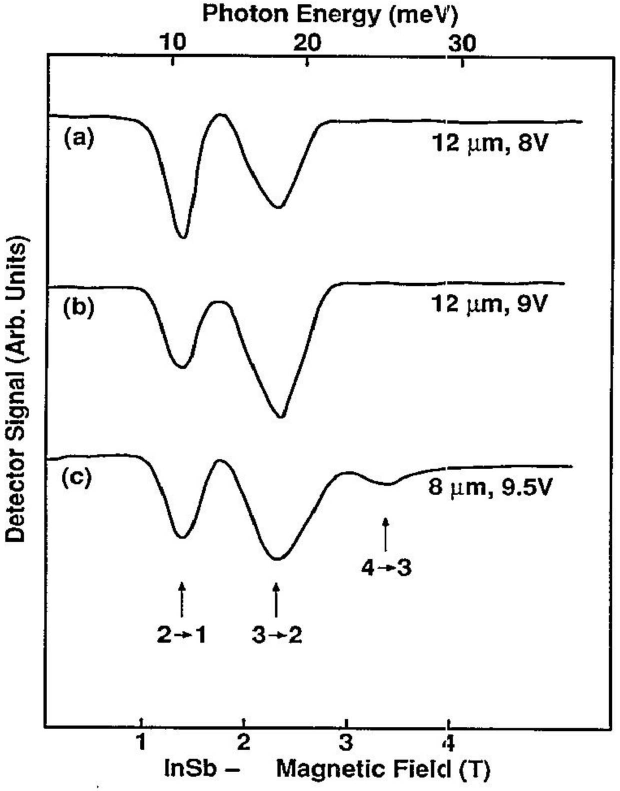


→ **Population inversion is obtained at an unstable point of the I-V curve !**

R.F. Kasarinov and R. A. Suris, Soviet Physics (1971)

First intersubband luminescence





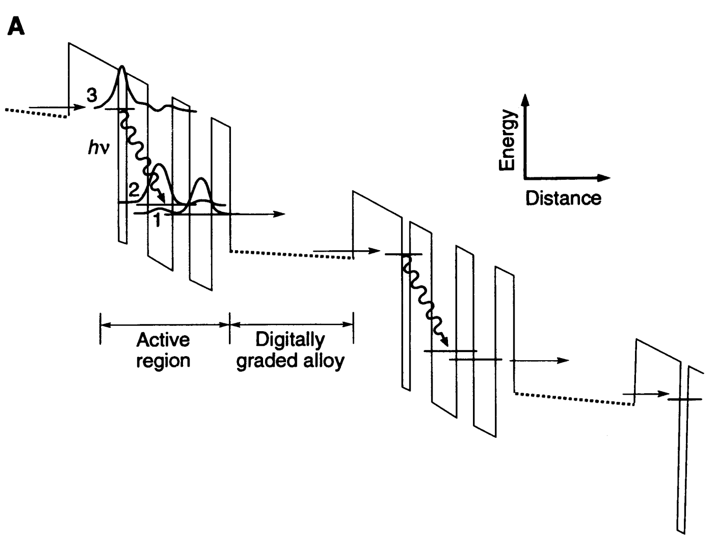
- Resonant tunneling in a periodic superlattice
- Emission observed in the Far-Infrared

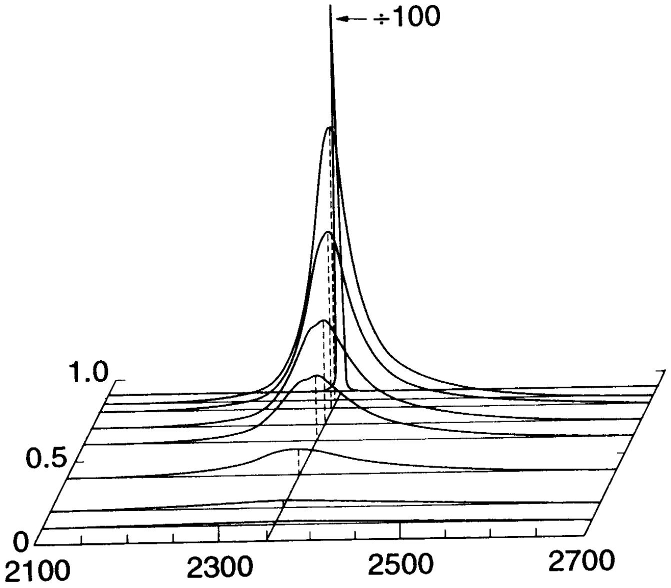
M. Helm et al, PRL **63**, 74 (1989)

First quantum cascade laser

1994: First intersubband laser (quantum cascade laser) is demonstrated in Bell Labs

Tmax = 125K (pulsed), Pmax = 10mW, $\lambda = 4.26\mu m$





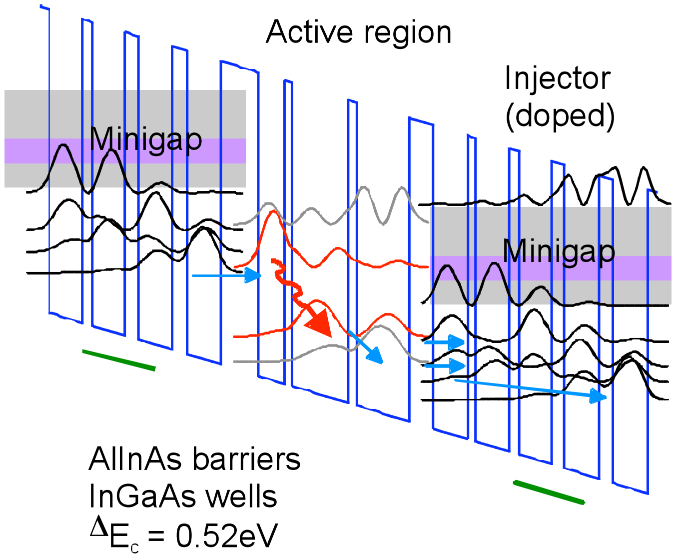
J. Faist, F. Capasso, D. L. Sivco, C. Sirtori, A.L. Hutchinson, A. Y. Cho, Science **264**, 553 (1994)

Outline

- A small look at history
- Computing energy states
- Rate equations and the parameters
- Active region optimization
- Injection mechanism: the Kazarinov and Suris model

Active region: electrons interacting

$$H = \frac{P^2}{2m} + V_{crystal} + V_{heterostructure} + V_{field} + H_{e-phonon} + H_{e-photon} + H_{scatt}$$



Solve first this part

Intersubband transition in QW's: textbook 1D potential

Envelope function approximation: the wavefunction is the product of an envelope function and the Bloch periodic part

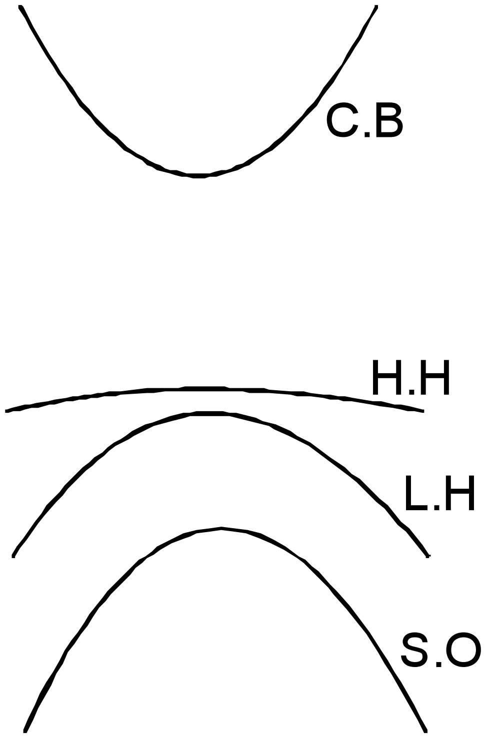
$$| \Psi > = | f_{env} > | \phi_{Bloch} >$$

Matrix elements involve mostly the envelope part

- Electron wavelength (~10nm) "averages" the interface (0.3nm)
- Charges are free in the plane -> no Coulomb charging effects
- Dominant non-radiative scattering are one particule effect

Optical transitions in QW

Kane kp approach at k_{perp}=0



$$H=\begin{pmatrix} E_c(z) & \sqrt{\frac{2}{3}}\frac{p_{cv}}{m_0}p_z & -\sqrt{\frac{1}{3}}\frac{p_{cv}}{m_0}p_z \\ -\sqrt{\frac{2}{3}}\frac{p_{cv}}{m_0}p_z & E_{lh}(z) & 0 \\ \sqrt{\frac{1}{3}}\frac{p_{cv}}{m_0}p_z & 0 & E_{so}(z) \end{pmatrix}$$

Optical transitions in QW

If one is only interested in the conduction band part, one can reduce the hamiltonian
with an “effective” valence band as

$$\mathbf{H} = \begin{bmatrix} E_c(z) & \frac{p_{cv}}{m_0} p_z \\ -\frac{p_{cv}}{m_0} p_z & E_v(z) \end{bmatrix}$$

with $p_{cv} = i\sqrt{m_0 E_p / 2}$ and Ep being the Kane energy (~ 20eV in usual III-V’s)

Matrix elements and energies

The matrix element for optical transitions is

$$P_{if} \quad \left\langle \phi^{i}{}_{c} \right| p_{z} \frac{m_{0}}{m(E_{i},z)} \quad \frac{m_{0}}{m(E_{f},z)} p_{z} \left| \phi_{c}^{f} \right\rangle$$

with ${}_{c}$ solution of the one- dimentional equation

$$p_{z} \frac{1}{2m(E,z)} p_{z} \quad {}_{c} + E_{c}(z) \quad {}_{c} = E \quad {}_{c}$$

and the energy-dependant effective mass is

$$m_{0}(E,z) = m^{*}(1+\frac{E(z)}{E_{c} - E_{v}})$$

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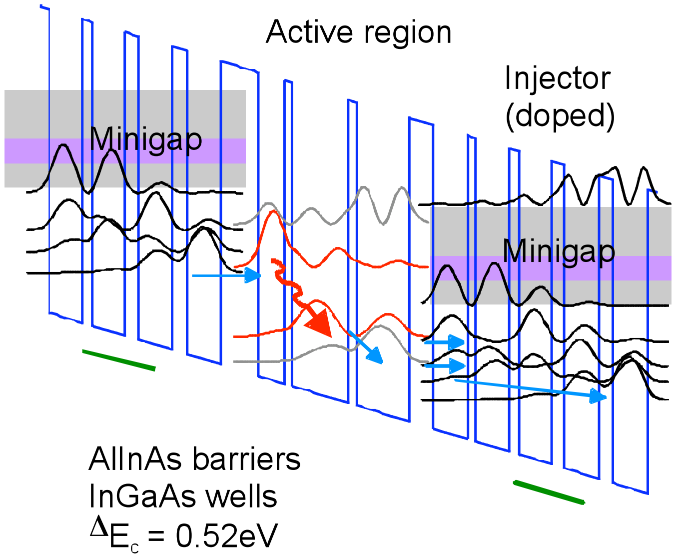
Electron transport and gain

$$H = \frac{P^2}{2m} + V_{crystal} + V_{heterostructure} + V_{field} + H_{e-phonon} + H_{e-photon} + H_{scatt}$$



Rate equations in the basis of the electronic states (Perturbation and independent Electrons)

Rate equations

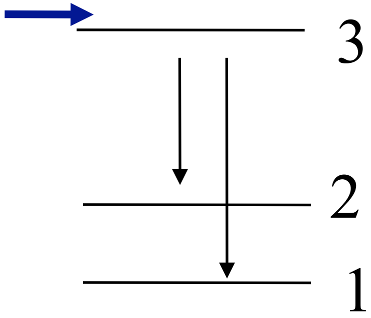
Atomistic model captures nevertheless key elements

$$\frac{dn_3}{dt} = J/q_0 - n3/\tau_3 - gS(n_3 - n_2)$$

$$\frac{dn_2}{dt} = n_3/\tau_{32} - n_2/\tau_2 + gS(n_3 - n_2)$$

$$\frac{dn_1}{dt} = n_3/\tau_{31} - n_1/\tau_1$$

$$\frac{dS}{dt} = \frac{c}{n_g}(g(n_3 - n_2) - \alpha_{tot})S + \beta n_3/\tau_{spon}$$



All the population is lumped together in k=0 state!

Lifetimes: Fermi's golden rule

$$\frac{\hbar}{2\tau\pi} = \sum_f |\langle \psi_i | V(r) | \psi_f \rangle|^2 \delta(\epsilon_f - \epsilon_i)$$

Optical phonon scattering rate

Fermi's golden rule, Froelich interaction

Scattering Rate: $$\frac{1}{\tau_i} = \frac{m^* e^2 \omega_{LO}}{2\hbar^2 \epsilon_P} \sum_f \int_0^{2\pi} d\theta \frac{I^{ij}(Q)}{Q}$$

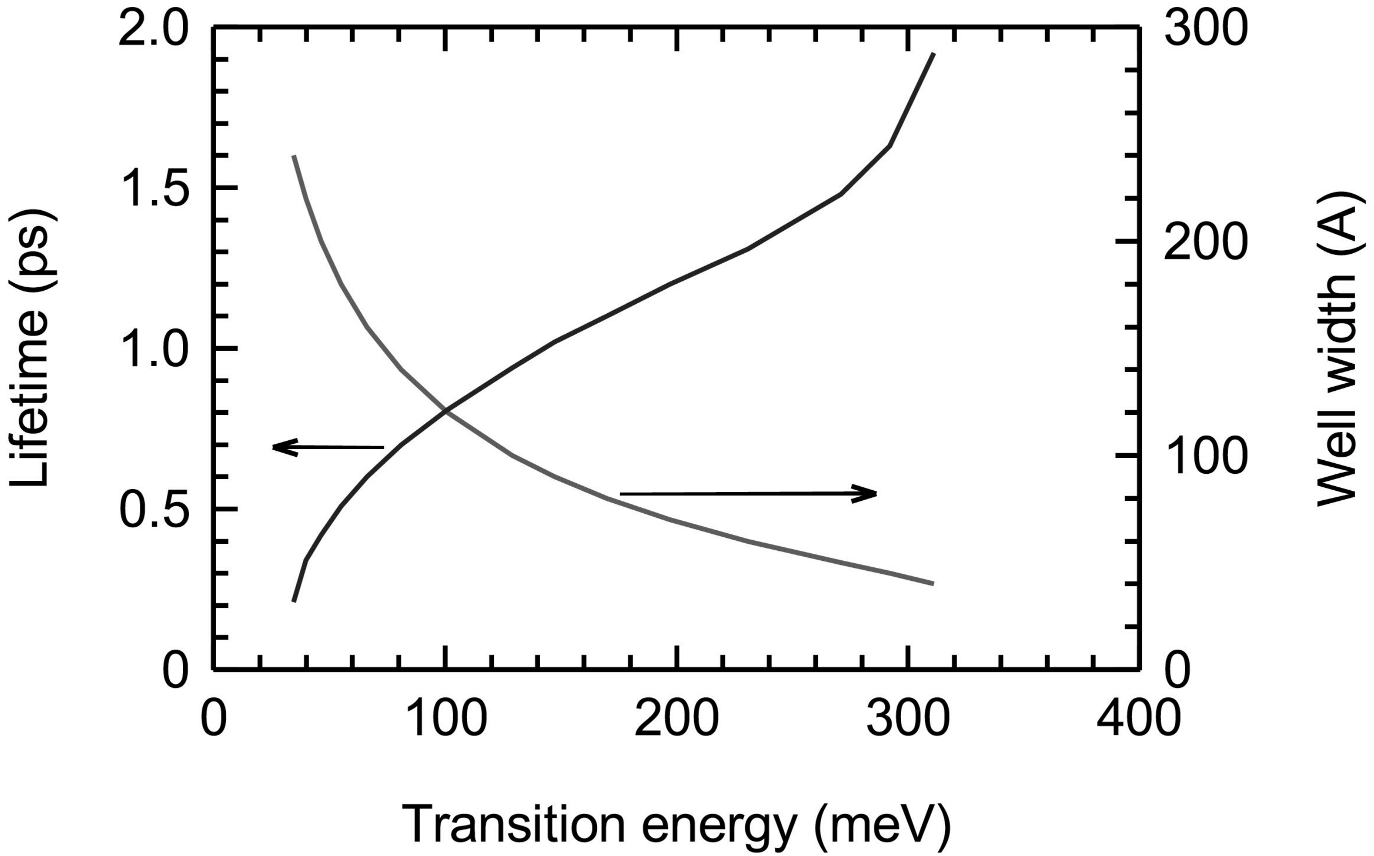
Form factor

$$I^{ij}(Q) = \int dz \int dz' \phi_i(z)\phi_j(z) e^{-Q|z-z'|} \phi_i(z')\phi_j(z')$$

Using $\epsilon_P^{-1} = \epsilon_\infty^{-1} + \epsilon_s^{-1}$ $\quad Q = \sqrt{k_i^2 + k_f^2 - 2k_i k_f \cos\theta}$

P. J. Price, Surface Sience 113, 199 (1982); R. Ferreira and G. Bastard Phys. Rev. B 40, 1074 (1982)

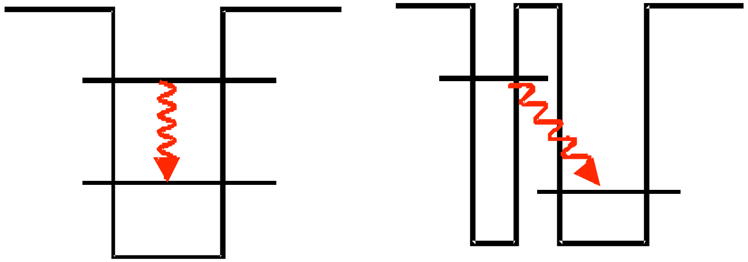
Lifetime in a square well



Threshold current (set S=0)

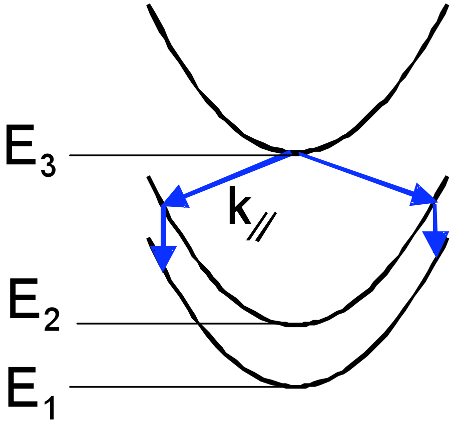
$$J_{th} = \frac{1}{\tau_3(1-\underbrace{\tau_2/\tau_{32}}_{\text{Extraction}})}\left(\frac{\varepsilon_0\,\lambda\,nL_p\overbrace{\gamma}^{\text{Linewidth}}}{4\pi q\Gamma z^2}\underbrace{(\alpha_m+\alpha_w)}_{\text{Loss}}\right)$$

How does one engineer lifetimes?



Diagonal transitions in real space:

Reduction of matrix elements due to a decrease overlapp between wavefunctions.



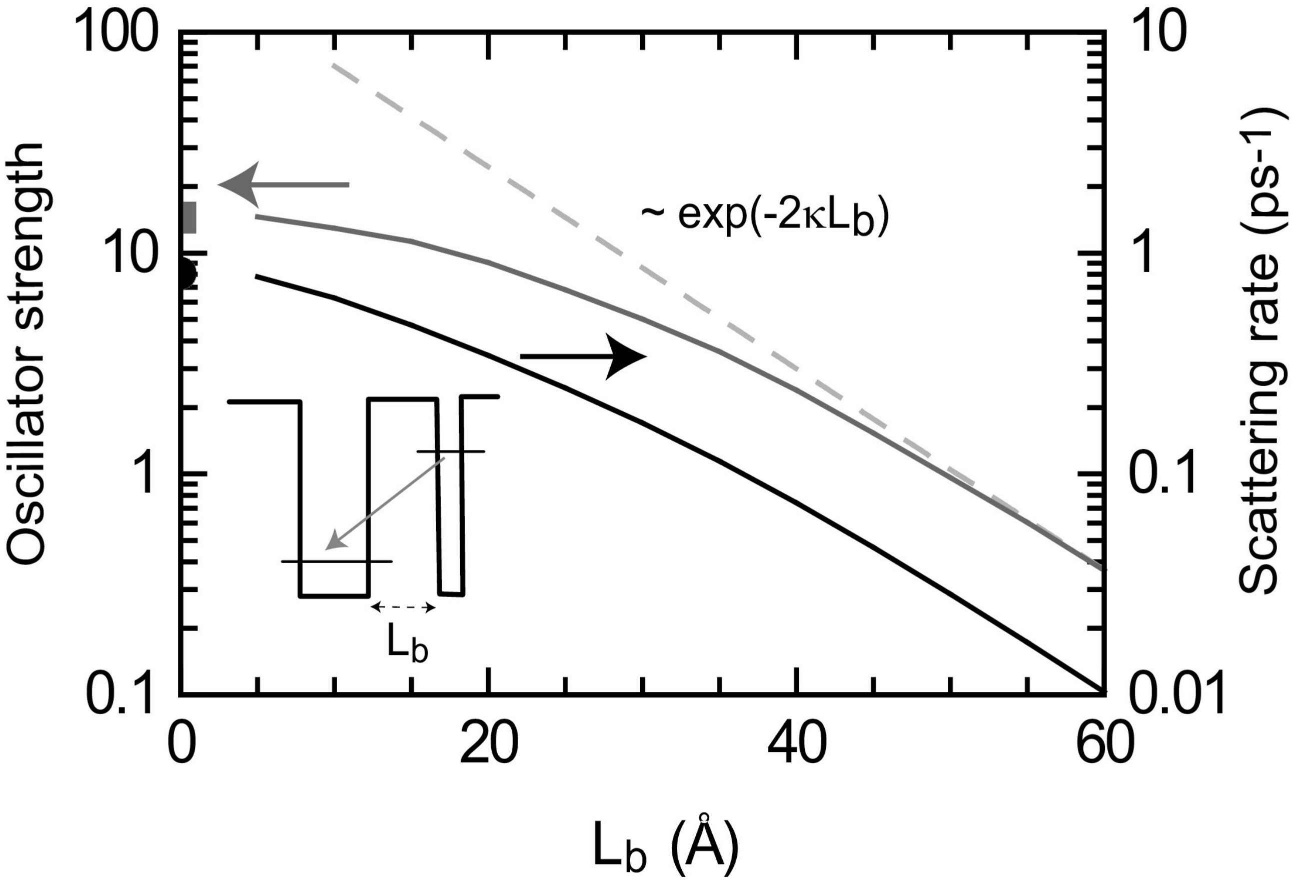
$\tau_{ij} \div k_{\parallel}^2$

$\boxed{\tau_{32} > \tau_{21}}$

Phonon momentum transfer:

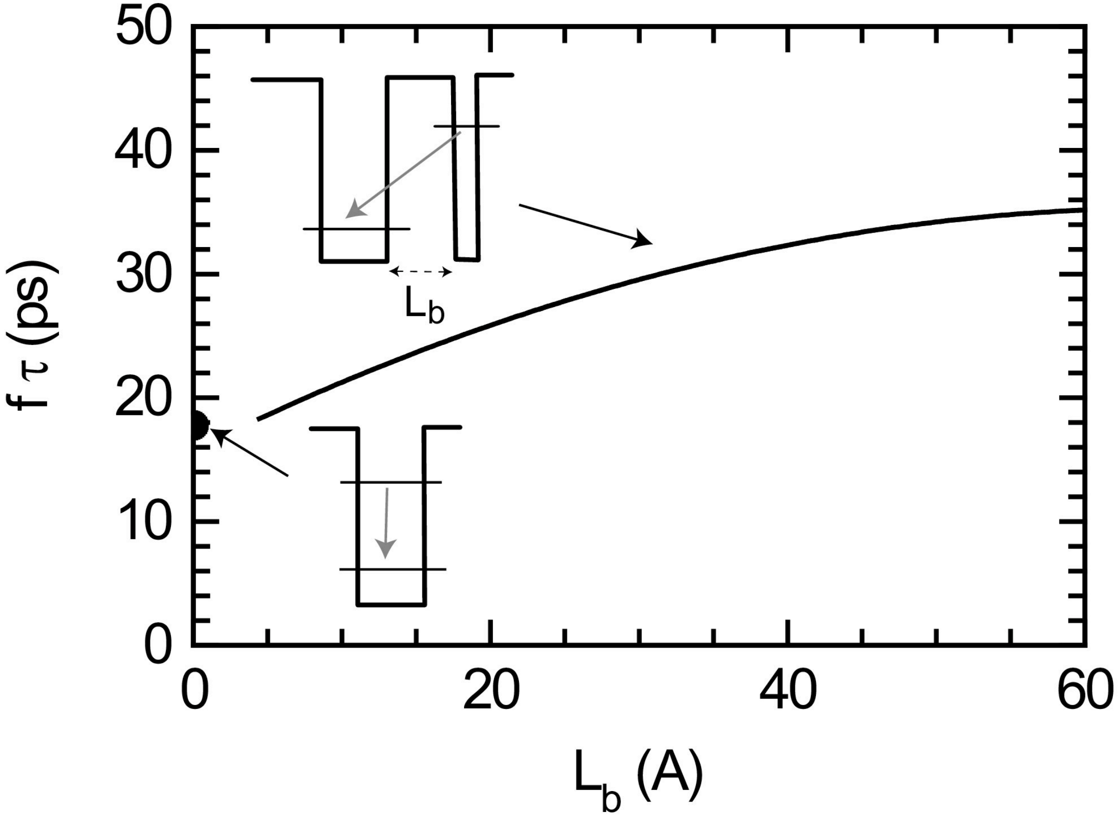
Electron lifetime on excited subbands is a function ($\sim k_{\parallel}^2$) of the momentum exchanged with the lattice by the emission of an optical phonon.

Tunneling

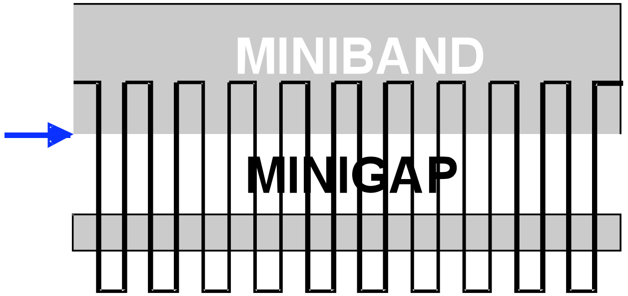


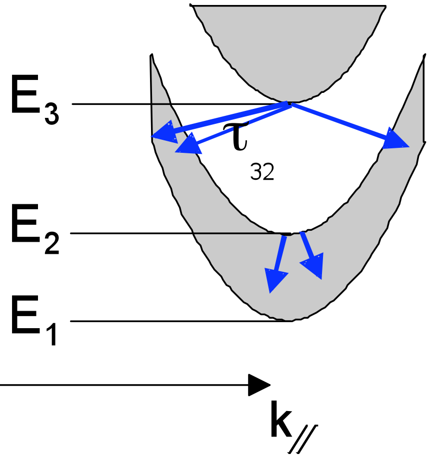
100
10
1
0.1
0
20
40
60
10
1
0.1
0.01
Oscillator strength
Scattering rate (ps-1)
~ exp(-2κL$_b$)
L$_b$
L$_b$ (Å)

Improves also the figure of merit



Engineering lifetimes (II)



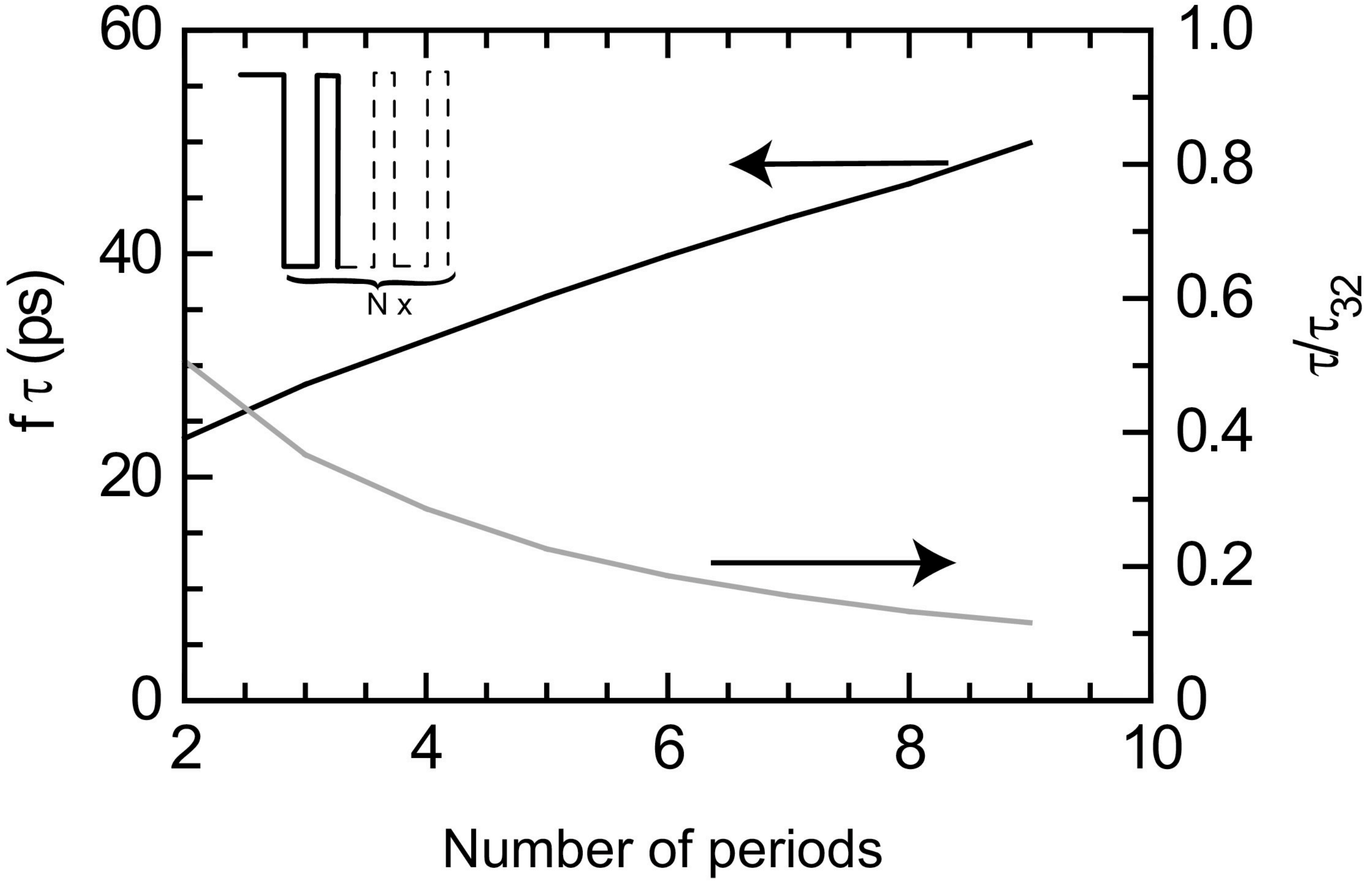


Phase space in superlattice:

The probability of injecting the electron in the upper state of the lower miniband is very small. However, once there, the electron has a large phase space to scatter out of this state.

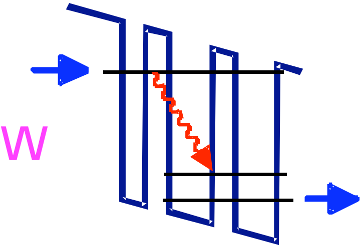
$$\boxed{\tau_{32} >> \tau_{2}}$$

Superlattice



Architectures

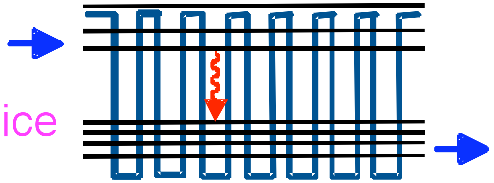
3QW



- Optical phonon resonance
- tunneling

J.Faist et al. Science 94

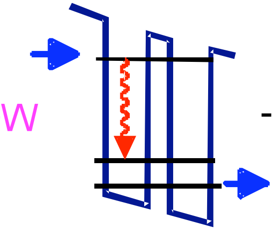
Superlattice



- Phase space

G. Scamarcio et al. Science 97

2QW



- Optical phonon resonance

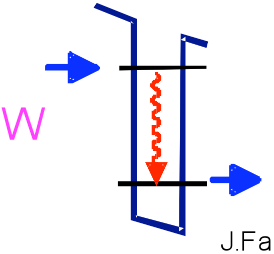
C.Sirtori e t al. PTL 97

Chirped Superlattice

- Phase space

Tredicucci et al. Appl. Phys. Lett. (1998)

1QW



- tunneling + non-parabolicity

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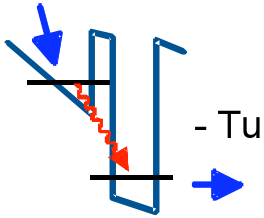
Diagonal



- Tunneling

J.Faist et al. Nature 97

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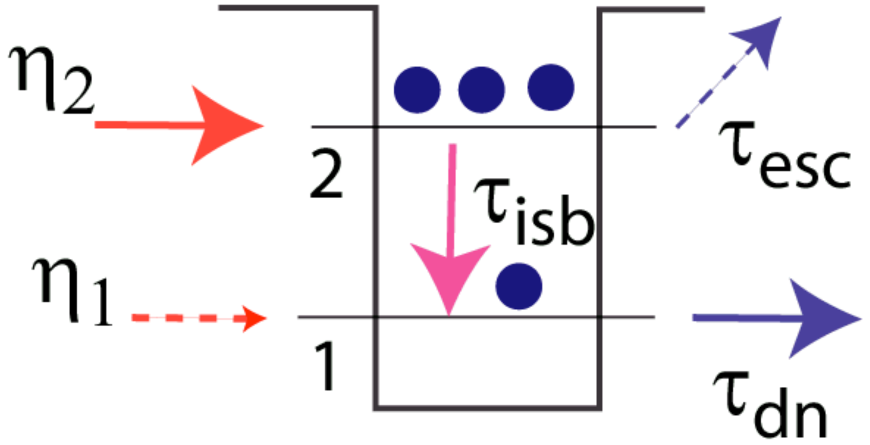
Active region design rules

- Avoid electron escape
- Avoid backfilling
- Discontinuity
- Injection efficiency
- Extraction efficiency/bottleneck effects

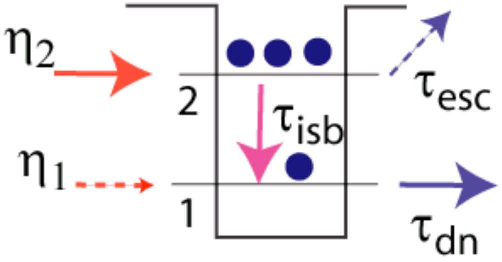
Active region optimization

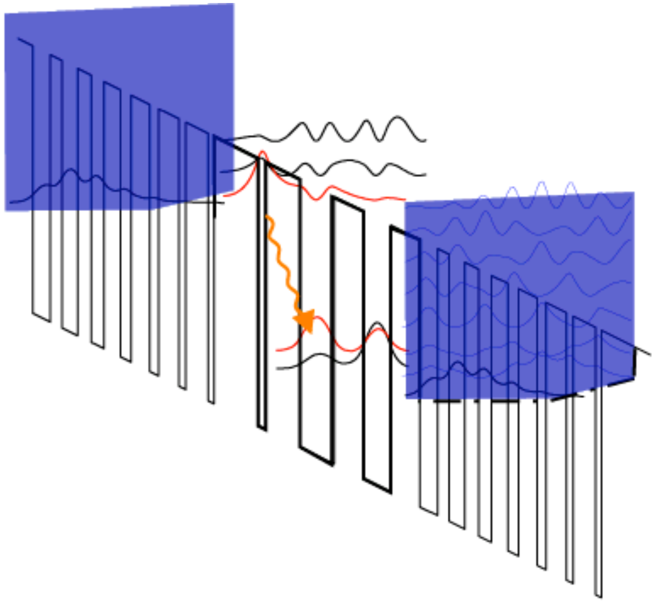


gain ~ $(n_2 - n_1)$

Since τ_{isb} is fixed by the intersubband physics, the optimization will concentrate on minimizing the "parasitic" factors η_1 and τ_{esc}

First QC laser at 4.26µm



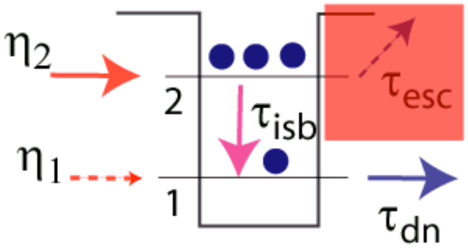


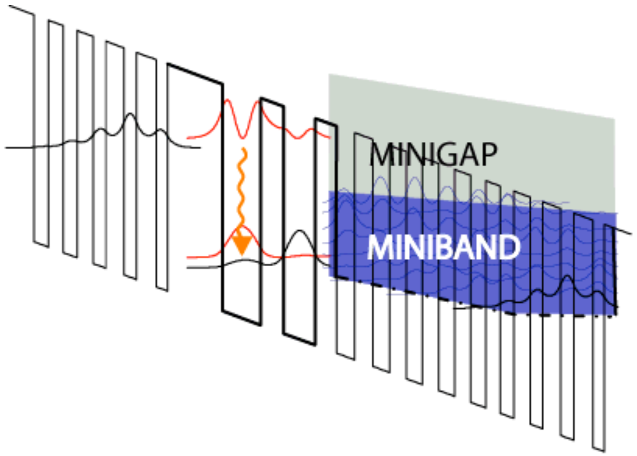
$J_{th} = 15\text{kA/cm}^2$

First QC laser structure based on three quantum wells:
Big escape problem!

J. Faist et al., Science 1994

Vertical transition (1995)



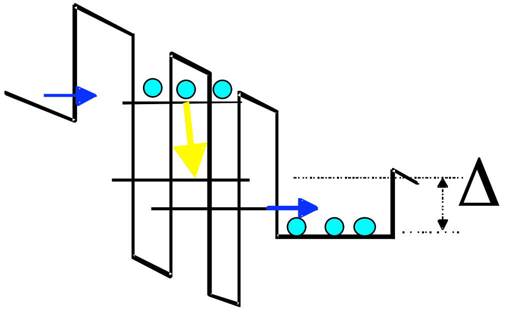


Vertical transition, two quantum well active region
Bragg reflection reduced escape

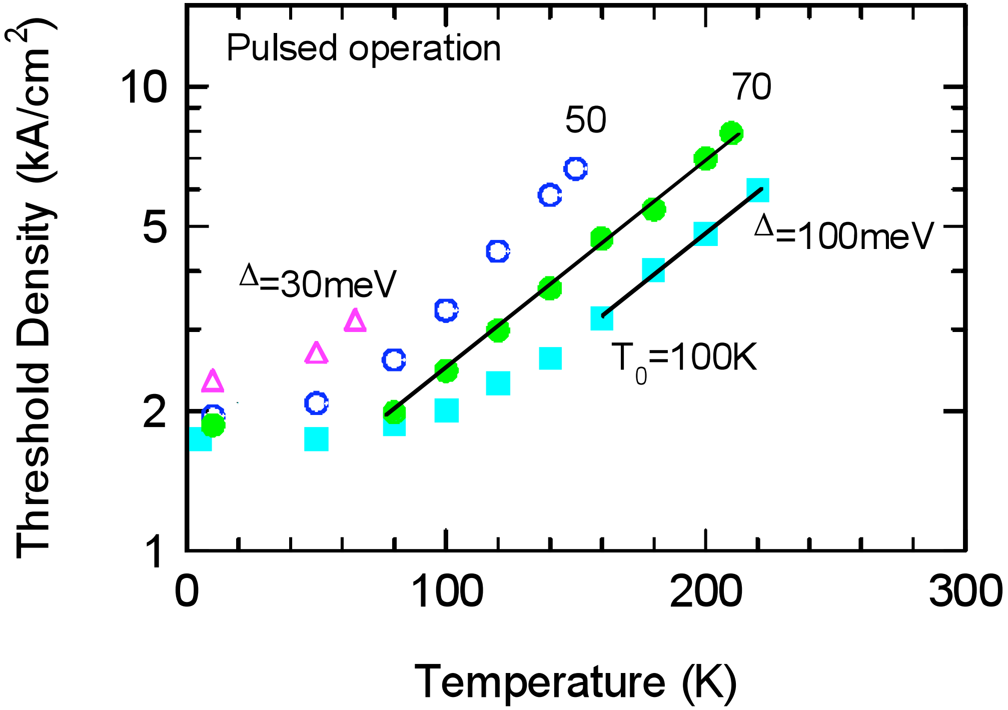
$J_{th} = 2\text{kA/cm}^2$ @ 10K

(J. Faist et al., APL 1995)

Avoid Backfilling



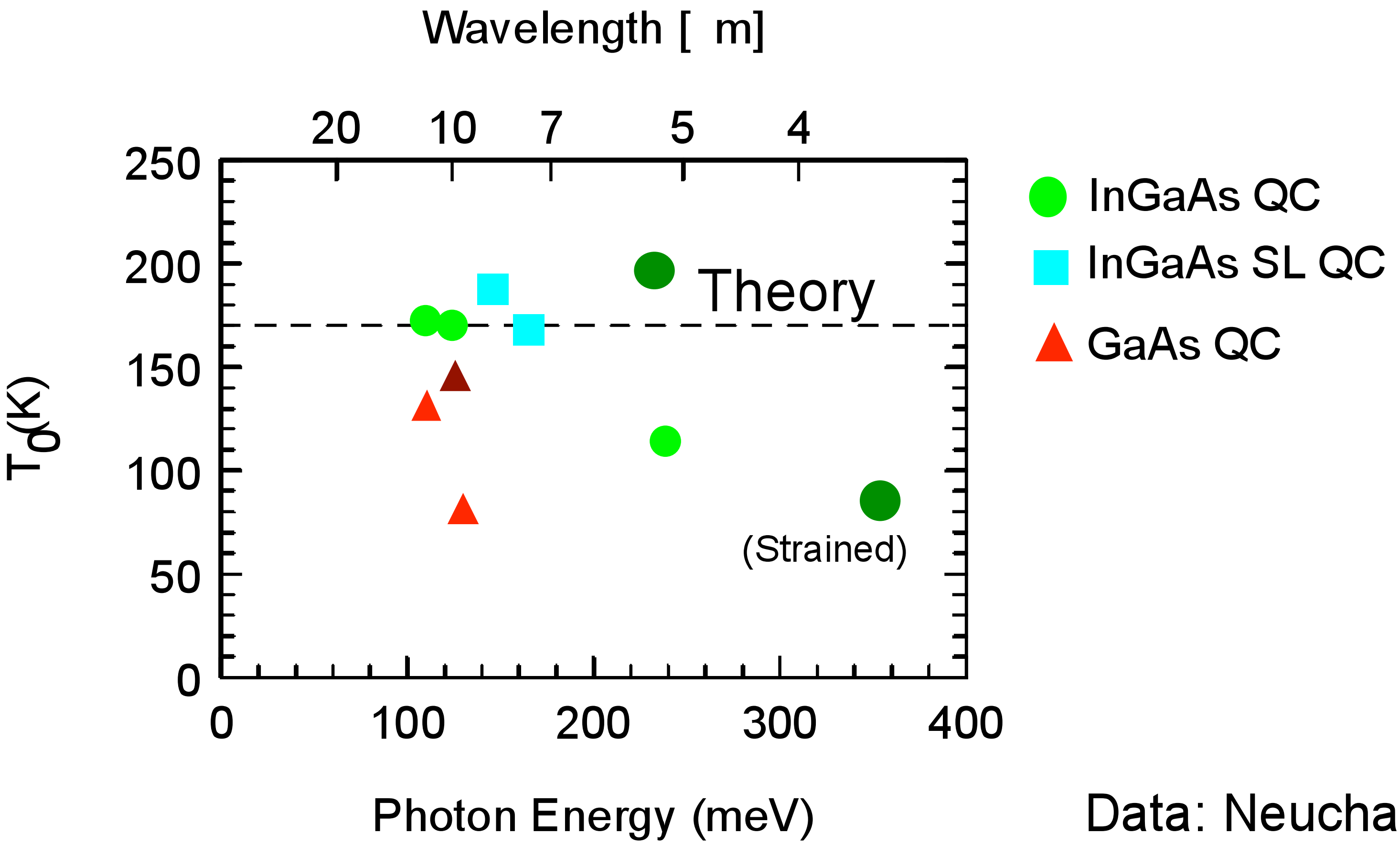
- Vertical $\lambda = 4.6 \mu m$ laser



– Δ is the activation energy for electrons into the lowest lasing state
- "Backfilling" must be avoided

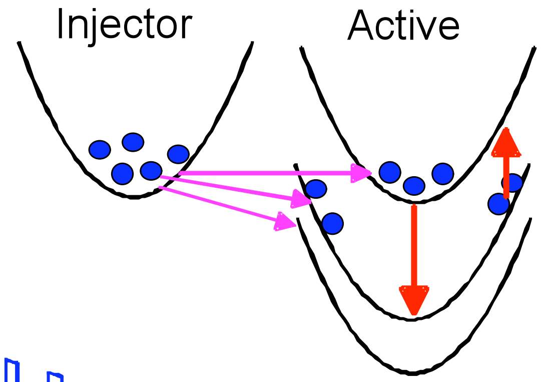
Semiconductor and semimetals, Vol 66

Influence of the discontinuity

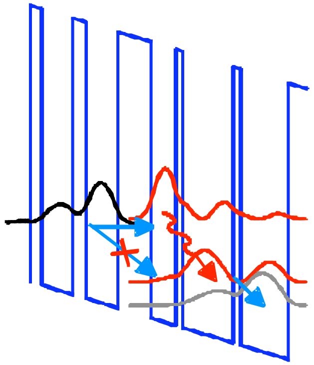


Data: Neuchatel,
Bell Labs
Thomson

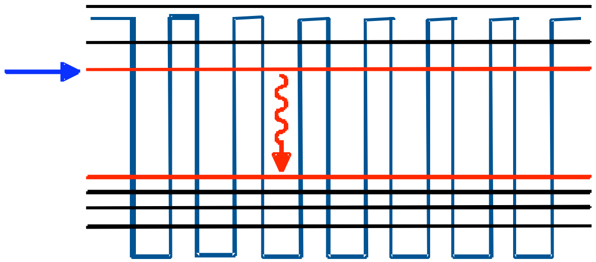
Injection efficiency



Gain depends in a critical way in the ration between the current injected in the lower and upper subband

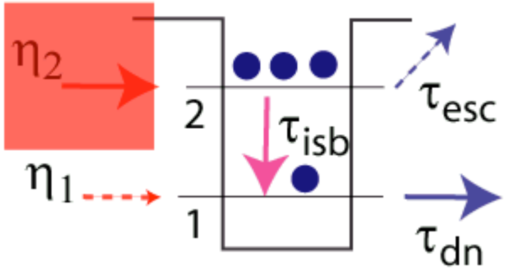


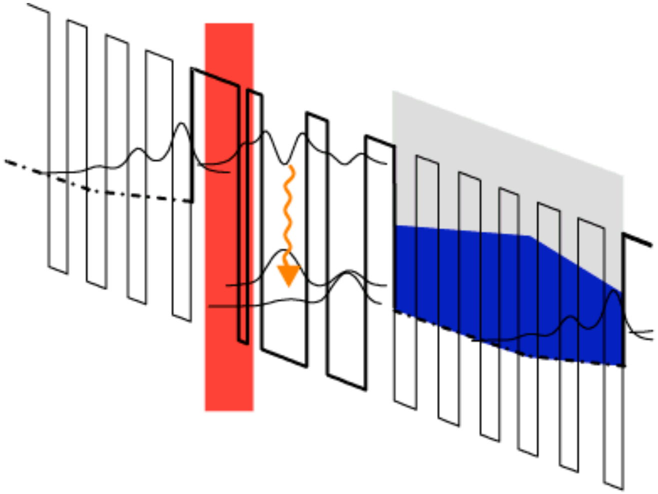
3QW vertical or anticrossed designs: optimize the overlap between the n=3 and injector levels



Superlattices: electrons injected in lower levels have a very low probability of bein at an energy where they would reabsorb (phase space argument)

Three QW active region



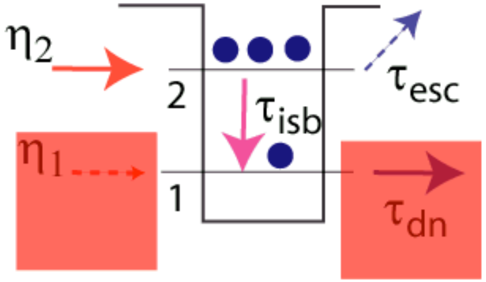


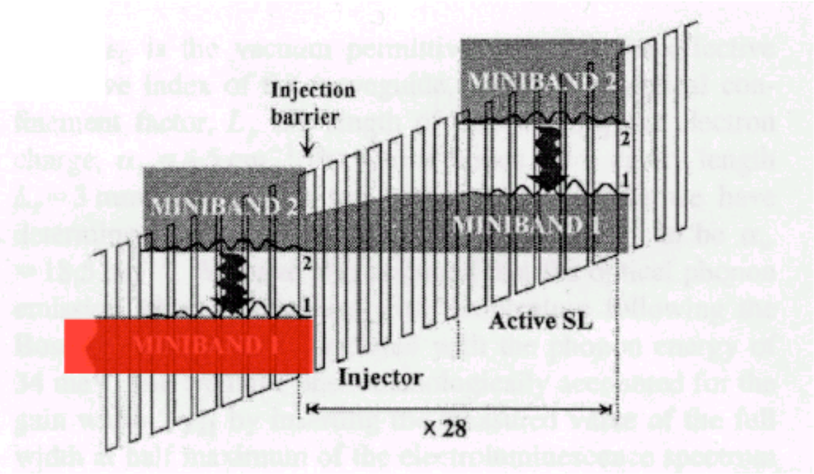
Three quantum well active region
High injection efficiency (large η_2)

J_{th} = 5-10kA/cm^2 @300K

(J. Faist et al., APL 1996)

Chirped Superlattice (1998)



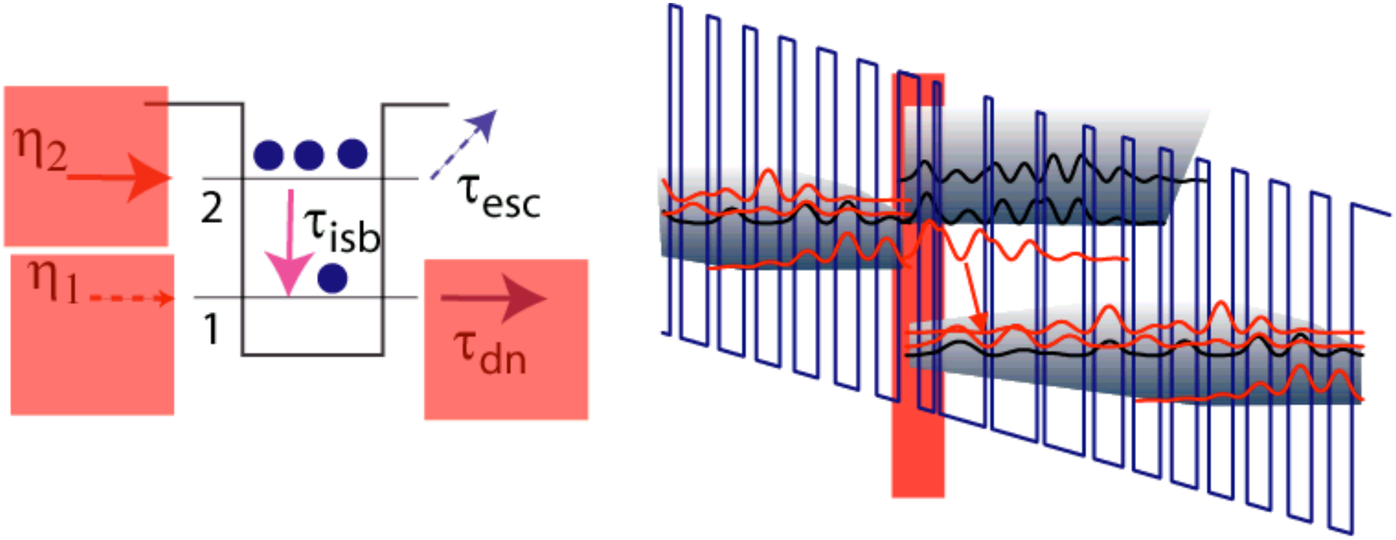


Chirped superlattice
Efficient miniband extraction

$J_{th} = 4.6 kA/cm^2$ @300K

(A.Tredicucci et al., APL 1998)

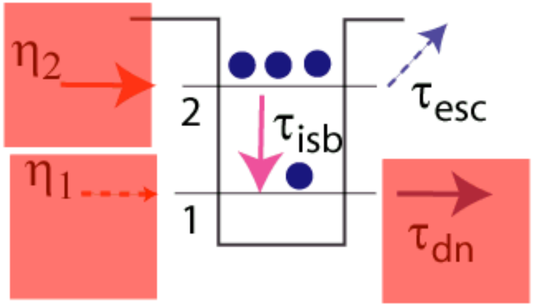
Bound-to-continuum

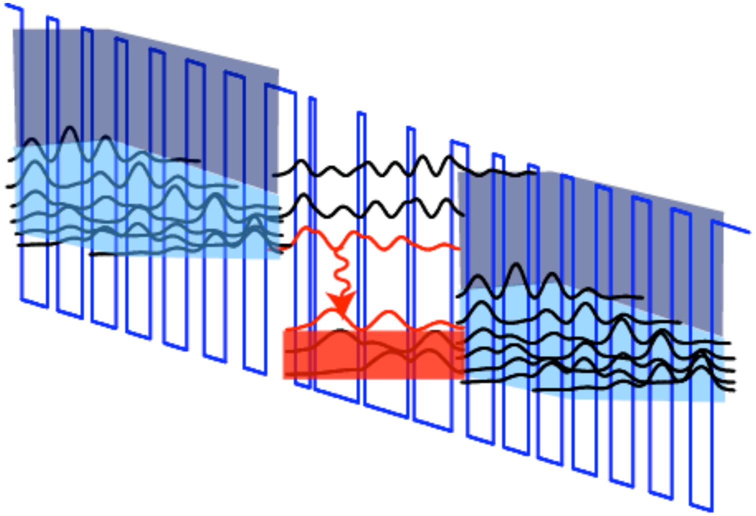


Bound-to-continuum
Efficient miniband extraction and high injection efficiency

(J. Faist et al., APL 2001)

Two phonons





Two phonon resonance
Double resonant phonon extraction and high injection efficiency

(D. Hofstetter et al., APL 2001)

Maximum wallplug efficiency

Wallplug efficiency good figure of merit

$$\eta_{wp} = \frac{P_{opt}}{UI}$$

Slope efficiency

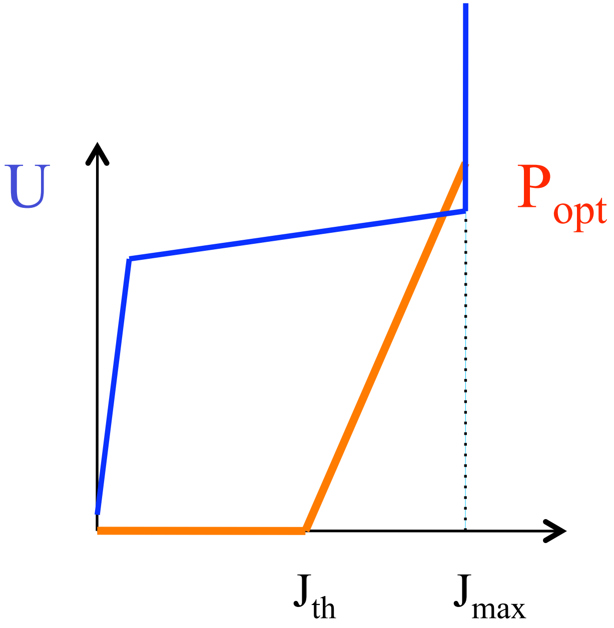
$$\frac{dP}{dI} = \eta_q N_p \frac{h\nu}{q} \frac{\alpha_m}{\alpha_m + \alpha_w}$$

“Voltage defect“

$$U = N_p(h\nu + \Delta_{inj})$$

Transition efficiency

$$\eta_q \approx (1 - \frac{\tau_{dn}}{\tau_{updn}})$$



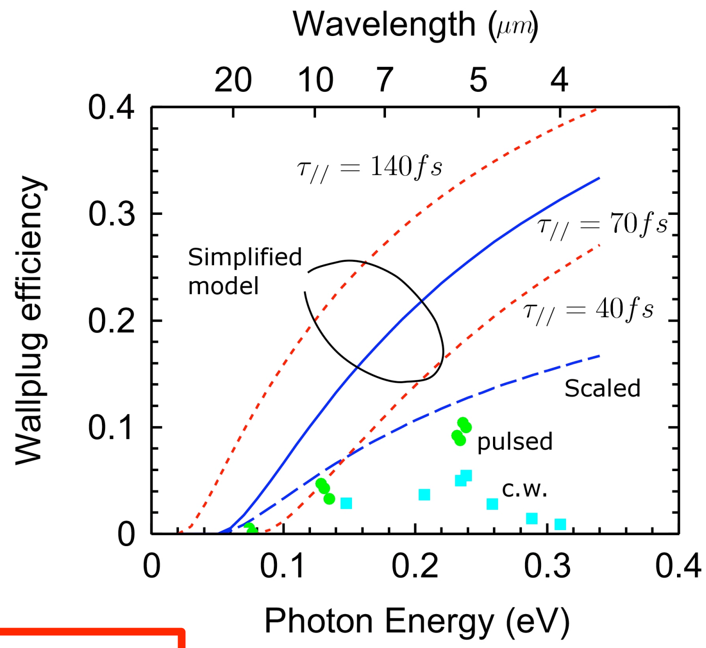
Doping dependence

$$\alpha_w \approx n_{dop} \qquad j_{max} \approx n_{dop}$$

Maximum wallplug efficiency in QCLs

Rate equation approach

$$\eta_{wp} = \frac{(J_{max} - J_{th})}{J_{max}} \frac{dP/dI}{U}$$



Free carrier absorption is proportional to doping

Mirror losses are optimum

$$\eta_{wp,max} = \eta_{tr} \frac{1}{1 + \Delta_{inj}/(\hbar\omega)} \left[\frac{\sqrt{g^*\tau^*} - 1}{\sqrt{g^*\tau^*}}\right]^2$$

$$g^* = \frac{1}{2}\omega^2 \tau_{//} \tau_{fc} f'$$

$$\tau^* = \tau_{up}/\tau_{trans}$$

J.Faist, Appl. Phys. Lett. (2007)

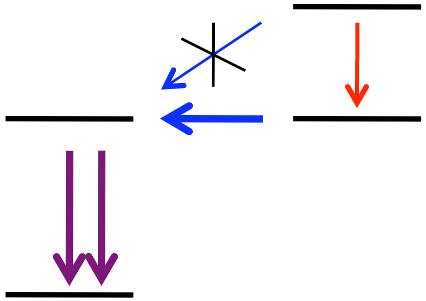
Outline

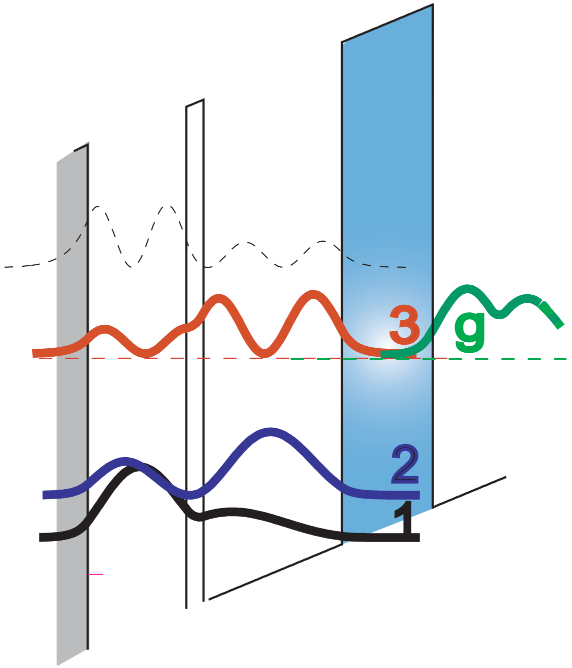
- A small look at history
- Computing energy states
- Rate equations and the parameters
- Active region optimization
- Resonant tunneling in QCLs

Resonant tunneling

Enables selective depopulation

Mid-infrared: used only
For the injection



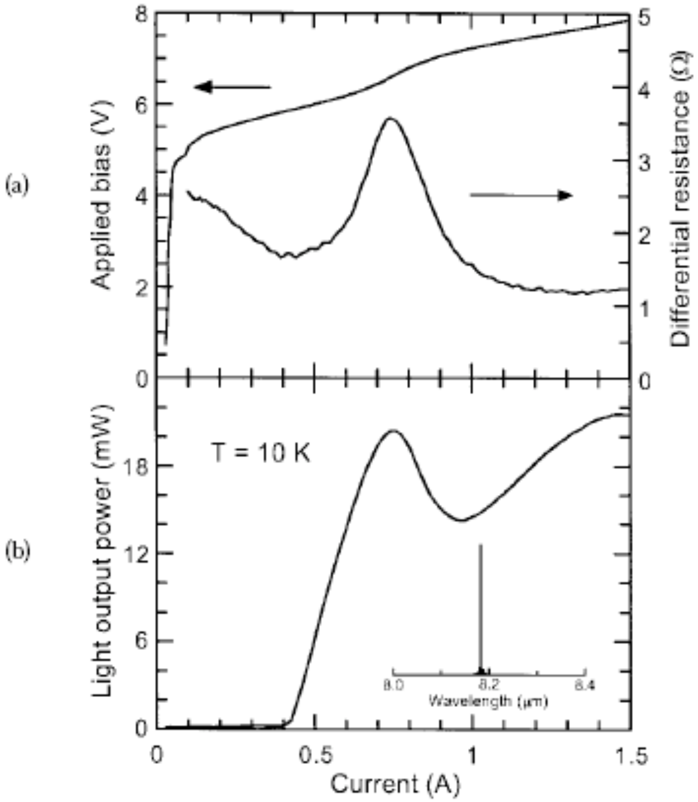


$$\tau_2, \tau_1 \ll \tau_3$$

1722 IEEE JOURNAL OF QUANTUM ELECTRONICS, VOL. 34, NO. 9, SEPTEMBER 1998

Resonant Tunneling in Quantum Cascade Lasers

Carlo Sirtori, *Member, IEEE,* Federico Capasso, *Fellow, IEEE,* Jérôme Faist, *Member, IEEE,*
Albert L. Hutchinson, *Member, IEEE,* Deborah L. Sivco, and Alfred Y. Cho, *Fellow, IEEE*



$$J = qN_s \frac{2|\Omega|^2\tau_\perp}{1+\underbrace{\Delta^2}_{\text{Detuning}}\underbrace{\tau_\perp^2}_{\text{Dephasing}}+4\underbrace{|\Omega|^2}_{\text{Coupling}}\underbrace{\tau_3}_{\text{Upper state lifetime}}\tau_\perp}$$

Limits at resonance

Jmax: $$J_{\max} = eN_s \frac{2|\Omega|^2\tau_\perp}{1+4|\Omega|^2\tau_3\tau_\perp}.$$

Weak coupling: $4|\Omega|^2\tau_3\tau_\perp \ll 1$

$$J_{\max} \;=\; (eN_s/2)4|\Omega|^2\tau_\perp$$

Strong coupling $4|\Omega|^2\tau_3\tau_\perp \;\gg\; 1$

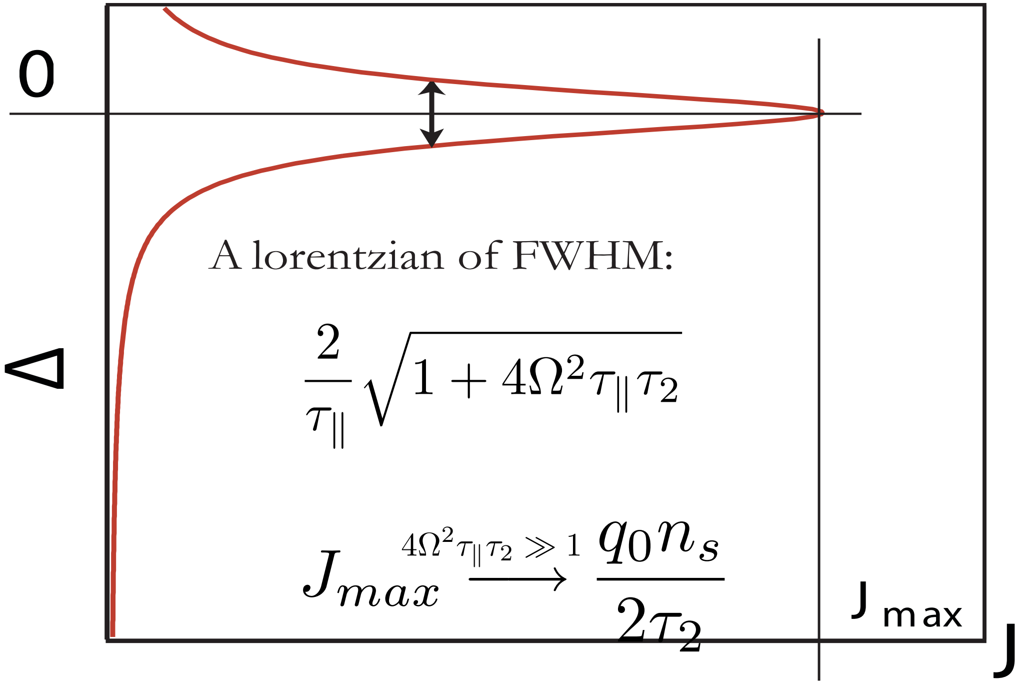
$$J \;=\; eN_s/(2\tau_3)$$

Kazarinov-Suris model: single barrier

Resonant tunneling current through a barrier (tight-binding):

Kazarinov and Suris., Sov. Phys. Semicond. 6, 120 (1972)

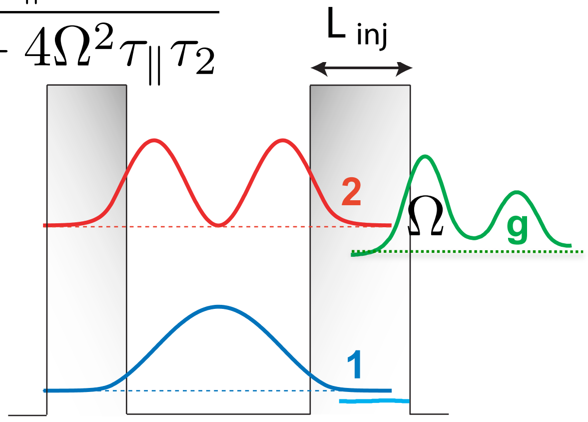
$$J = q_0 n_s \frac{2\Omega^2\tau_\parallel}{1+\Delta^2\tau_\parallel^2+4\Omega^2\tau_\parallel\tau_2}$$



A lorentzian of FWHM:

$$\frac{2}{\tau_\parallel}\sqrt{1+4\Omega^2\tau_\parallel\tau_2}$$

$$J_{max} \xrightarrow{4\Omega^2\tau_\parallel\tau_2 \gg 1} \frac{q_0 n_s}{2\tau_2}$$



Ω Coupling frequency

Δ Detuning

$\tau_\parallel$ In-plane dephasing time

τ_2 Scattering time of $|2\rangle$

C. Sirtori, F . Capasso, J. Faist, A. Hutchinson, D. Sivco, and A. Cho, IEEE J. Quantum Electron. 34, 1722 (1998)

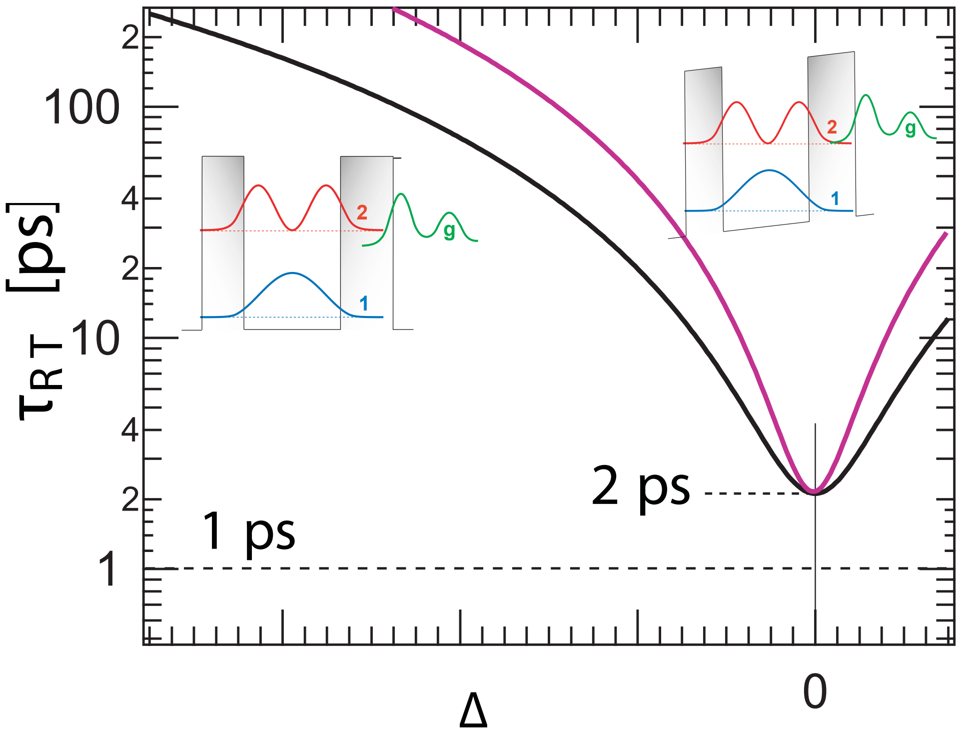
Total transport time:

As an effective lifetime

$\hbar\Omega = 3$ meV

$\tau_2 = 1$ ps

$$\tau_{RT} = \underbrace{\frac{1+\Delta^2\tau_{\|}^2}{2\Omega^2\tau_{\|}}}_{\text{Tunneling time}} + \underbrace{2\tau_2}_{\text{Lifetime distributed over states } |2\rangle \text{ and } |g\rangle}$$

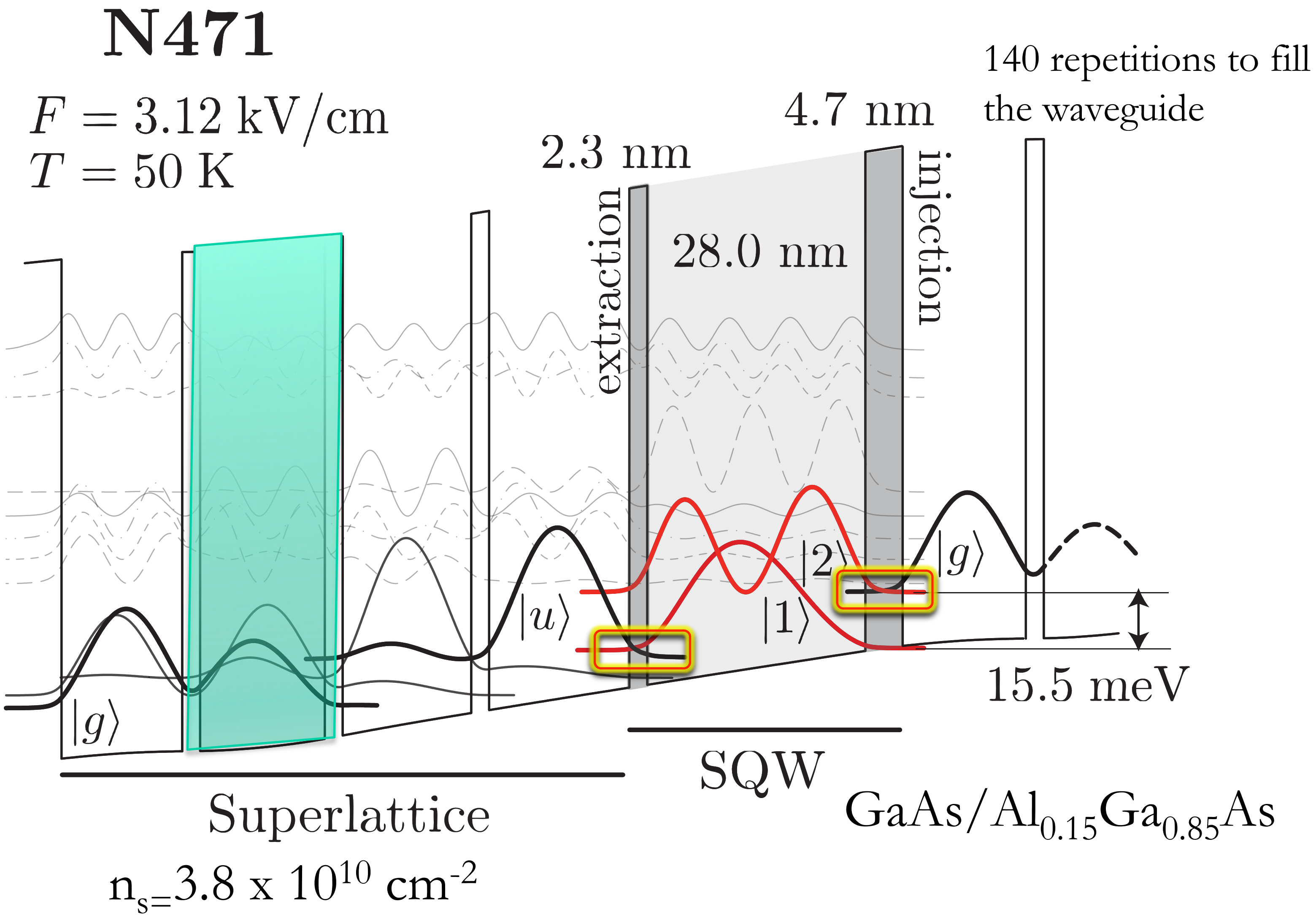


$\tau_{\|} = 0.2$ ps

$\tau_{\|} = 0.5$ ps

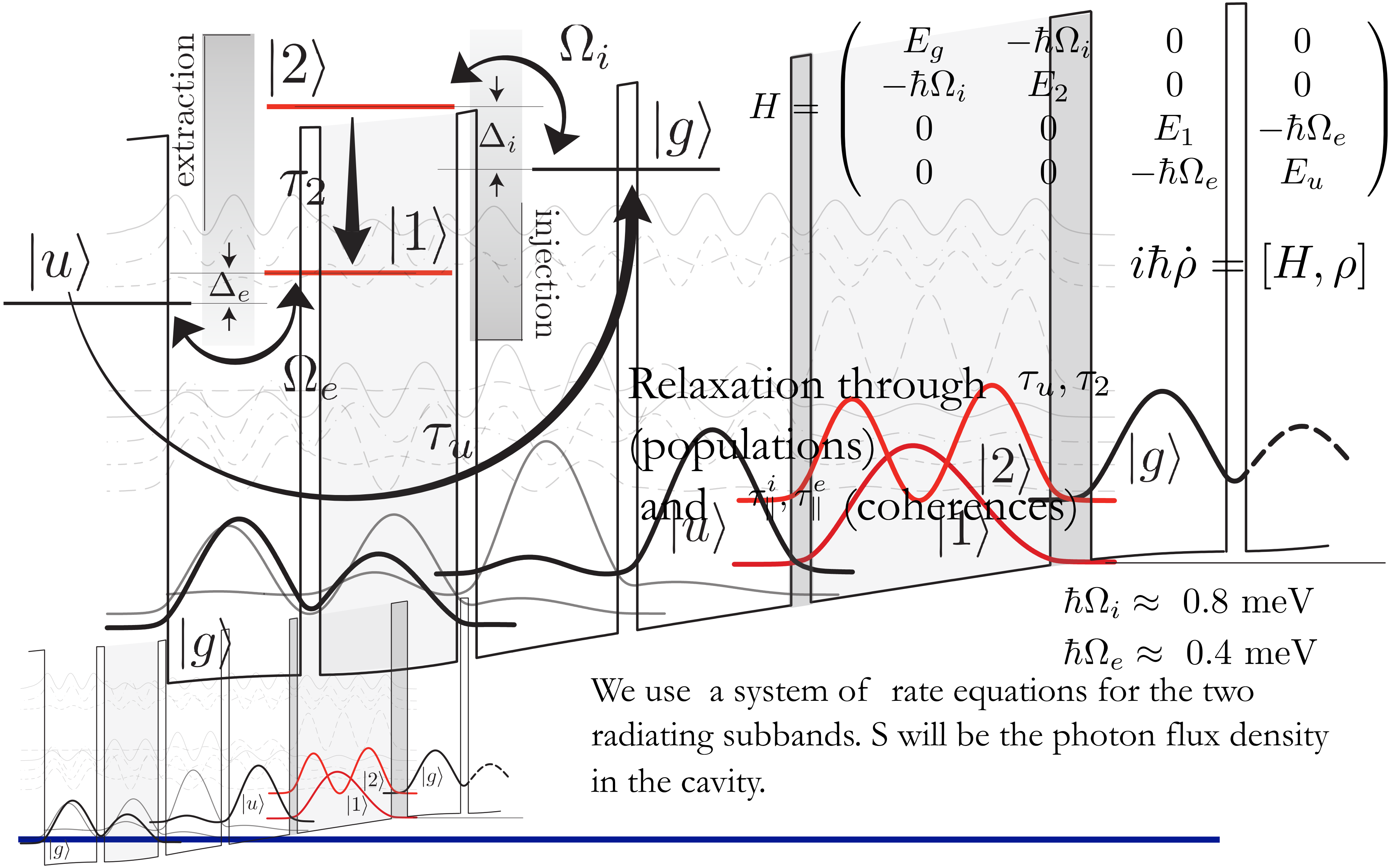
critical role of the in-plane scattering time $\tau_{\|}$

Single quantum well emitting at 3.7 THz



Very similar to Rochat et al., Appl. Phys. Lett., Lett. 73, 3724 (1998)

Density matrix at injection and extraction on a tight-binding basis



$$H = \begin{pmatrix} E_g & -\hbar\Omega_i & 0 & 0 \\ -\hbar\Omega_i & E_2 & 0 & 0 \\ 0 & 0 & E_1 & -\hbar\Omega_e \\ 0 & 0 & -\hbar\Omega_e & E_u \end{pmatrix}$$

$$i\hbar\dot{\rho} = [H, \rho]$$

Relaxation through τ_u, τ_2 (populations) and $\tau_\parallel^i, \tau_\parallel^e$ (coherences)

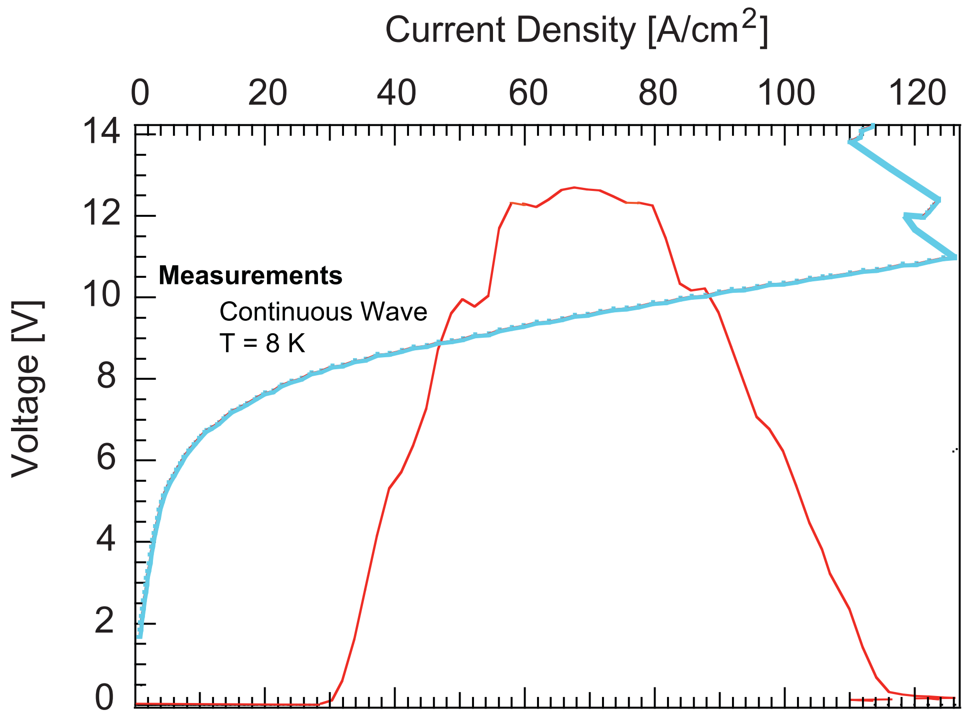
$\hbar\Omega_i \approx\ 0.8$ meV

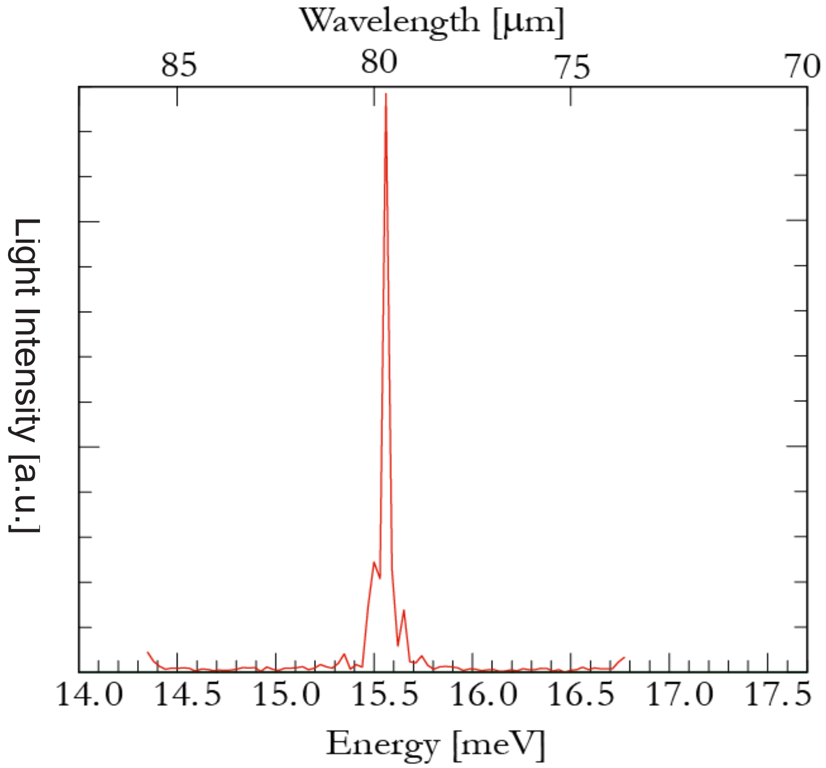
$\hbar\Omega_e \approx\ 0.4$ meV

We use a system of rate equations for the two radiating subbands. S will be the photon flux density in the cavity.

G. Scalari, R.Terazzi et al., *Appl. Phys. Lett.*, **91,** 032103 (2007), R. Terazzi, *unpublished* (2008)

Experimental results





Laser action with extremely reduced threshold (J_{th}< 30 A/cm^2) at 80 µm (3.7 THz) in a double metal configuration

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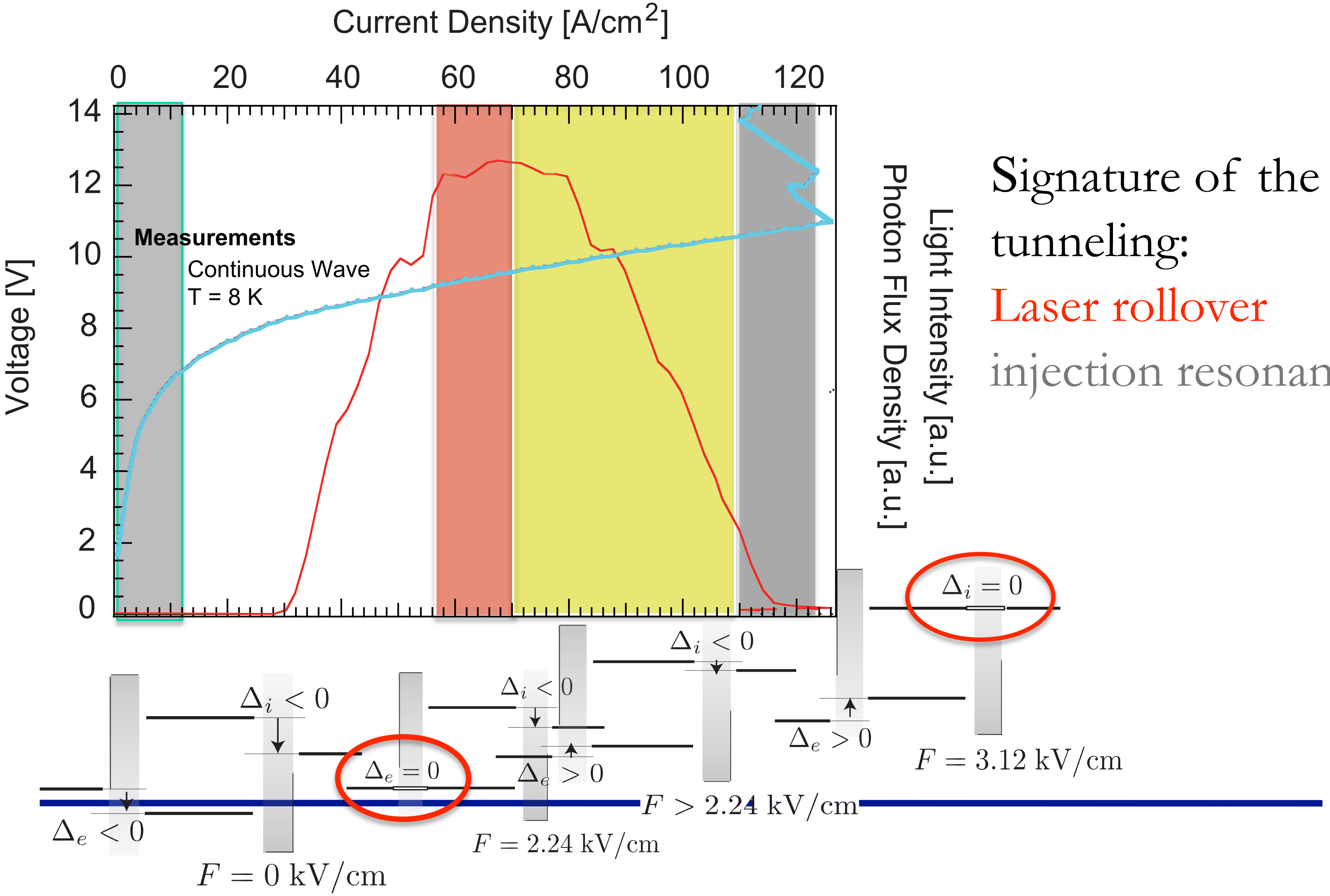
G. Scalari, R.Terazzi et al., *Appl. Phys. Lett.*, **91,** 032103 (2007)

Couplings of the doublets as a function of electric field



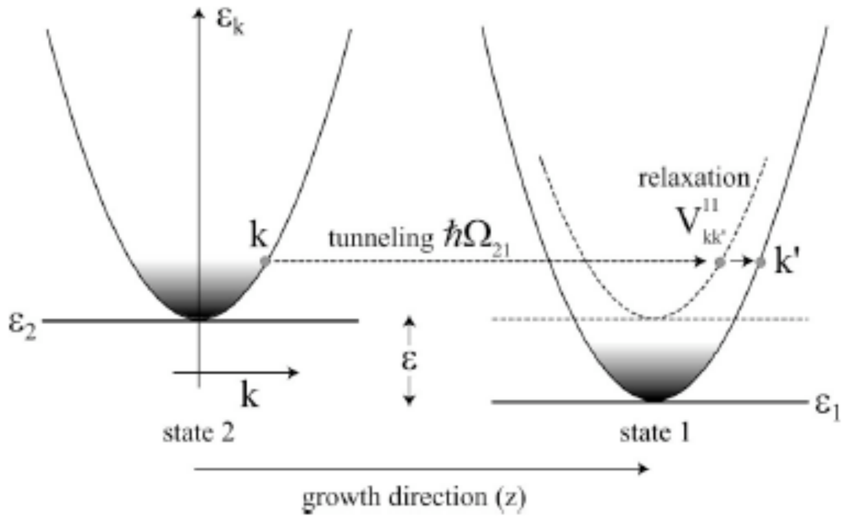
Signature of the resonant tunneling:

Laser rollover

injection resonance

Density Matrix derivation

- Elements: two states coupled by tunneling
- In-plane scattering



$$H_k^{ij} = \begin{pmatrix} \epsilon_{2k} & \hbar\Omega_{21} \\ \hbar\Omega_{12} & \epsilon_{1k} \end{pmatrix}^{ij}, \quad V_{kk'}^{ij} = \begin{pmatrix} V_{kk'}^{22} & 0 \\ 0 & V_{kk'}^{11} \end{pmatrix}^{ij}$$

- Density matrix equation

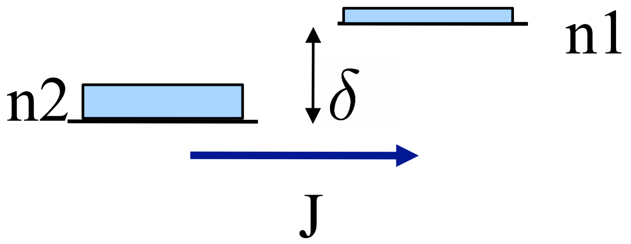
$$i\hbar\,\partial_t\hat{\rho} = [\mathcal{H}, \hat{\rho}]$$

- Keep off-diagonal elements

(H. Willenberg et al., Phys Rev. B 67, 085315 (2003))

Resonant tunneling current (ver II)

- Assume classical distributions in both subbands (same mass)

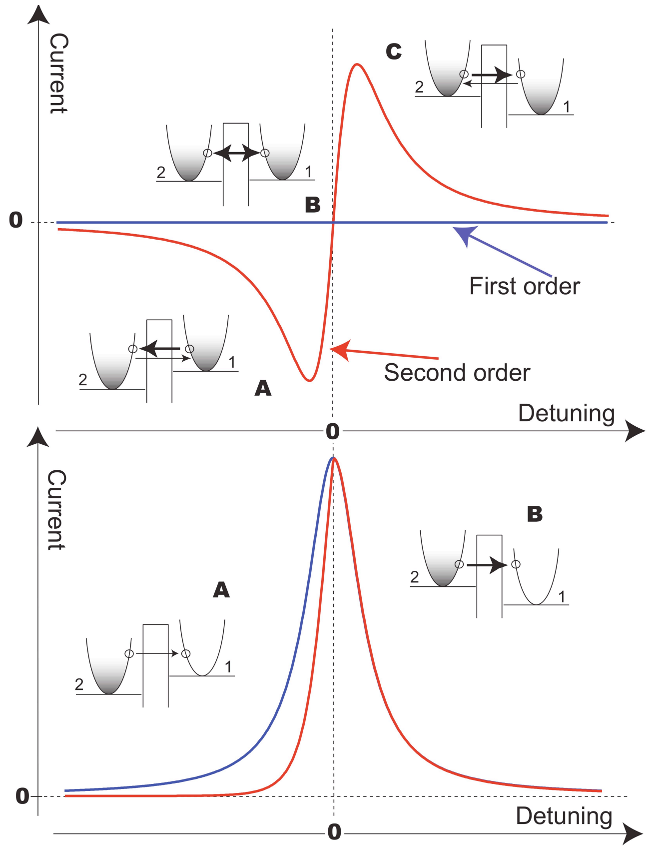


$\delta < 0$ $$J(\delta), = A\frac{\gamma}{\gamma^2 + \delta^2}(n_2 \exp(-\delta/kT) - n_1)$$

Kazarinov: $$J(\delta), = A\frac{\gamma}{\gamma^2 + \delta^2}(n_2 - n_1)$$

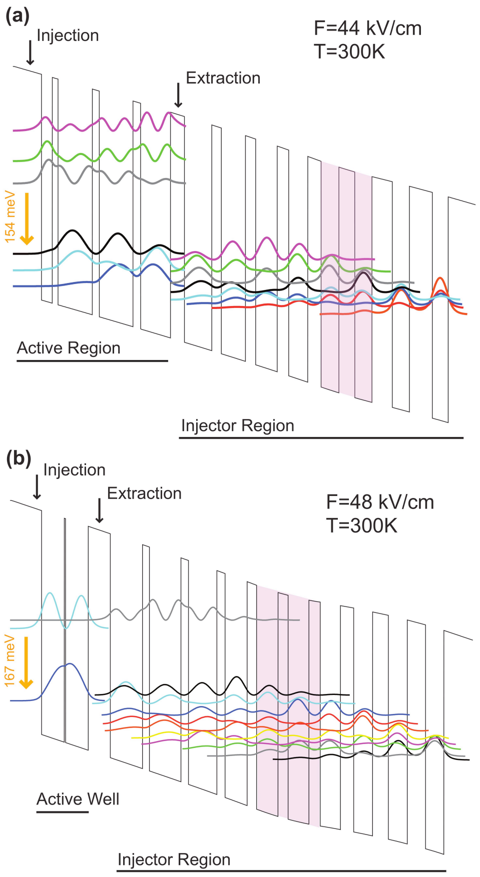
Equal for high temperatures $\delta << kT$

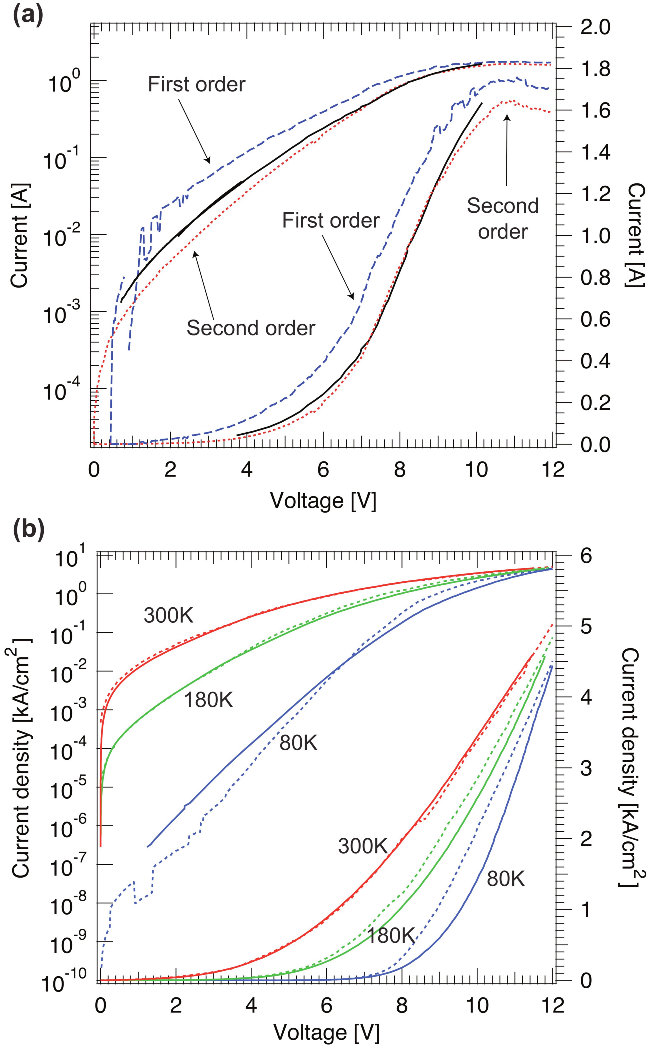
Enables computation of the I-V laser characteristics



R. Terazzi et al., submitted

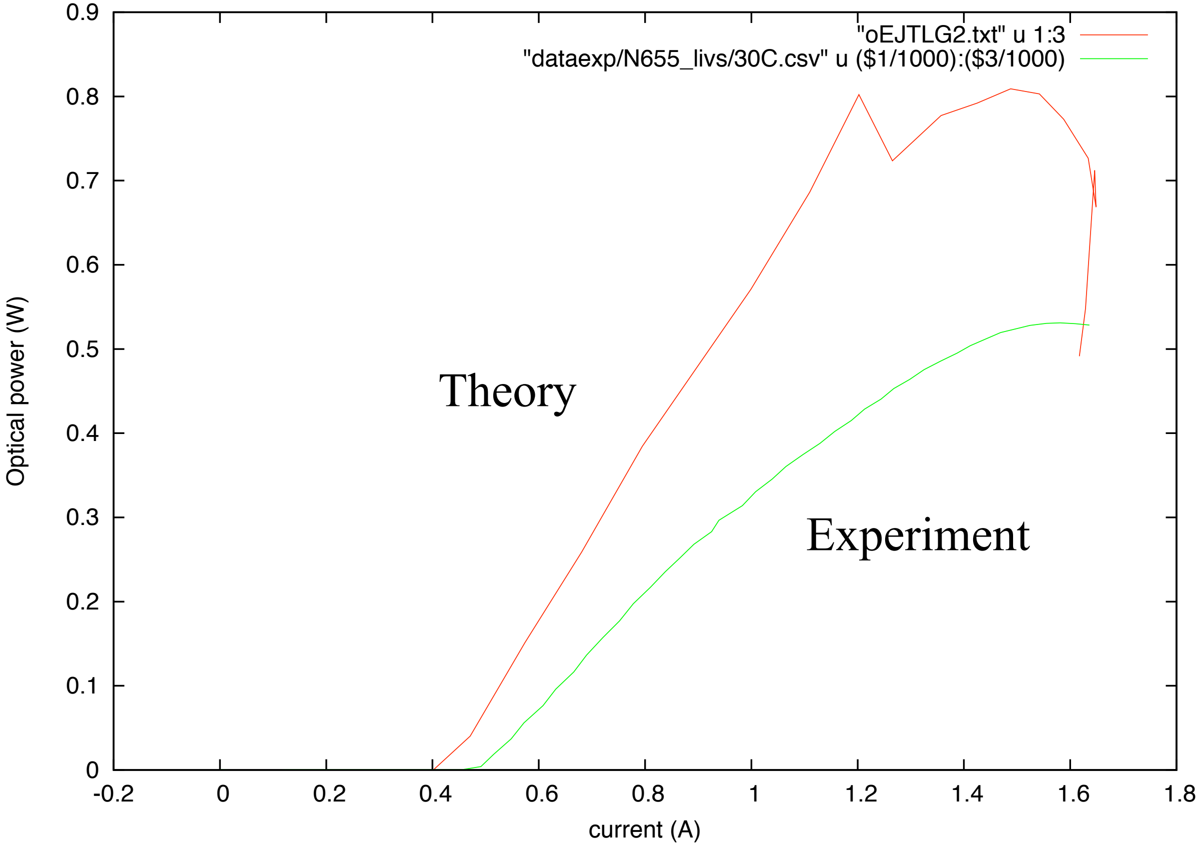
IV curves predictions





R. Terazzi, A. Wittmann, T. Gresch et al., submitted

Also possible to include the light



One “free” parameter: waveguide roughness scattering 1cm^{-1}

R. Terazzi, A. Wittmann, unpublished

Conclusion

- Designability of intersubband
- In the mid-IR, “ab initio” computations are now possible

Collaborators

FIR team: G. Scalari, M. Amanti, C. Walther,
J. Lloyd-Hughes
MIR team: A. Wittmann, Y. Bonetti, T.Gresch, R.Terazzi,
A. Bismuto, A. Hugi, A. Mohan

Growth Team: M. Beck, M. Fischer, V. Liverini