
Modeling of Transport and Gain in Quantum Cascade Lasers

Andreas Wacker



LUNDS UNIVERSITET

in collaboration with:

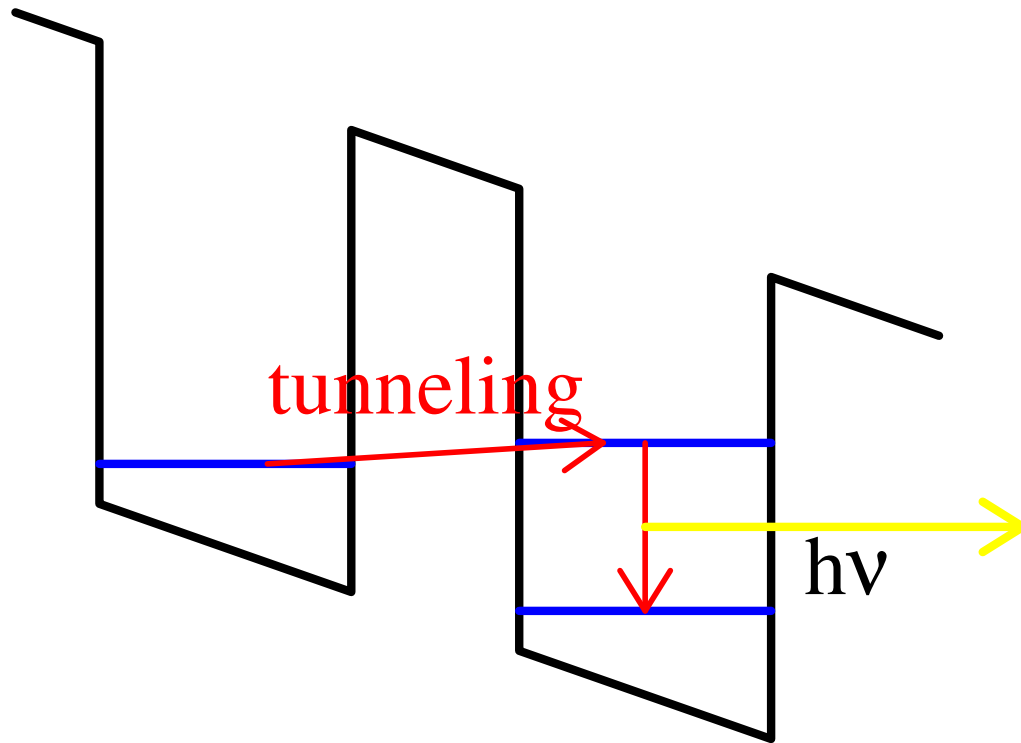
M.P. Pereira Jr., NMRC, Cork



Introduction



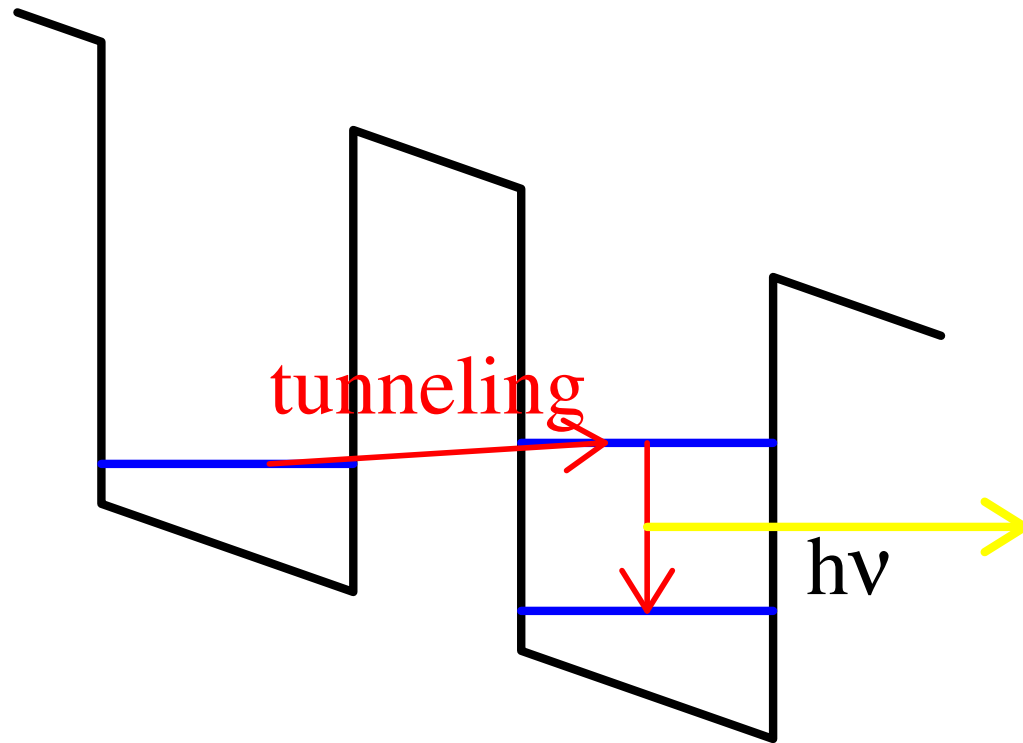
The Challenge: Intersubband Lasing



Kazarinov and Suris,
1971



The Challenge: Intersubband Lasing

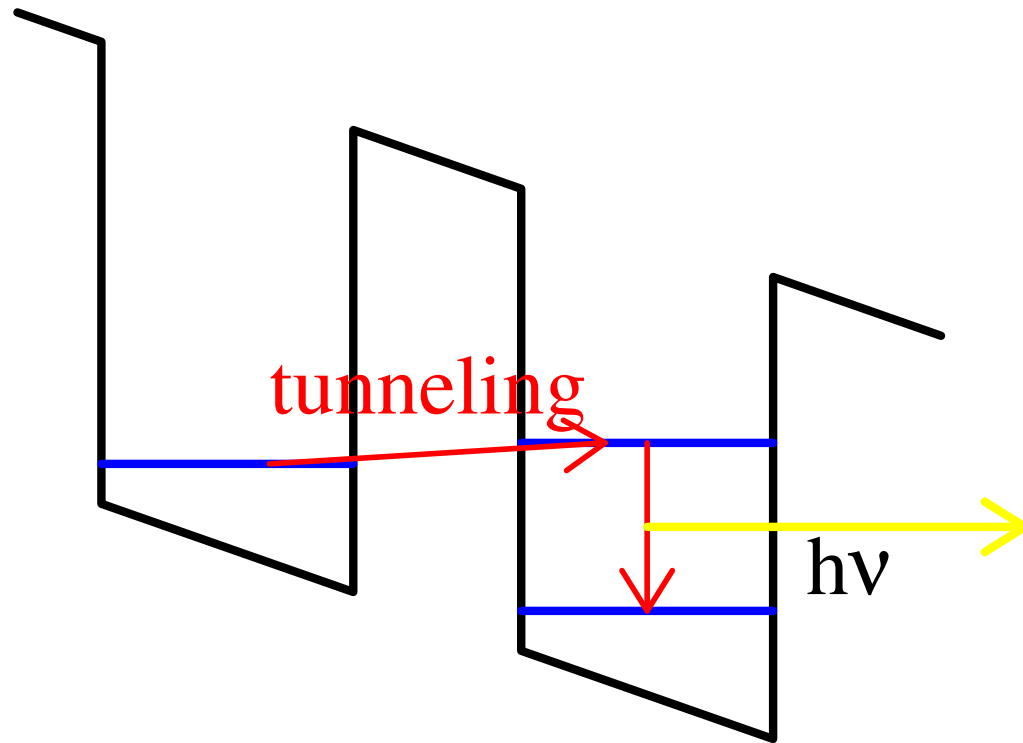


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Advantage: Photon energy tunable by well width:
 $h\nu \sim 100 \text{ meV} \pm ?? \rightarrow$ molecular spectroscopy



The Challenge: Intersubband Lasing



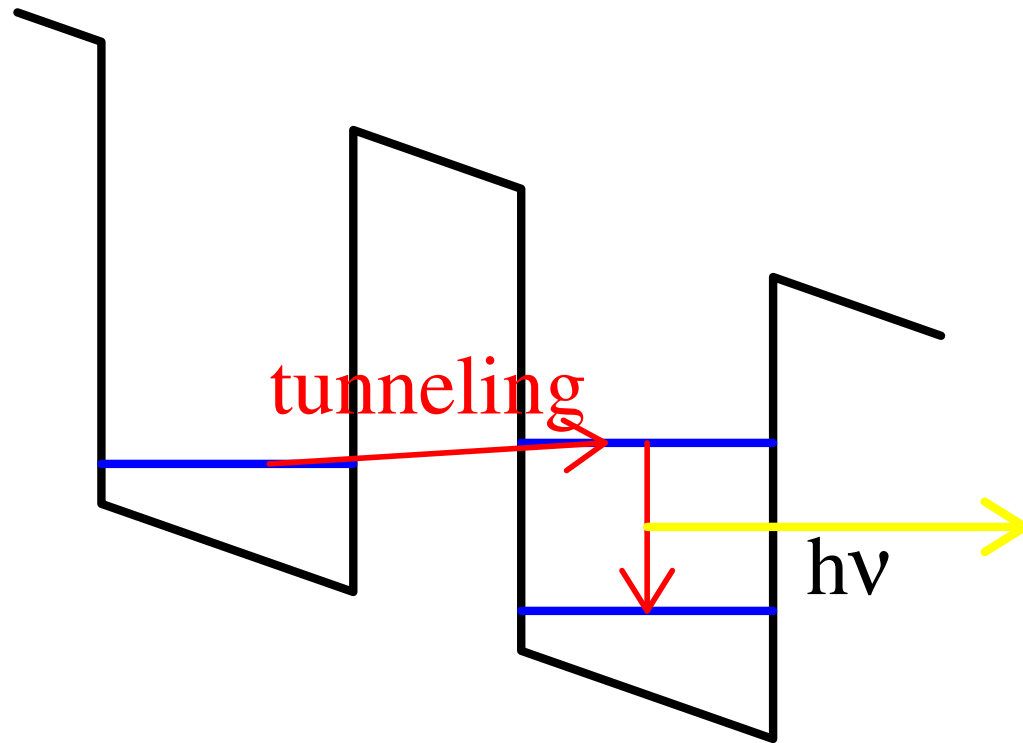
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Escape to continuum



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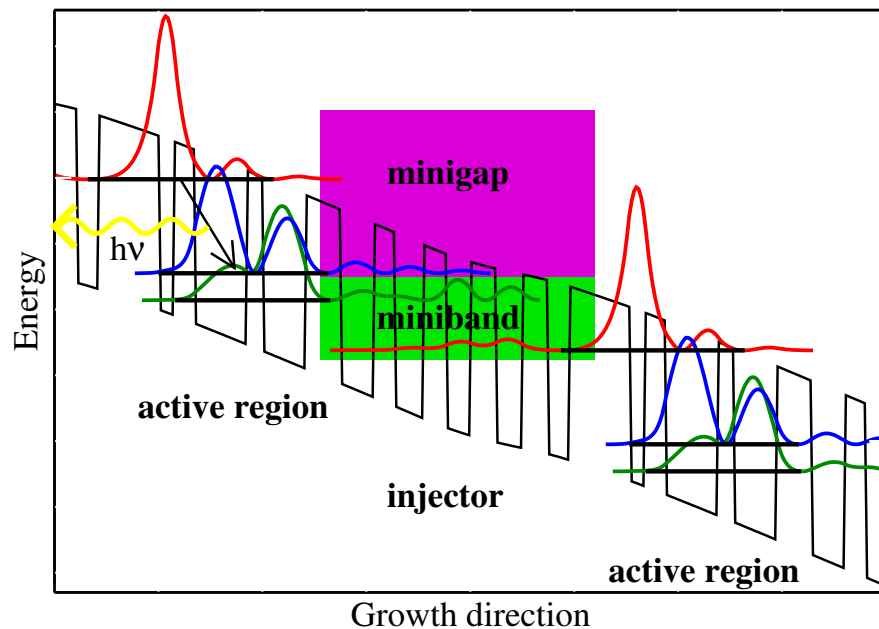
It took 23 years to achieve such a laser...



The Quantum Cascade Laser

First realized by

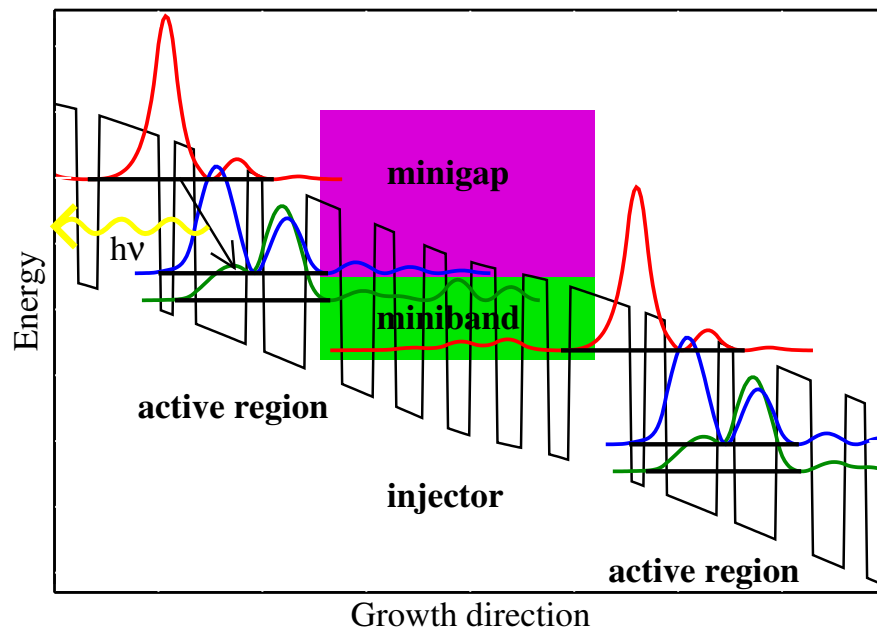
Faist, Capasso et al: 1994



The Quantum Cascade Laser

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Key design features:

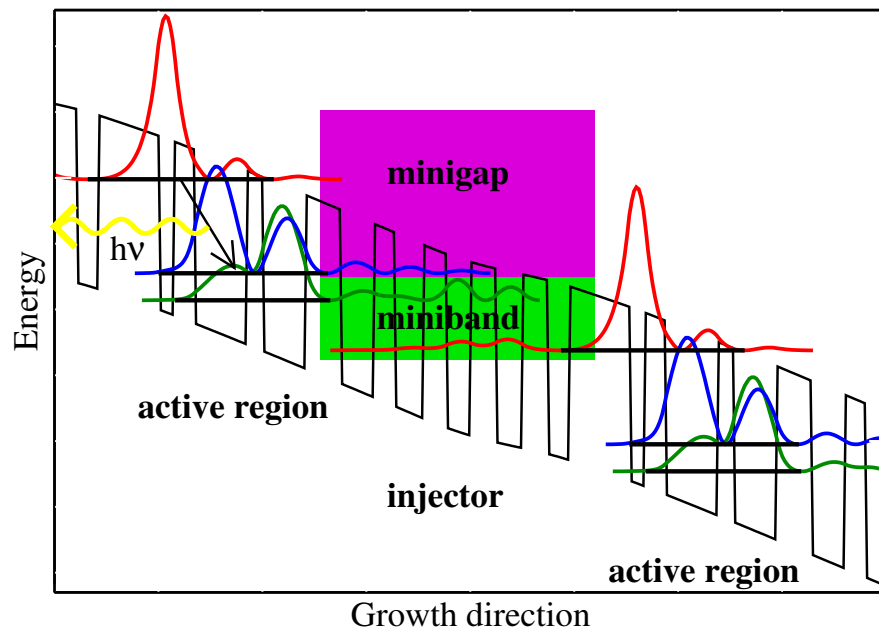
- **3 levels** in active region
- **Injector region**
 - efficient electron transfer into level 3
 - prevents escape into continuum
- **Cascading:**
 - ~ 30 repetitions of (active region + injector)



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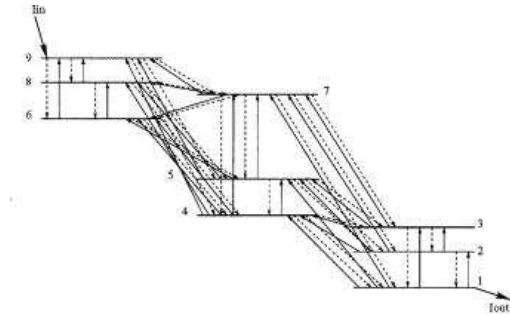
Current state of the art:

- Wavelength: $3.5\mu\text{m} < \lambda < 24\mu\text{m}$ and $\approx 60\mu\text{m}$
Energy: $350\text{ meV} > h\nu > 50\text{ meV}$ and $\approx 16\text{ meV}$
- Operation temperature: $> 300\text{ K}$ for IR, $> 77\text{ K}$ for THz



Transport Models

Semiclassical rate equation

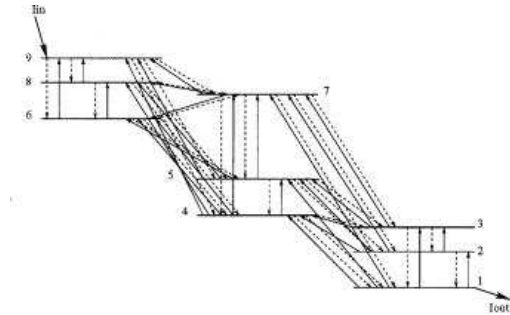


Donovan,
Harrison,
and Kelsall:
JAP 2001



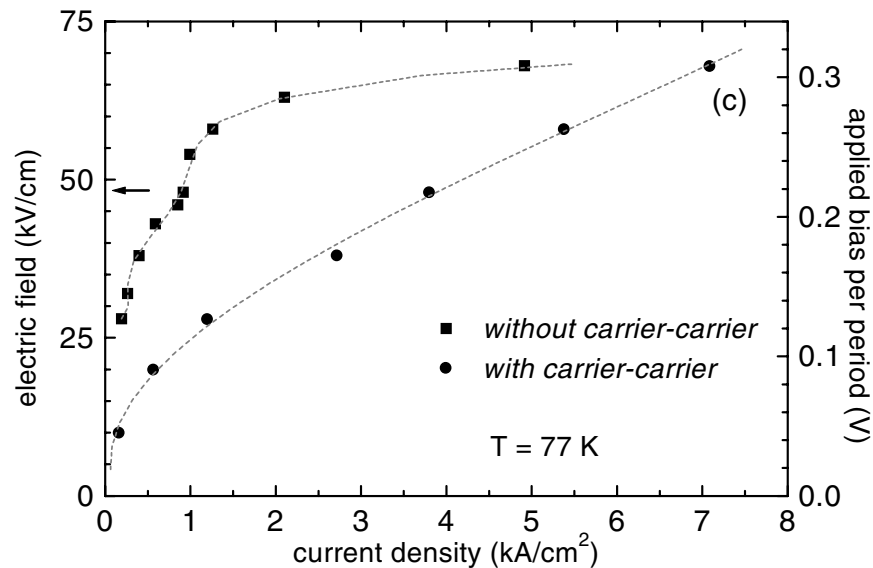
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MC-simulation for $f_n(\mathbf{k})$

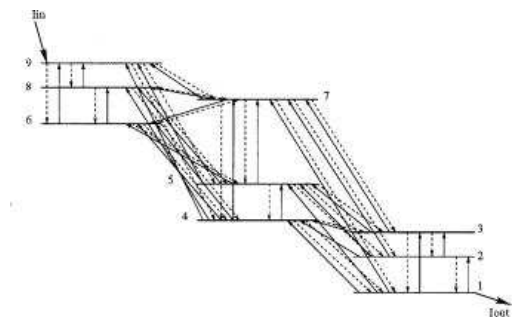


Iotti and Rossi: PRL 2001



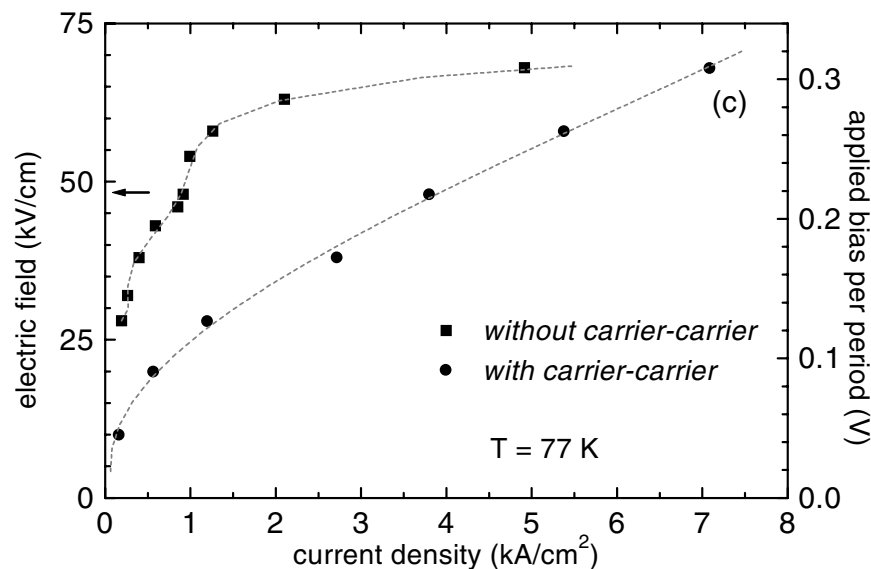
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Semiclassical rate equation



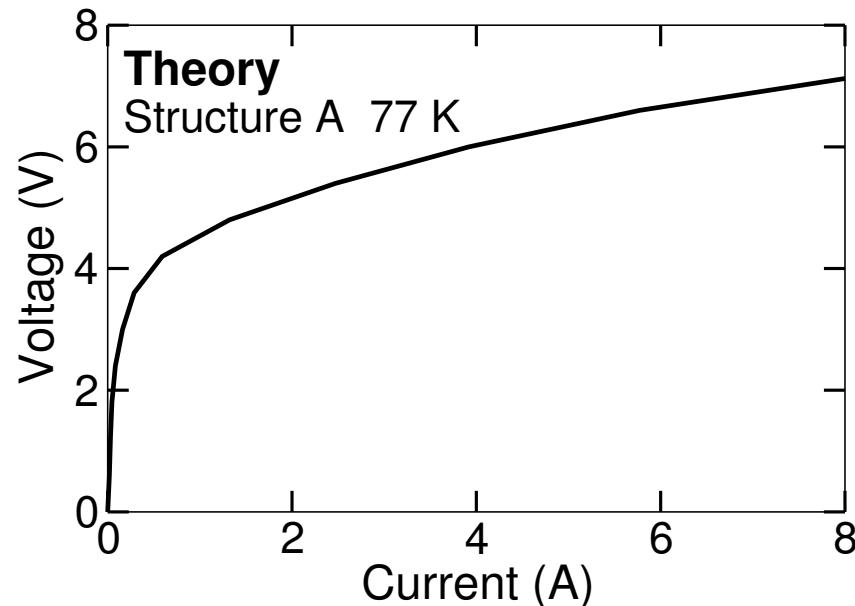
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JAP 2001

MC-simulation for $f_n(\mathbf{k})$



Iotti and Rossi: PRL 2001

Quantum transport



Lee and Wacker: PRB 2002

Good agreement with experiment
(Sirtori *et al.*: PRB 1998)



The Quantum Transport Model



Why Quantum Transport?

Interplay between

- Tunneling transitions
 - Scattering processes
 - Optical transitions
- } $\Rightarrow$ Operation of QCL

- **Broadening** of tunneling resonances and optical transitions by scattering
- **Electronic distribution** modified by transitions $\rightarrow$ modified scattering rates

Combine **quantum evolution**, **scattering**, and **carrier distribution**

$\rightarrow$ Quantum Transport Theory



Nonequilibrium Green Functions

Start with (single particle) **basis** $\Psi_{\alpha}(z)e^{i(k_x x + k_y y)}$

$$\hat{H} = \hat{H}^o + \hat{H}_{\text{scatt}} \quad \text{with} \quad \hat{H}^o = \sum_{\alpha, \beta, k} H_{\alpha\beta}^o(k) a_{\alpha k}^{\dagger} a_{\beta k}$$

Aim: $f_{\alpha k}(t) = \langle a_{\alpha k}^{\dagger}(t) a_{\alpha k}(t) \rangle$, $J = \frac{e}{V} \langle \frac{d\hat{z}}{dt} \rangle = \frac{ie}{\hbar V} \langle [\hat{H}, \hat{z}] \rangle = \dots$



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Concept: Green functions

$$G_{\alpha, \beta}^<(k; t, t') = i \langle a_{\beta k}^\dagger(t') a_{\alpha k}(t) \rangle \stackrel{\text{steady state}}{=} \int \frac{dE}{2\pi} G_{\alpha, \beta}^<(k, E) e^{-iE(t-t')/\hbar}$$

Dyson equation $(E - \mathbf{H}^o(k) - \Sigma^{\text{ret}}(k, E)) \mathbf{G}^{\text{ret}}(k, E) = \mathbf{1}$

Keldysh relation $\mathbf{G}^<(k, E) = \mathbf{G}^{\text{ret}}(k, E) \Sigma^<(k, E) \mathbf{G}^{\text{adv}}(k, E)$



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Self-energies (in self-consistent Born approx.)

$$\Sigma^{\text{ret,imp}}(k, E) = \sum_{k'} \langle \mathbf{V}(k, k') \mathbf{G}^{\text{ret}}(k', E) \mathbf{V}(k', k) \rangle_{\text{imp}}$$

$$\begin{aligned} \Sigma^{<,\text{phon}}(k, E) = & \sum_{\vec{p}} \mathbf{M}(\vec{p}) n_B \mathbf{G}^<(k + p, E - \hbar\omega_p) \mathbf{M}_l(\vec{p}) \\ & + \mathbf{M}(\vec{p}) [n_B + 1] \mathbf{G}^<(E + \hbar\omega_p) \mathbf{M}_l(\vec{p}) \end{aligned}$$

Temperature enters only via phonon occupations $n_B(\hbar\omega_p)$

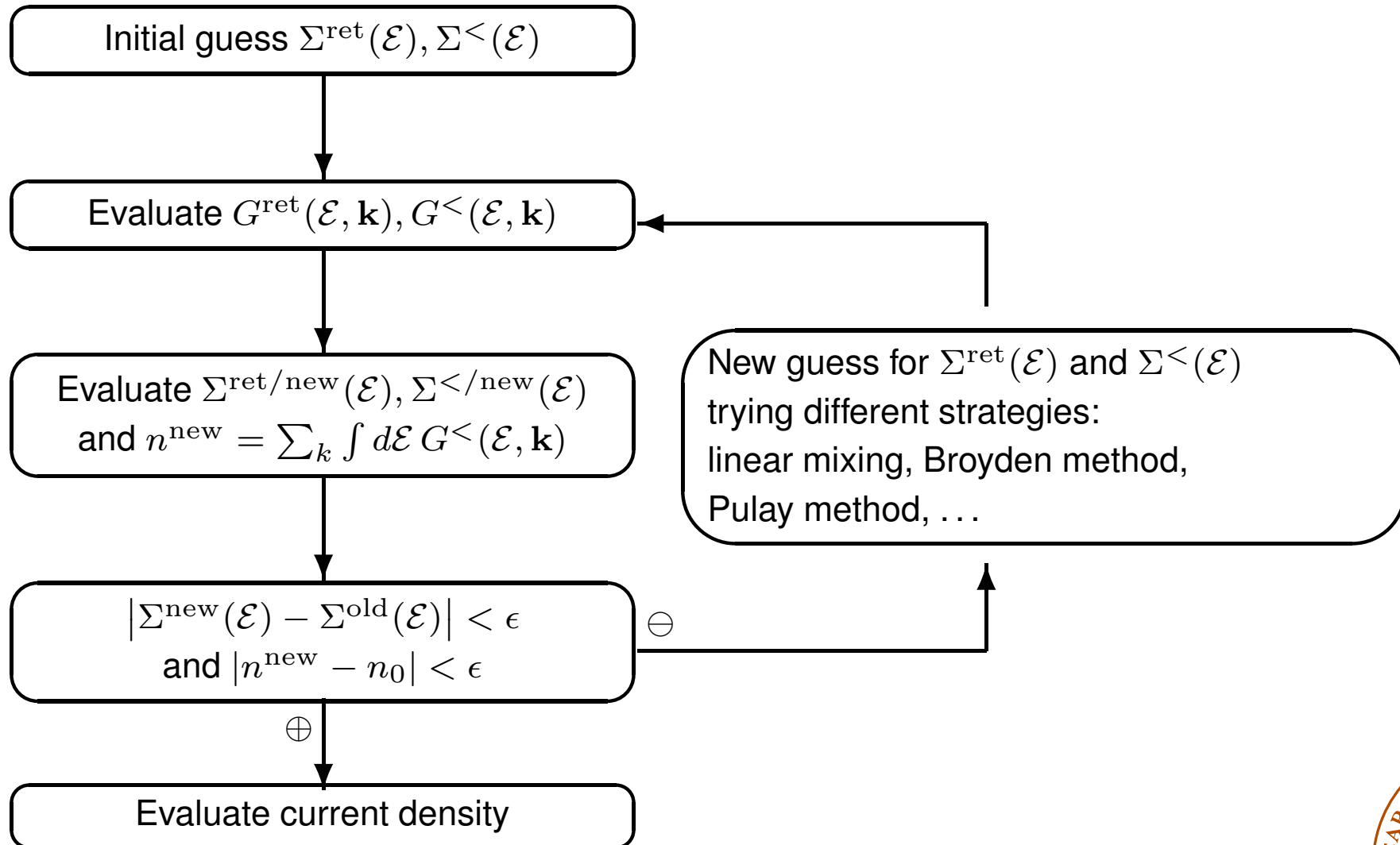


Calculation Details

- Scattering by optical phonons, interface roughness, charged impurities, artificial 'acoustic phonon'
- Electron-Electron interaction in mean field
- **Momentum-independent scattering matrix elements**
(Calculated for typical momentum transfer)
 $\Rightarrow$ Self-energies $\Sigma_{\alpha,\beta}(E)$ do not depend on k



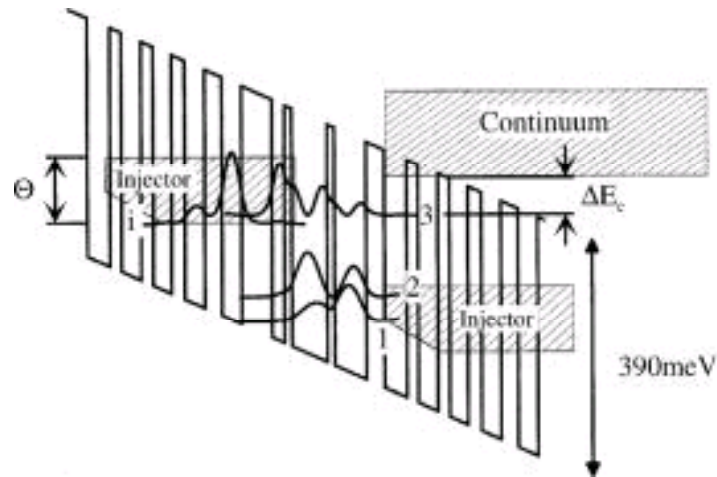
Numerical Implementation



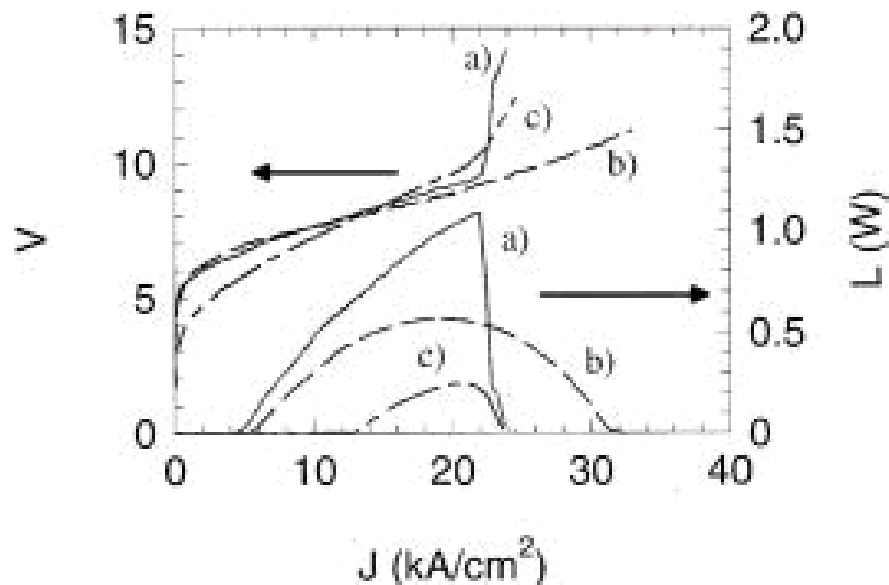
Transport and Electron Distribution



Current-voltage characteristic



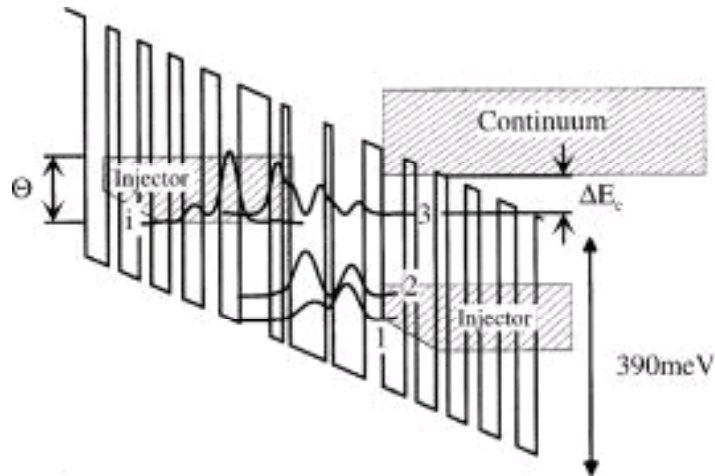
Page et al. APL01



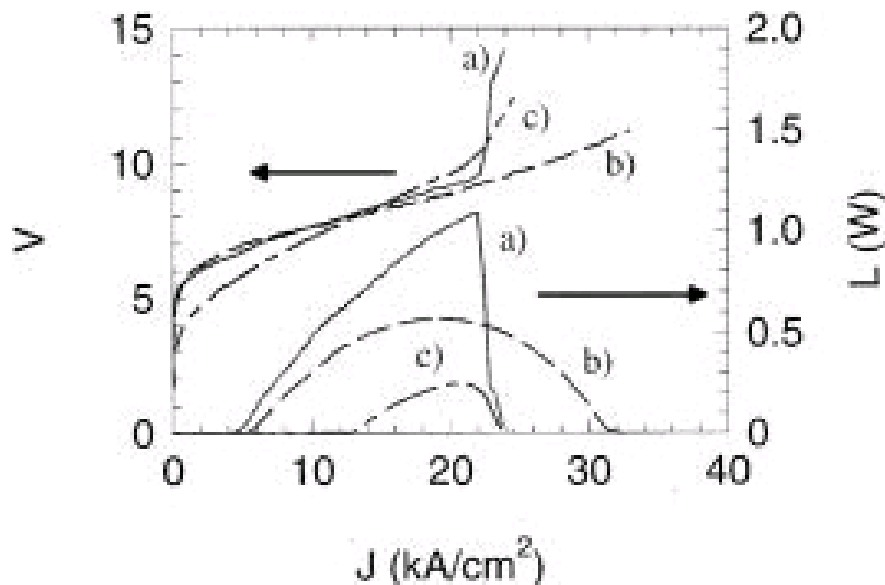
a)=77 K, c)=233 K



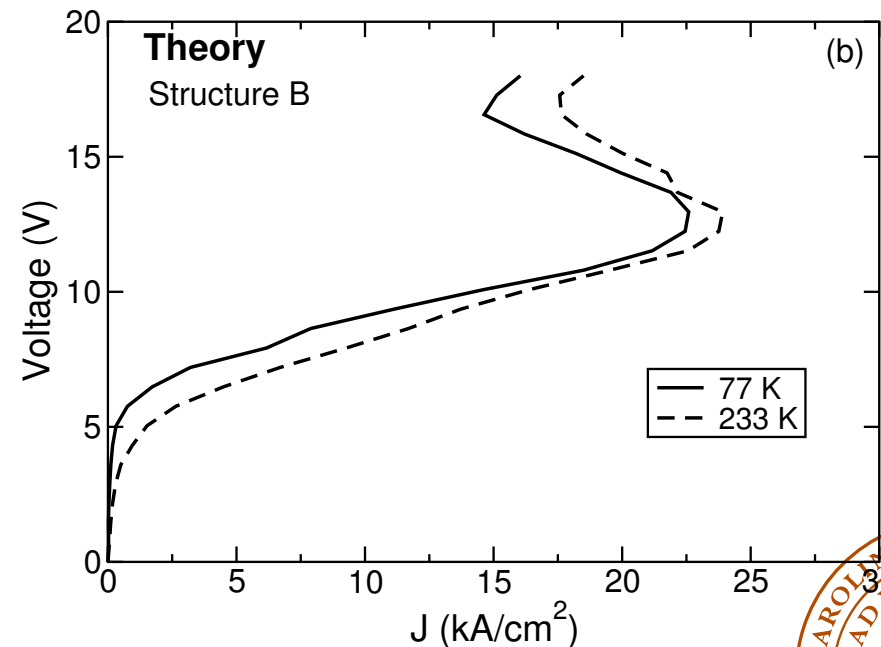
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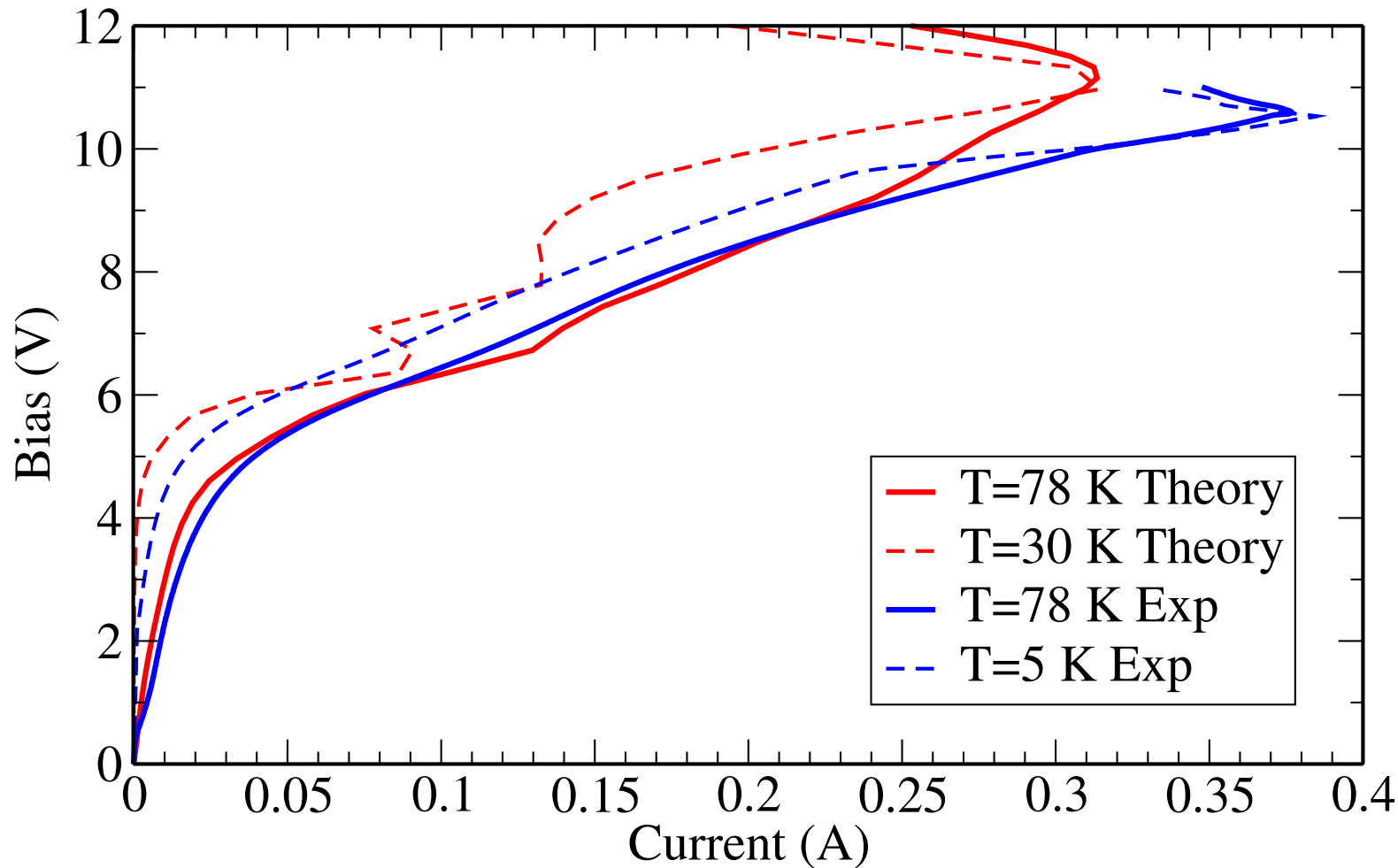


Quantitative agreement



THz-QCL operating at 77 K

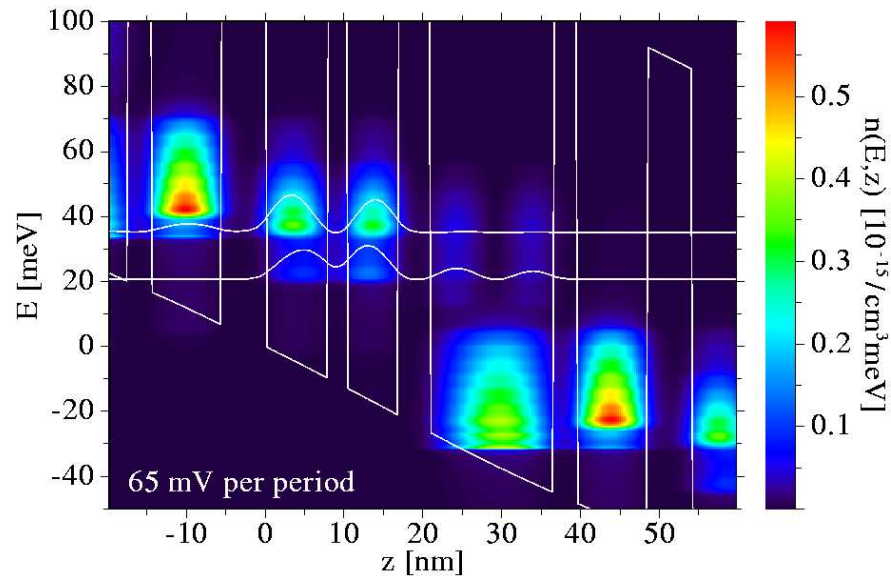
Data for sample of Kumar et al. APL 84, 2494 (2004)



See APL 86, 041108 (2005)



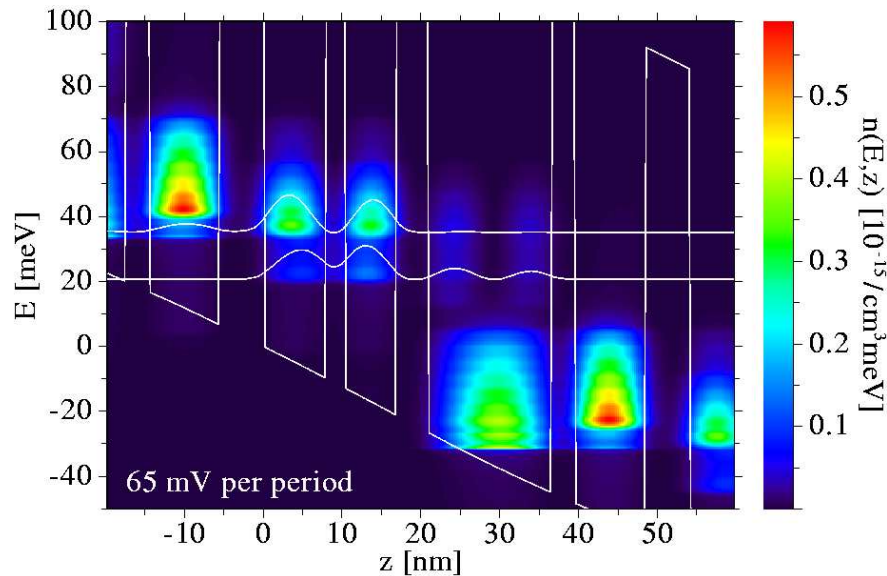
Spatial and energetical resolution



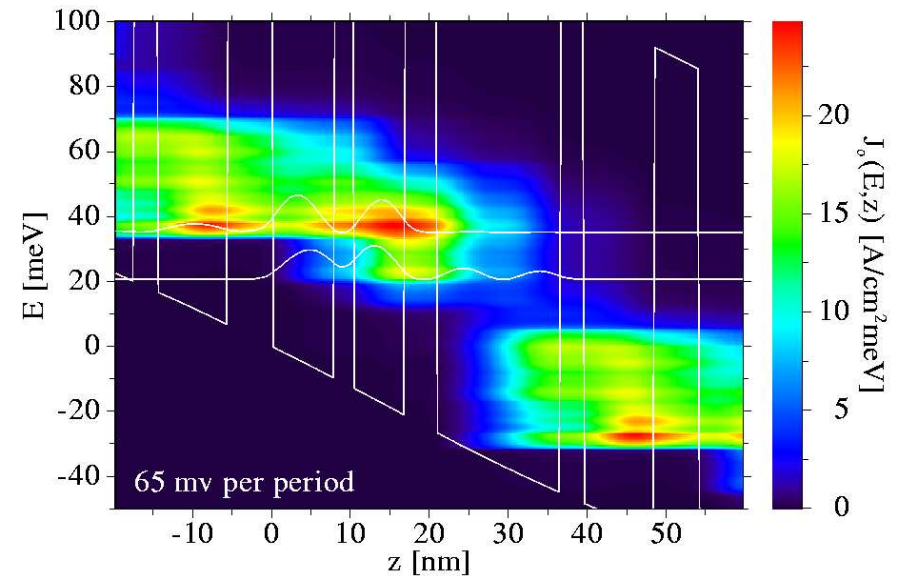
density localized in wells



Spatial and energetical resolution



density localized in wells
see [cond-mat/0507410](https://arxiv.org/abs/cond-mat/0507410)



Current through the structure



Calculation of Gain



Linear response

We know $\tilde{G}^{\text{ret}}(E)$, $\tilde{G}^{<}(E)$ in the nonequilibrium state



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Perturbation $\delta U(t) = -e\delta F(\omega)z_{\alpha,\beta}e^{-i\omega t}$



Linear response

We know $\tilde{\mathbf{G}}^{\text{ret}}(E)$, $\tilde{\mathbf{G}}^{<}(E)$ in the **nonequilibrium state**

Perturbation $\delta\mathbf{U}(t) = -e\delta F(\omega)z_{\alpha,\beta}e^{-i\omega t}$

Result within **linear response**

$$\delta\mathbf{G}^{\text{ret}}(\omega, E) = \tilde{\mathbf{G}}^{\text{ret}}(E + \hbar\omega) [\delta\mathbf{U}(\omega) + \delta\mathbf{\Sigma}^{\text{ret}}(\omega, E)] \tilde{\mathbf{G}}^{\text{ret}}(E)$$

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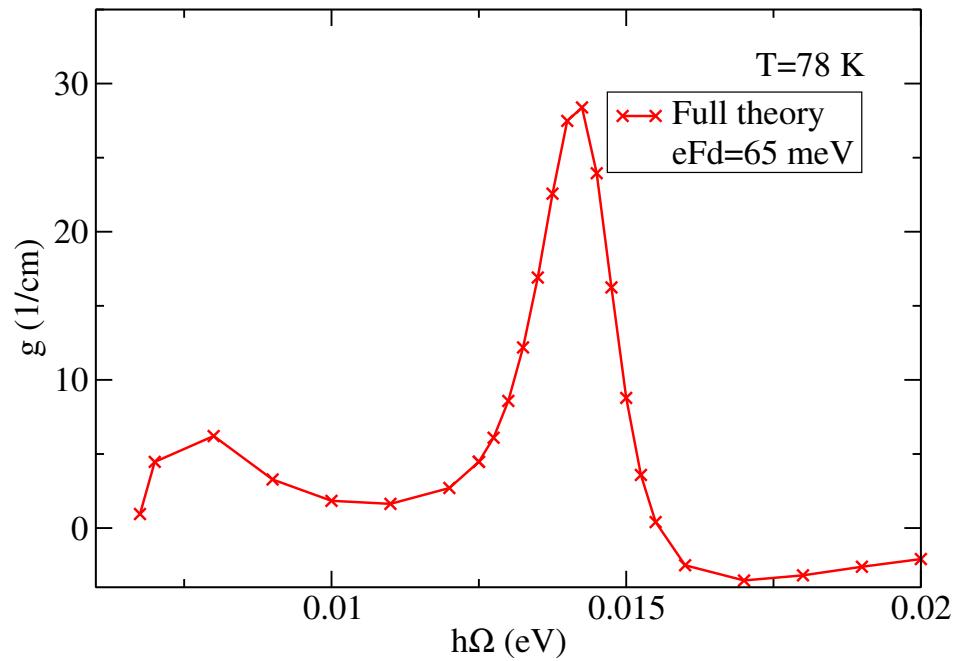
Change in current density $\delta J(\omega) \sim \int dE \delta G^<(E, \omega)$

Complex conductivity $\sigma(\omega) = \delta J(\omega)/\delta F$

→ **Material Gain** $G_m(\omega) \approx -\frac{\Re\{\sigma(\omega)\}}{c\epsilon_0\sqrt{\epsilon_r}}$



Result for Gain



Gain in the THz region
Exp: $3.2\text{ THz} \equiv 13.2\text{ meV}$



Width of Gain Peak

Compare with simple model

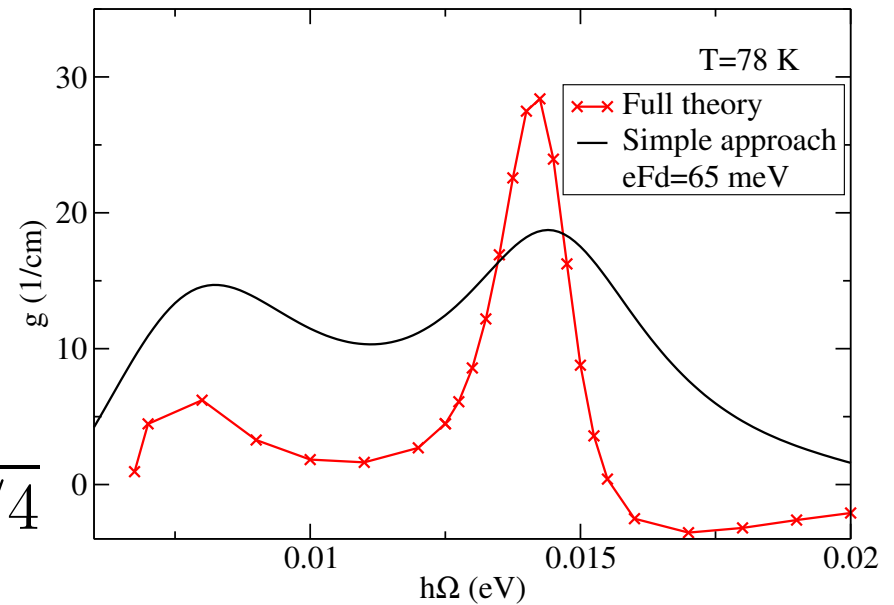
$$g(\omega) \propto \sum_{ij} |z_{ij}|^2 (n_i - n_j) \\ \times \frac{\Gamma_i + \Gamma_j}{(E_i - E_j - \hbar\omega)^2 + (\Gamma_i + \Gamma_j)^2/4}$$



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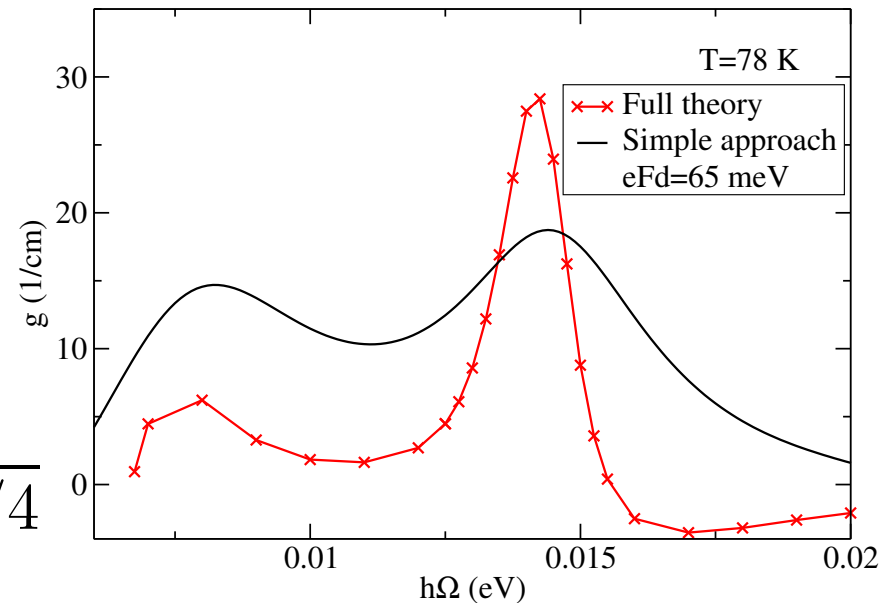
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Significantly reduced width

See [APL 86, 041108, \(2005\)](#)



Origin of main effect

$$\delta \mathbf{G}^<(\omega, E) = \tilde{\mathbf{G}}^{\text{ret}}(E + \hbar\omega) \delta \mathbf{U}(\omega) \tilde{\mathbf{G}}^<(E) + \tilde{\mathbf{G}}^<(E + \hbar\omega) \delta \mathbf{U}(\omega) \tilde{\mathbf{G}}^{\text{adv}}(E)$$

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Main correction $+ \tilde{\mathbf{G}}^{\text{ret}}(E + \hbar\omega) \delta \Sigma^<(\omega, E) \tilde{\mathbf{G}}^{\text{ret}}(E)$, in particular

$$\delta \Sigma_{12\mathbf{k}}^<(E) \approx \sum_{\mathbf{k}'} \underbrace{\langle V_{11}^{\text{imp}}(\mathbf{k} - \mathbf{k}') V_{22}^{\text{imp}}(\mathbf{k}' - \mathbf{k}) \rangle}_{=\hbar^2 \gamma_{1212} / (Am)} \delta G_{12\mathbf{k}'}^<(E)$$



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provides

$$g(\omega) \propto |z_{12}|^2 (n_2 - n_1) \frac{\Gamma_1 + \Gamma_2 - 2\gamma_{1212}}{(E_2 - E_1 - \hbar\omega)^2 + (\Gamma_1 + \Gamma_2 - 2\gamma_{1212})^2 / 4}$$

similar to Ando, J. Phys. Soc. Jpn. 54, 2671 (1985)



When is this of importance?

We have (for impurity scattering):

$$\gamma_{1212} \propto \langle V_{11}^{\text{imp}}(\mathbf{k} - \mathbf{k}') V_{22}^{\text{imp}}(\mathbf{k}' - \mathbf{k}) \rangle_{\text{imp}}$$

$$\Gamma_1 \approx \gamma_{1111} \propto \langle V_{11}^{\text{imp}}(\mathbf{k} - \mathbf{k}') V_{11}^{\text{imp}}(\mathbf{k}' - \mathbf{k}) \rangle_{\text{imp}}$$

γ_{1212} comparable to Γ_1, Γ_2 if
scattering environment is correlated
for states 1 and 2



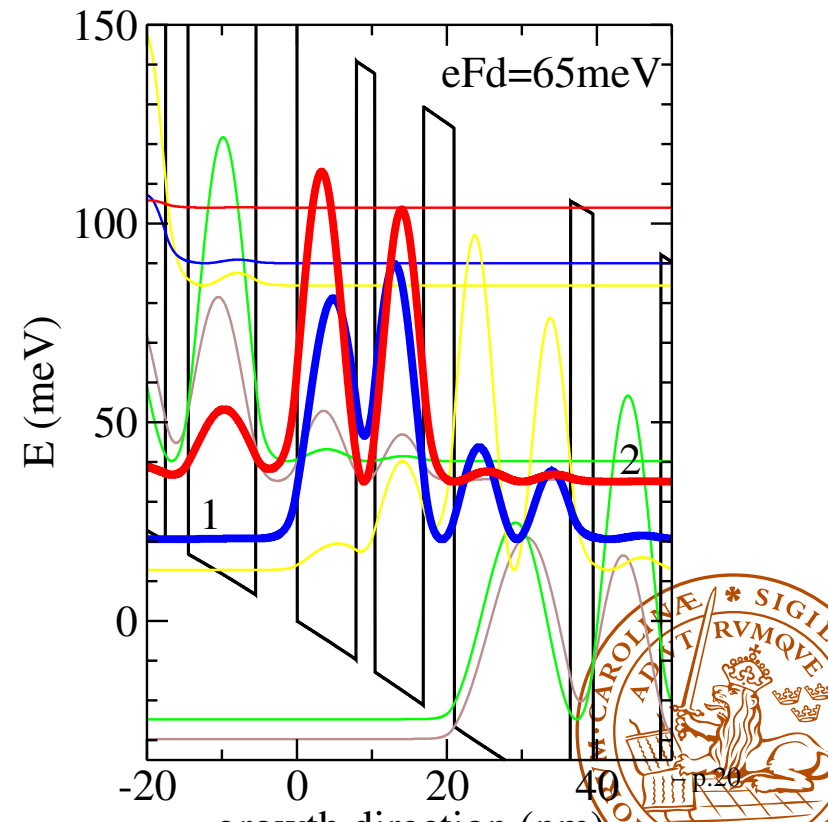
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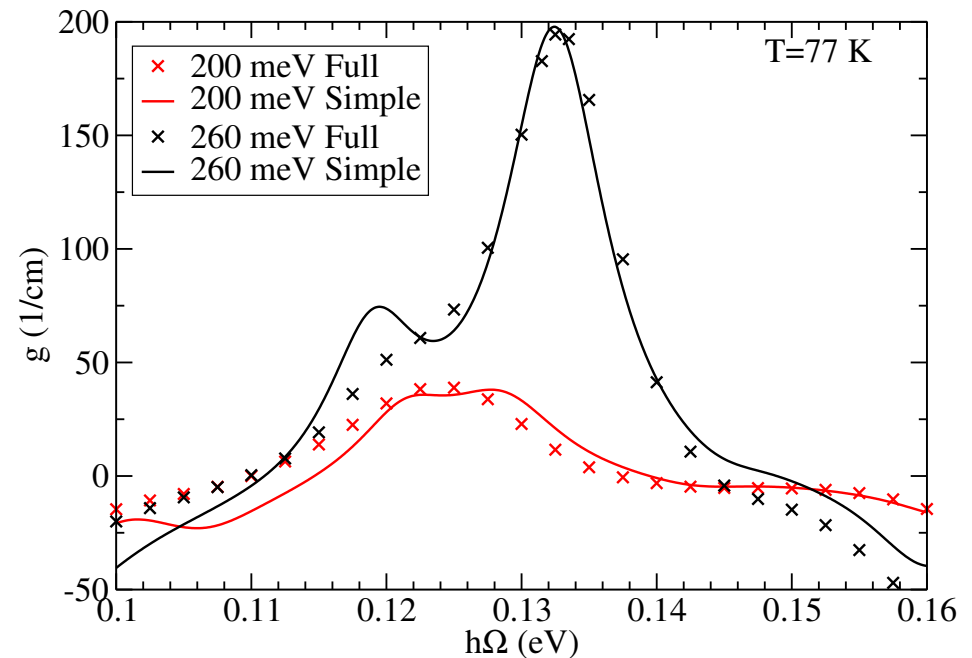
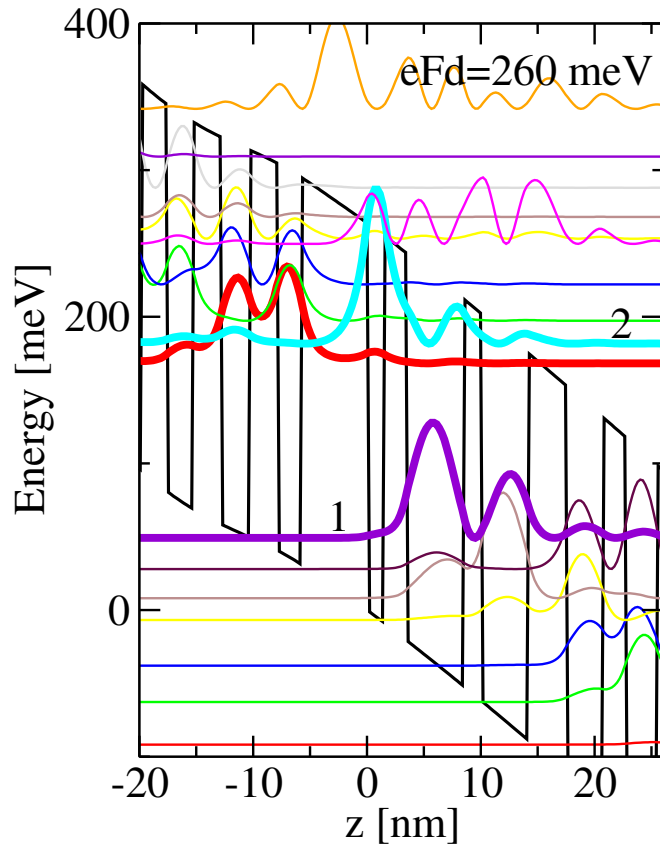
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Sample with less correlation

Standard QCL from Sirtori et al, APL 73, 3486 (1998)



Coulomb Shifts



Coulomb-corrections in Hartree Fock

Coulomb corrections in Hartree-Fock:

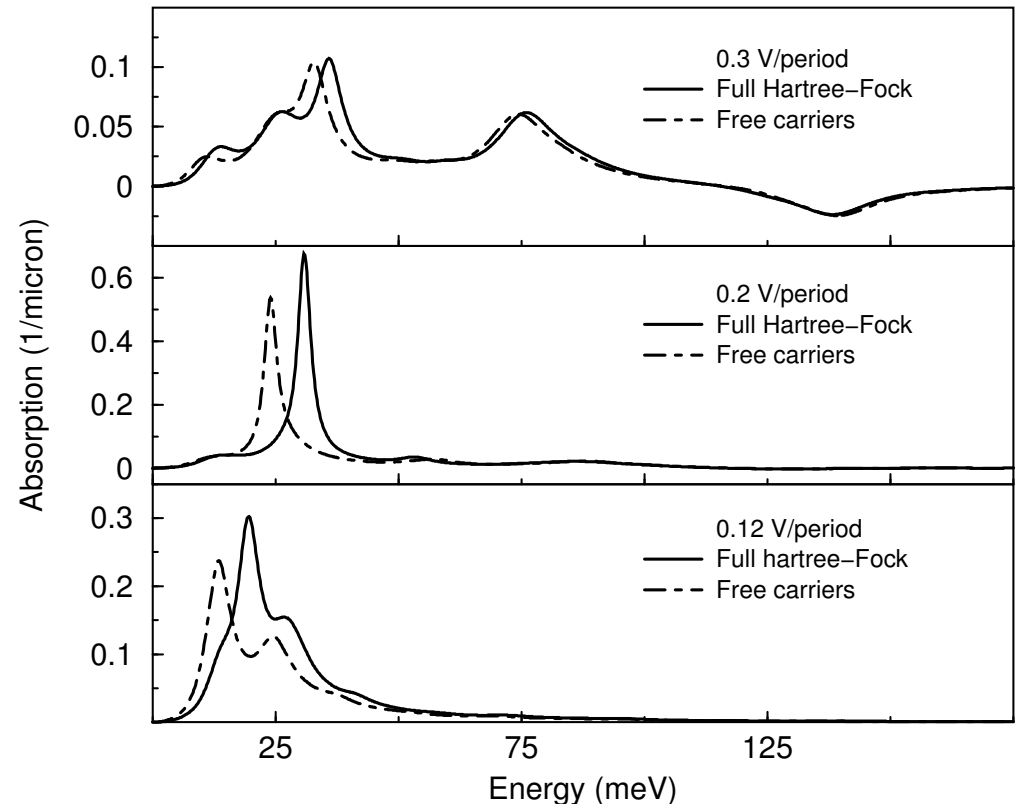
- Depolarization Shift (Hartree, dynamic)
- Subband shifts (Fock, static)
- Exchange correction (Fock, dynamic, like excitonic coupling)



Coulomb-corrections in Hartree-Fock

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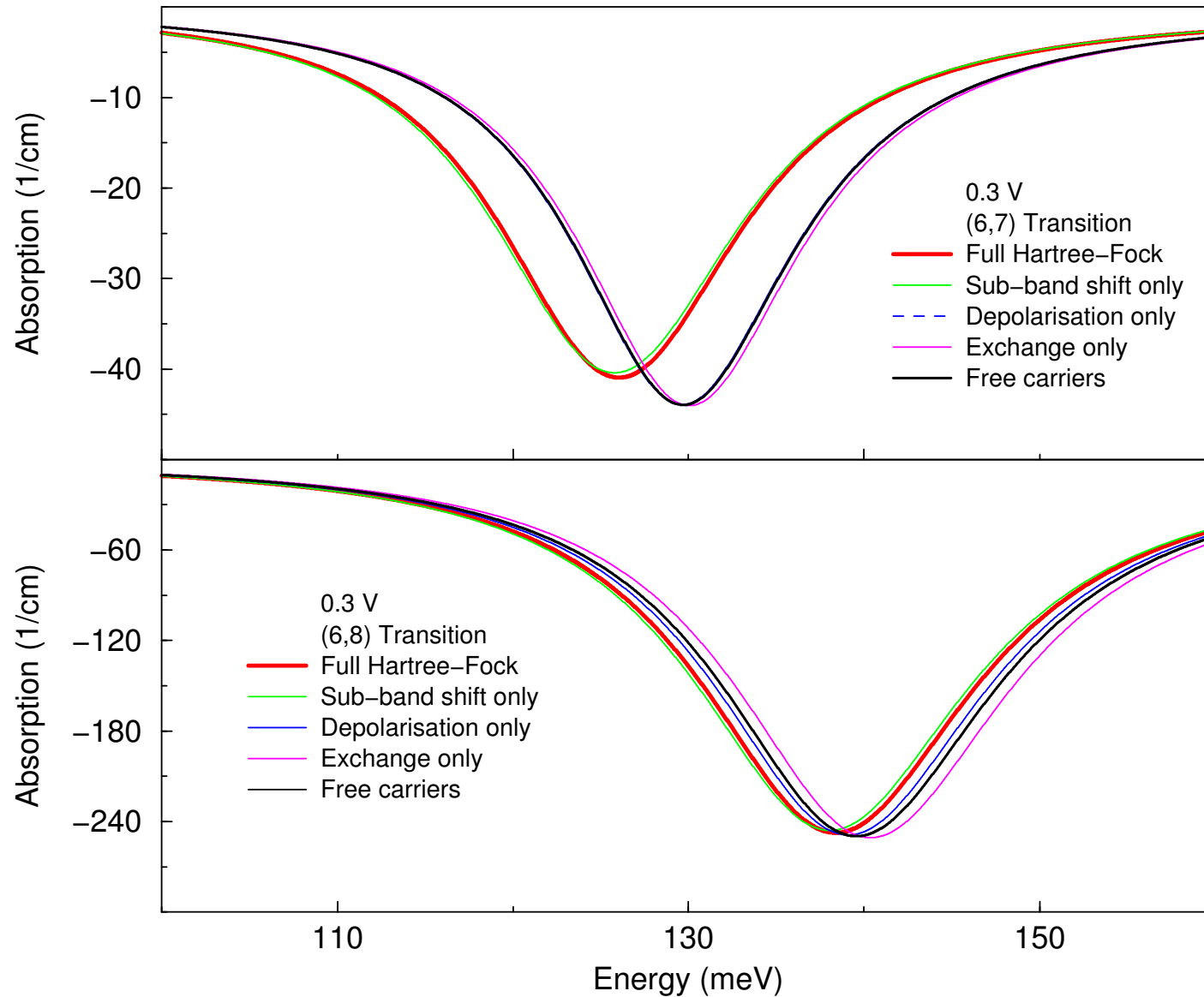
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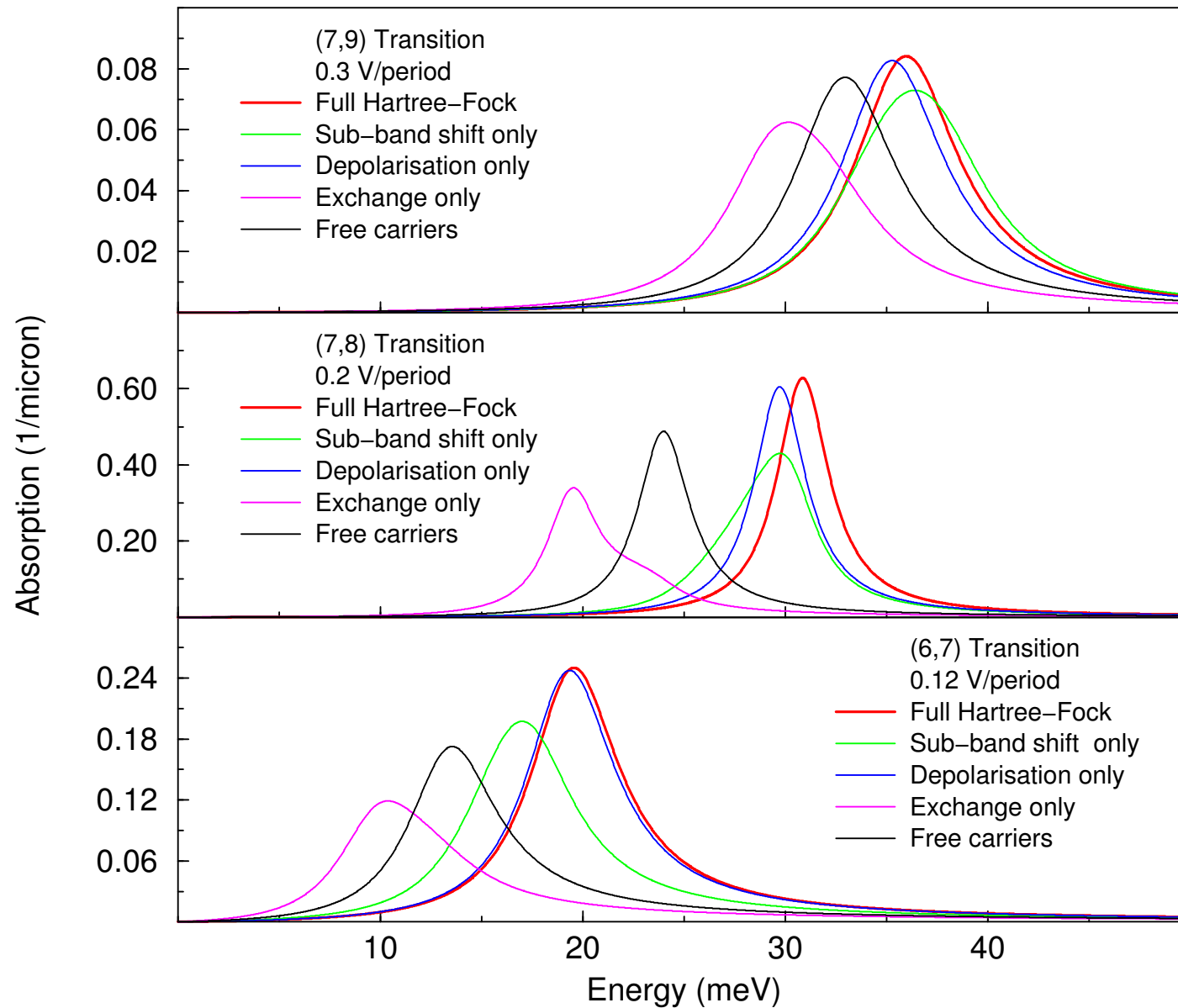
QCL from Sirtori et al, APL 73, 3486 (1998)



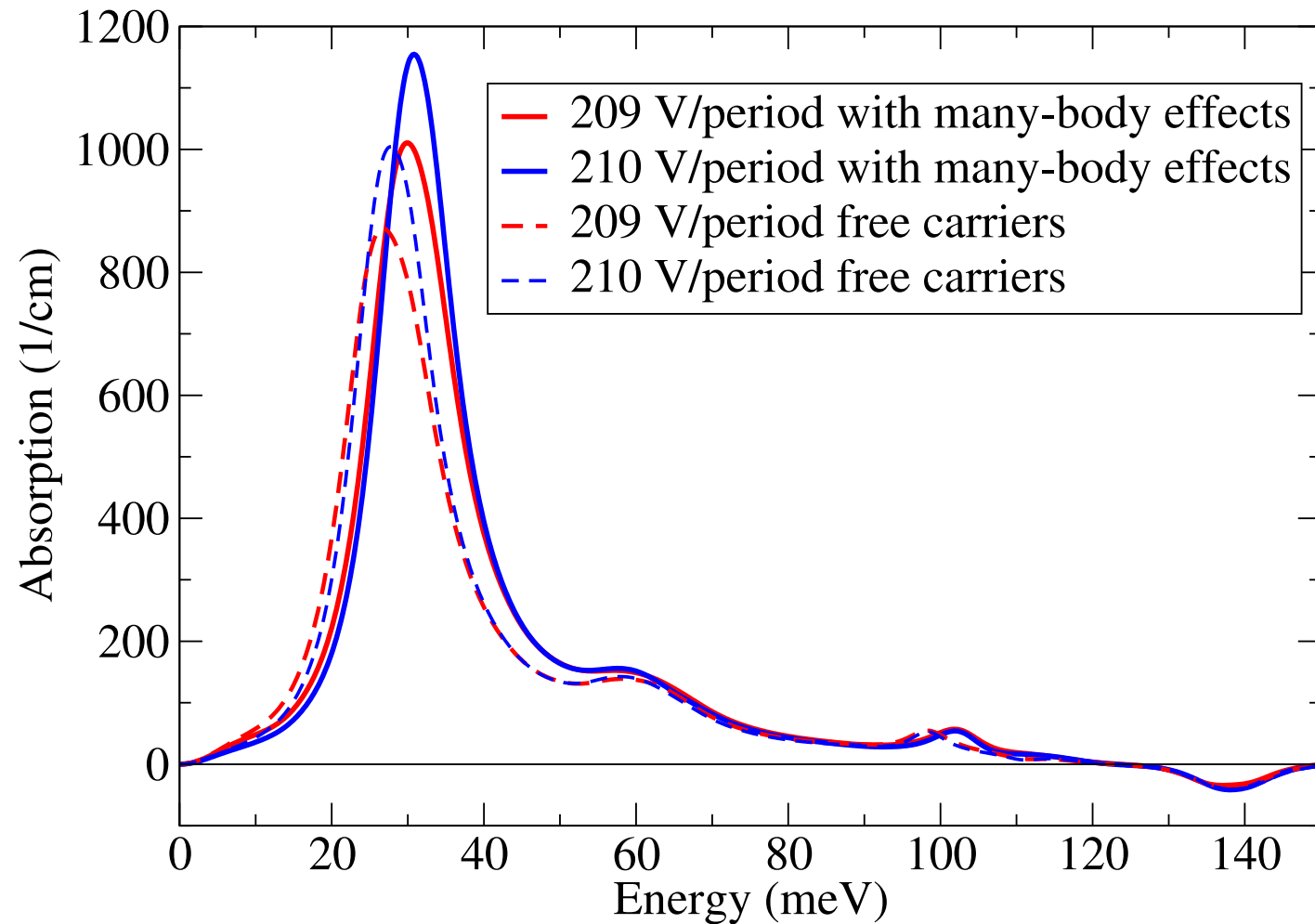
Resolved Gain Spectrum



Resolved Absorption Spectrum



Different sample



QCL from Gmachl et al., APL 72, 1430 (1998)



Conclusion

Development of a transport theory for Quantum cascade lasers using Nonequilibrium Green functions



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- Quantitative results for current-voltage characteristics and gain profile



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Blue shift in absorption

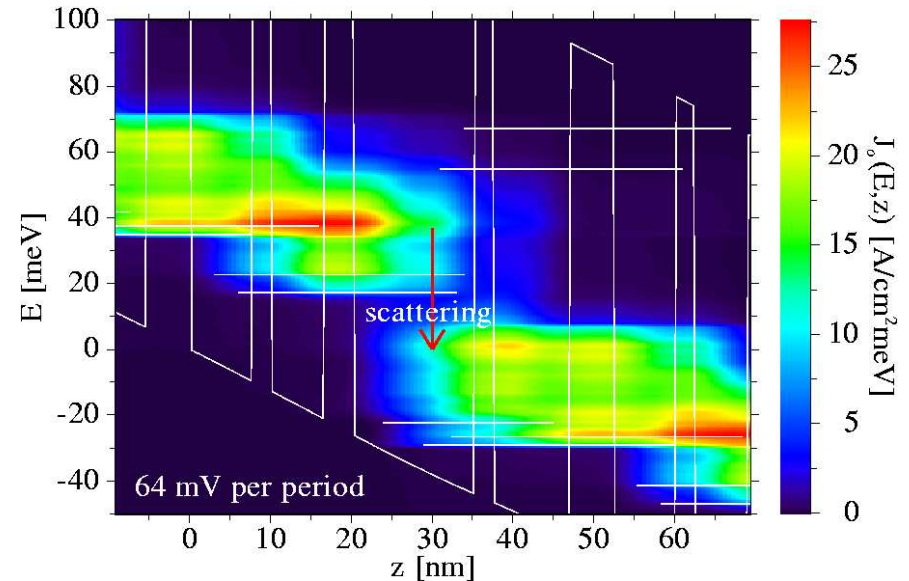


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- **Reduction of spectral width** due to correlations
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microscopic understanding of the device



PRB **66**, 245314 (2002); PRB **69**, 205310 (2004)
APL **86**, 41108 (2005); cond-mat/0507410

