Non-equilibrium quantum transport theory for quantum cascade lasers

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Motivation

- Realistic prediction of electronic transport in QCLs, treating quantum mechanical coherence and all relevant scattering mechanisms on an equal footing
- Fully self-consistent implementation of NEGF (Non-equilibrium Green function theory) to QCL

Open questions in transport through QCL

- Balance between coherence and dephasing
- Relevance of coherent tunneling

This work

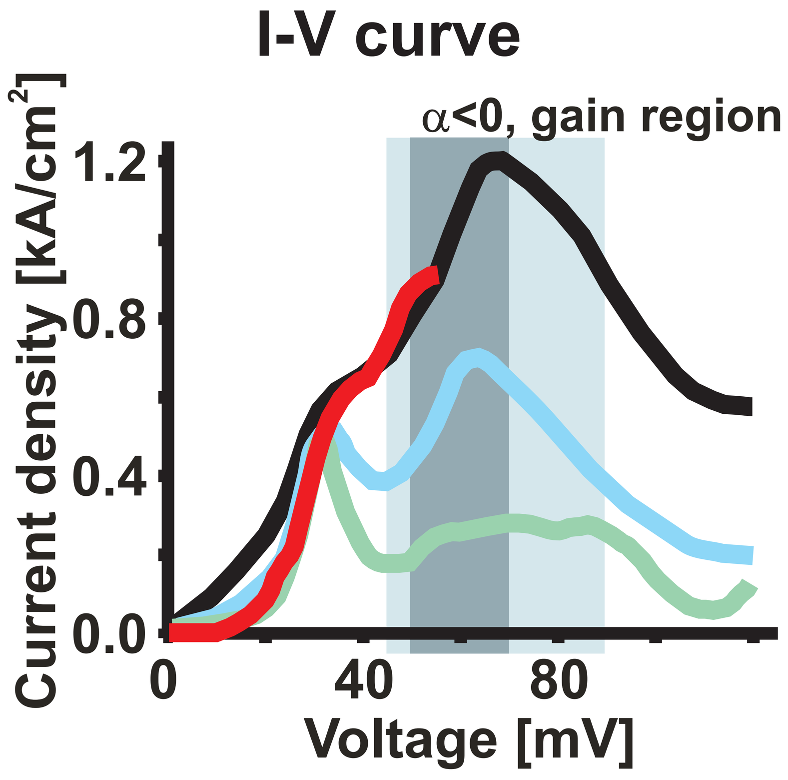
- Fully self-consistent implementation of NEGF:
  - Self consistent solution of $G^R \leftrightarrow \Sigma^R \leftrightarrow G^< \leftrightarrow \Sigma^<$
  - Self-consistent Born approximation
  - Momentum-dependent self-energies
  - Spatially off-diagonal self-energies
  - Acoustic phonon scattering
  - Optical phonon scattering
  - Impurity scattering
  - Interface roughness scattering
  - Electron-electron scattering (Hartree)
  - No fitting parameters

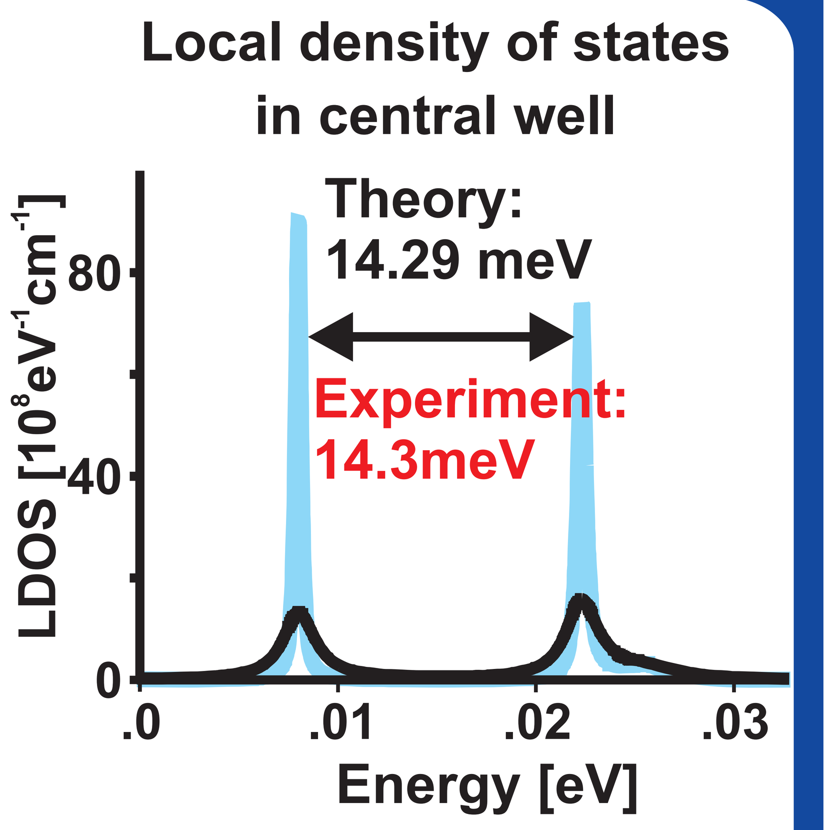
$$(E - H_0 - e\Phi - \Sigma^R)\,G^R = 1 \;\rightarrow\; G^< = G^R \Sigma^< (G^R)^\dagger$$

$$\Sigma^R = D^R G^R + D^< G^R + D^R G^< \;\leftarrow\; \Sigma^< = D^< G^<$$

Scattering states ↔ Occupation

- Study of active region of realistic QCL at 100K (Exp: Williams et al. APL 82, 1015 (2003))



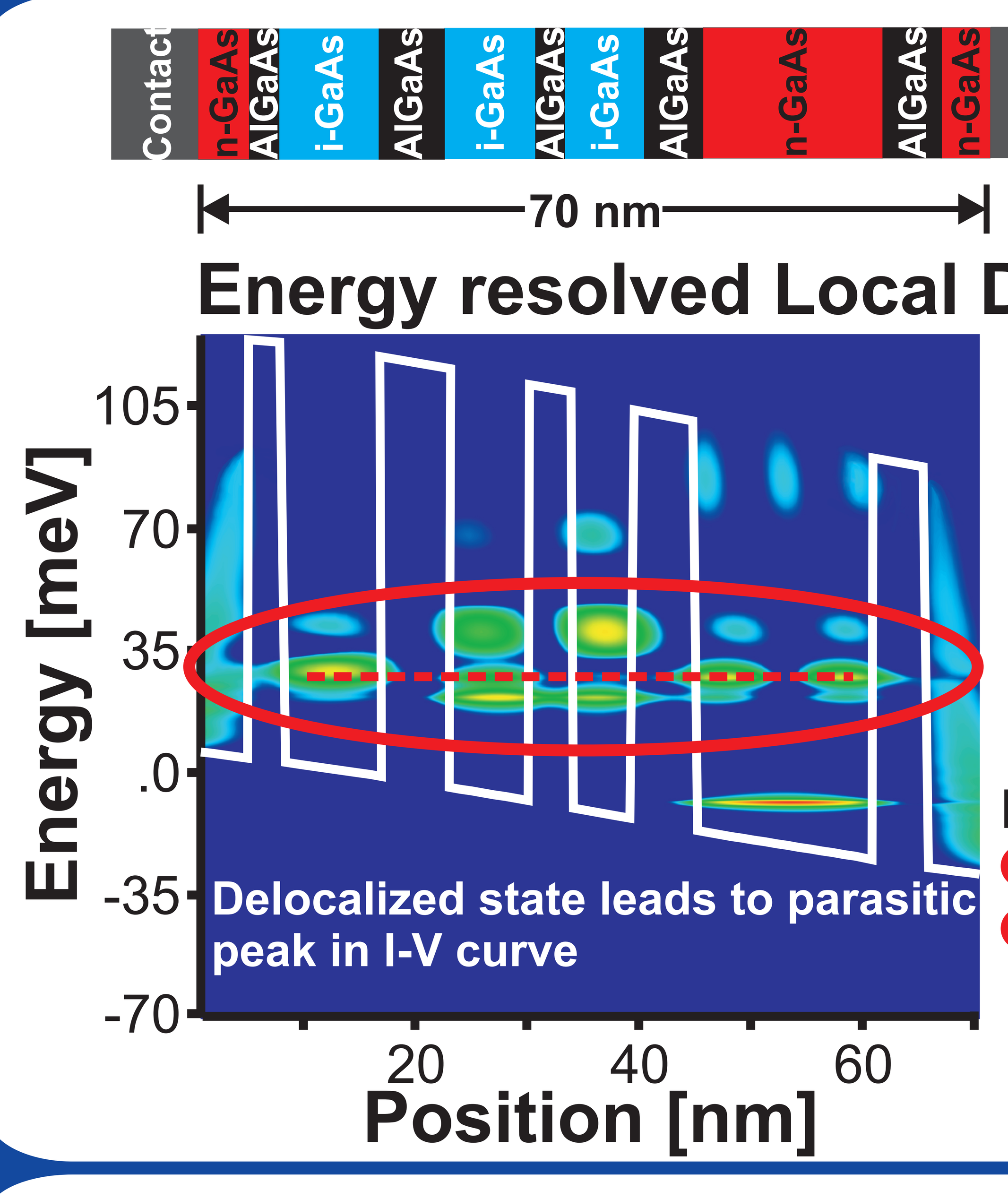


- NEGF including interface roughness
- NEGF ignoring interface roughness
- ballistic NEGF
- Experiment (Callebaut et al. APL 83, 207 (2003))

- Interface roughness
  - facilitates quantum mechanical tunneling due to momentum relaxation and delocalizes states ⇒ increases current
  - broadens energy states ⇒ reduces peak-to-valley ratio

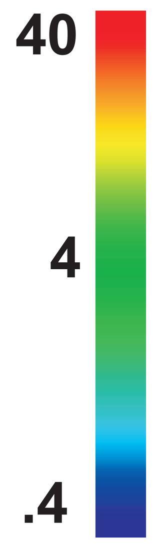
Results

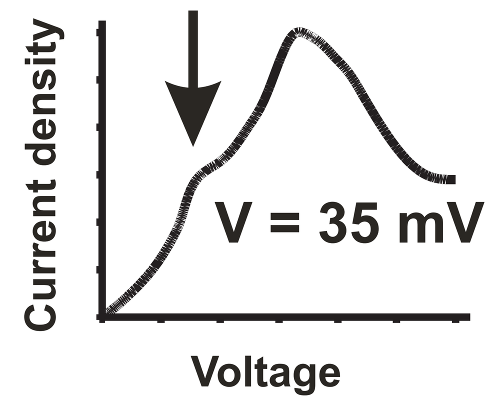
- Quantum mechanical effects play dominant role:
  - Tunneling across 3 and more quantum wells
  - Interface roughness increases current, but reduces gain
  - Occupation inversion arises mainly from coherent tunneling and not from incoherent scattering



Device dimensions [nm]: 6/2.4/10/5.4/8/2.4/7/3.8/15/3.8/6

A(z,E) $[10^8 eV^{-1}cm^{-1}]$

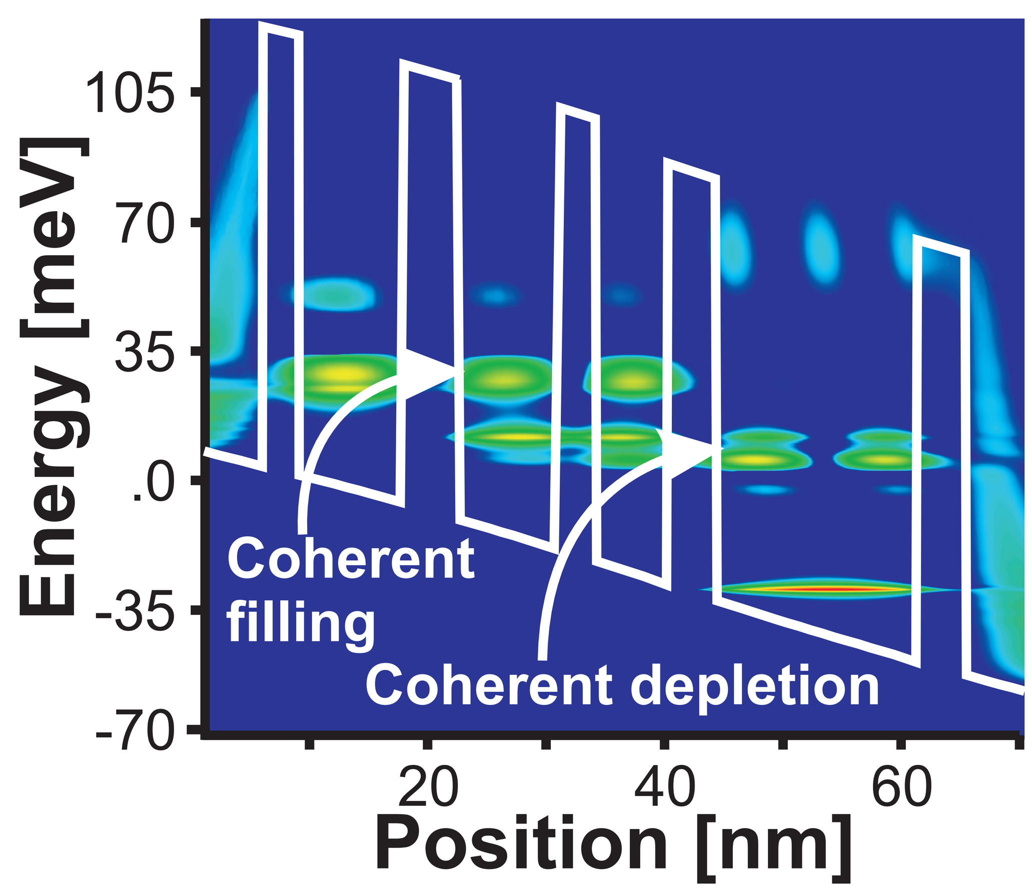


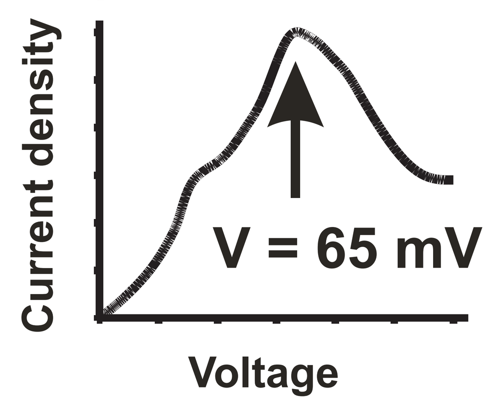


Relevant states remain delocalized
- in spite of dephasing
- lead to resonances in I-V curve

Resonant current is due to delocalized states

Energy resolved Local Density of States

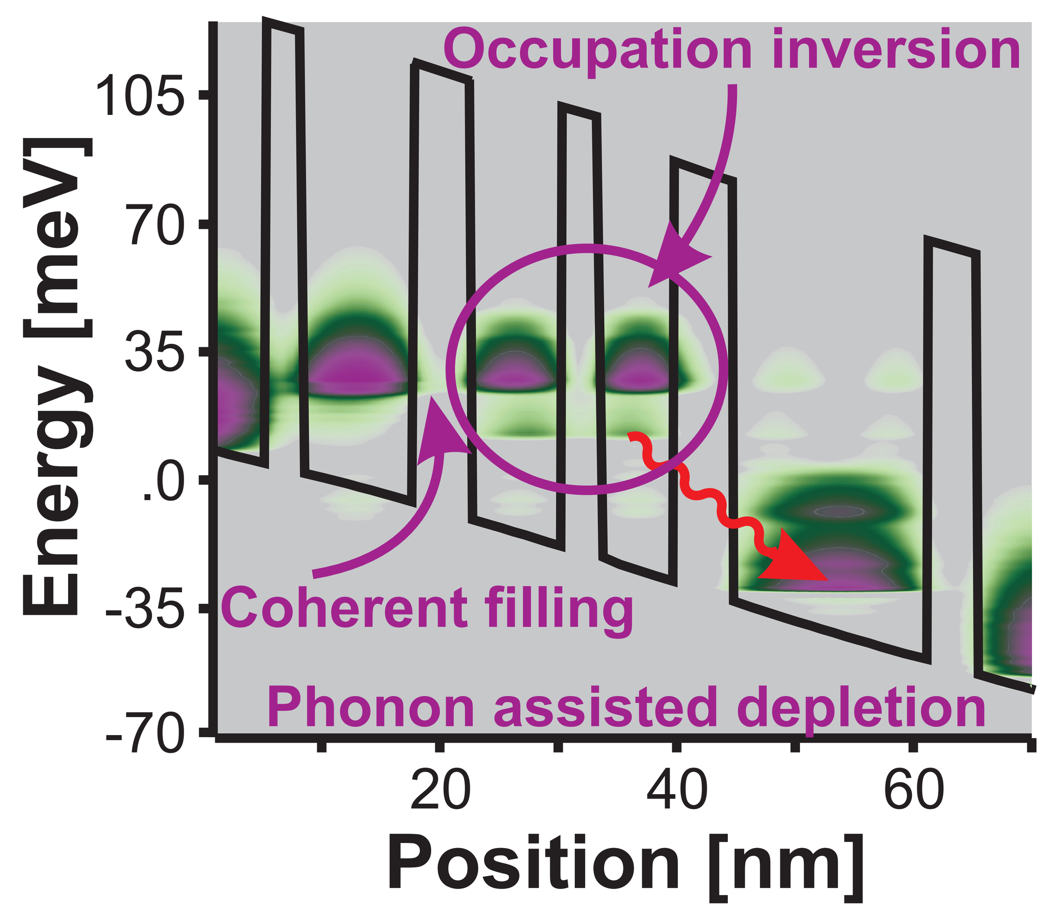




- Alignment leads to coherent
  - filling of upper laser state
  - depletion of lower laser state
- This is the basis mechanism leading to occupation inversion

States in resonance get coherently filled/emptied

Energy resolved density V = 65 mV



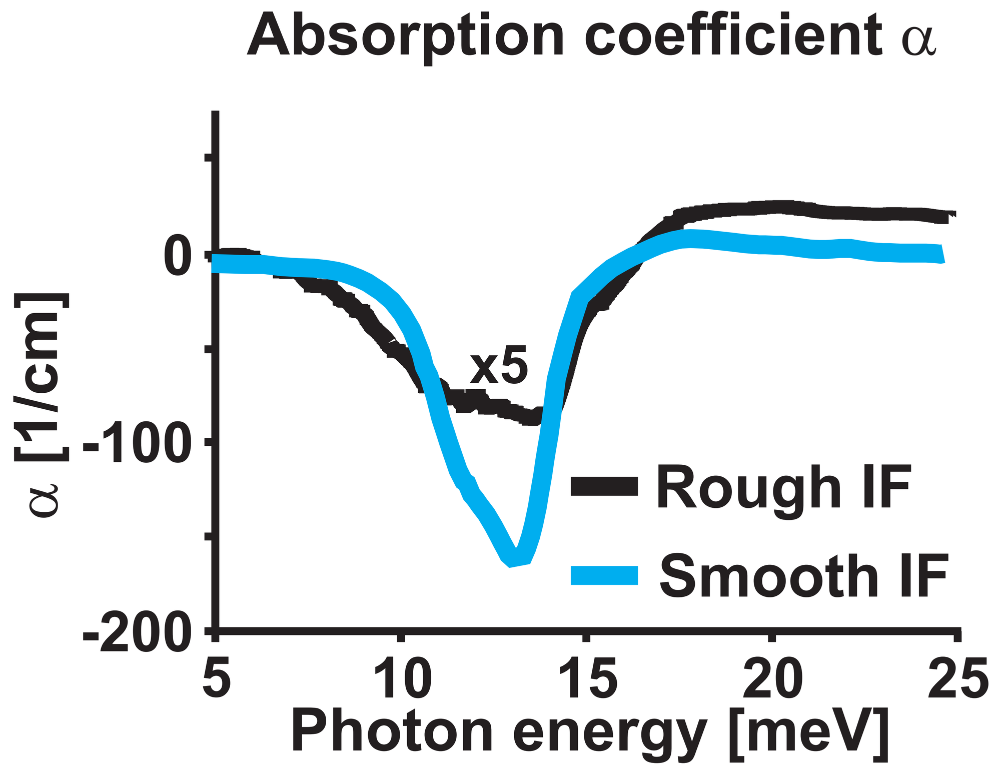
$$n(z,E) = \int dk\, k\, \mathrm{Im}[G^<(z,z,k,E)]$$

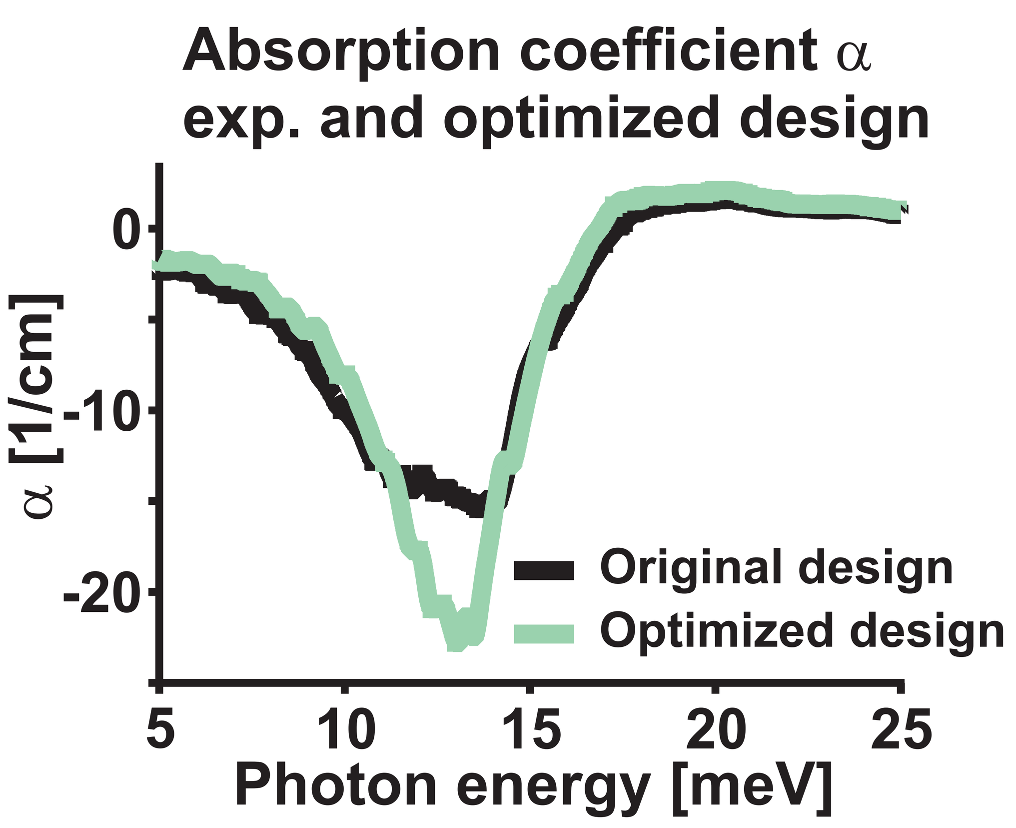
n(z,E) $[10^{18}\ cm^{-3}eV^{-1}]$

Phonon emission
- empties central well
- assists occupation inversion

Occupation inversion assisted by emission of polar optical phonons

Absorption coefficient α at V=65mV





- **Interface roughness reduces gain significantly**
- **Design optimization helps to increase gain**