Non-equilibrium Green's functions: Rough interfaces in THz quantum cascade lasers

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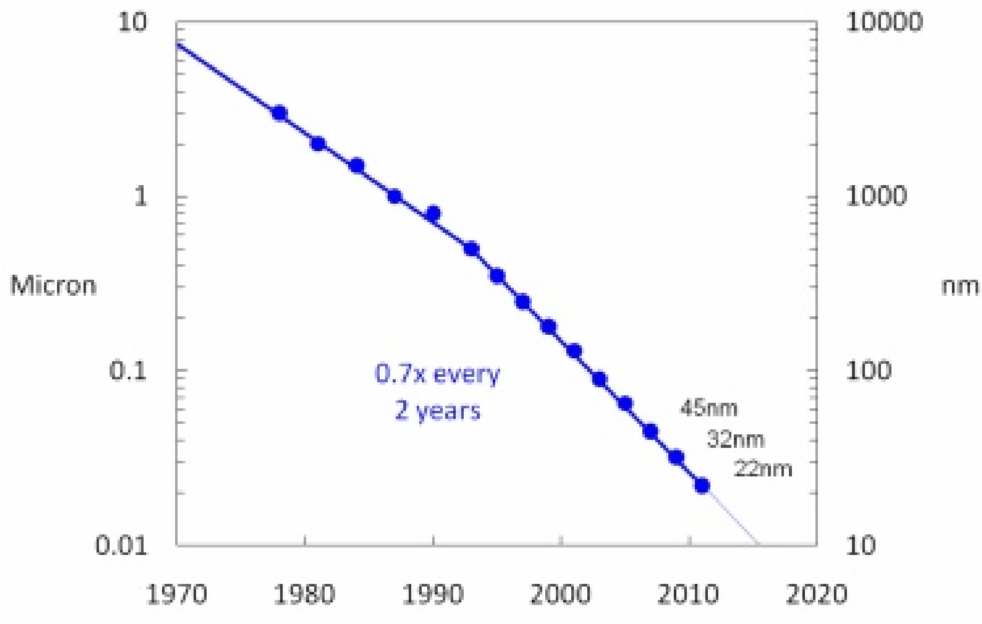
October, 2010

Why non-equilibrium Green's functions?

Transistor dimensions



www.intel.com/technology/mooreslaw/index.htm

State of the art semiconductor devices

- **utilize or suffer from quantum effects (tunneling, confinement, interference,…)**
- **are run in real world conditions (finite temperatures, varying device quality…)**

This requires a consistent description of

coherent quantum effects (tunneling, confinement, interferences,…)

and

incoherent scattering (phonons, impurities, rough interfaces,…)

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Why non-equilibrium Green's functions?

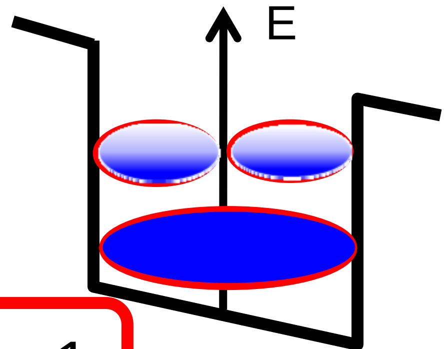
This talk:

Non-equilibrium Green's functions formalism (NEGF) is the method of choice

- **Covers quantum mechanics, particle statistics and incoherent effects on equal footing**
- **Offers reliable and consistent background information**

Example for application of NEGF: THz quantum cascade lasers

NEGF: Secret of success



Electronic states: retarded Green's function G^R

$$(E - H_0 - e\Phi - \Sigma^R)G^R = 1$$

Occupancy of states: "lesser than" Green's function $G^<$

$$G^< = G^R \Sigma^< G^{R\dagger}$$

Strength of NEGF:

- Calculates **consistently** resonant states and state occupancies
- Determines **reliable** energy resolved data (vital for device analysis)

Observables:

$$n(z) = \lim_{z \to z'} \int d^2k_{\|} \, dE \, \mathrm{Im}\left[G^<(z,z',k_{\|},E)\right]$$

$$j(z) = \lim_{z \to z'} \int d^2k_{\|} \, dE \, (\nabla_z - \nabla_{z'}) \mathrm{Re}\left[G^<(z,z',k_{\|},E)\right]$$

Observables: available in many methods, however…

NEGF: pitfalls (a few)

Approximations?

Full self-consistent Born approximation → current conservation

Full momentum and energy dependence →realistic relaxation

Full nonlocality of scattering → realistic scattering rates

(In-)elastic scattering mechanisms → realistic charge and current distributions

Fully coupled set of equations → many particle effects + Pauli blocking

Numerical implementation?

Usually requires

- **iterative solution schemes with possible convergence issues**
- **large memory storage and CPU load**
- **self refining discretizations in momentum and energy...**

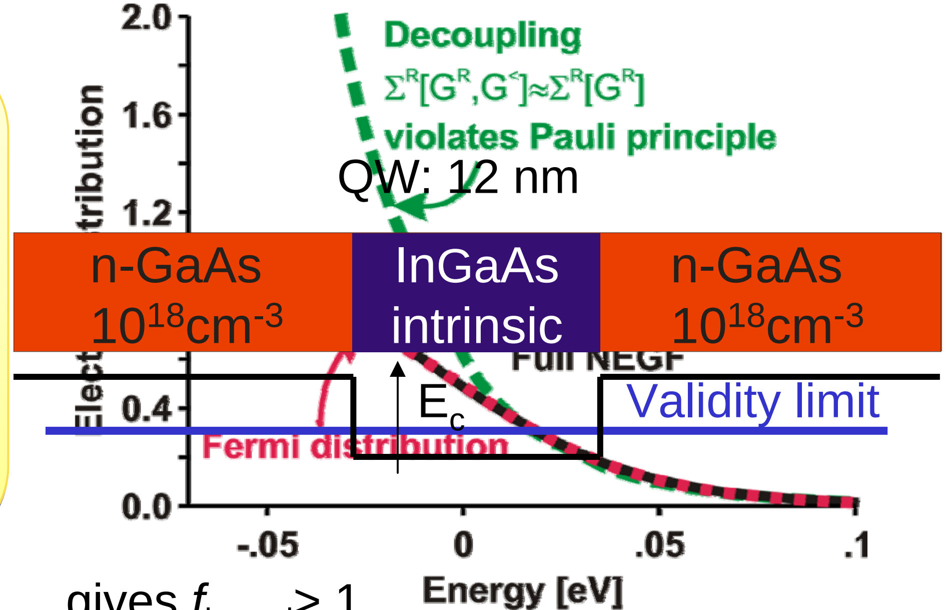
NEGF: pitfalls (1 example)

Approximations?

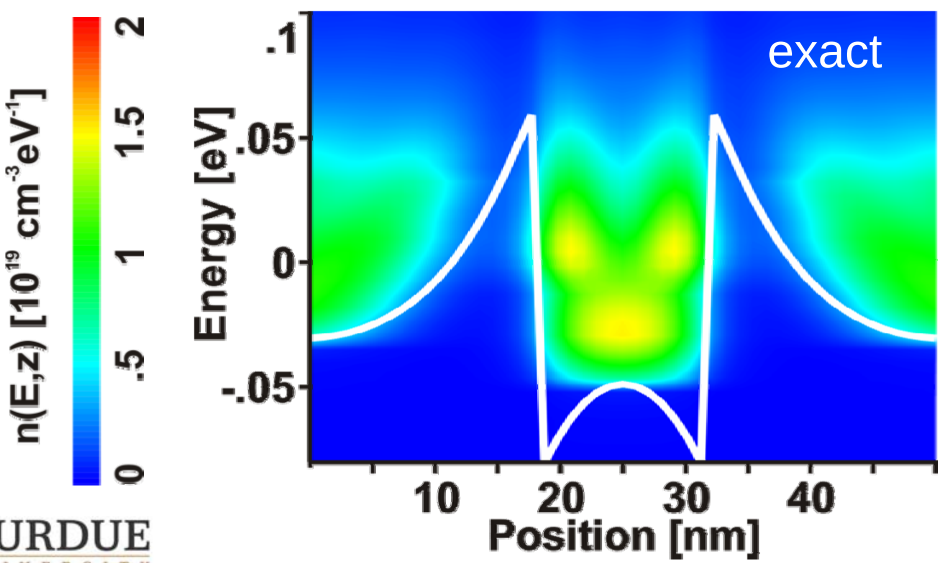
NEGF requires for the solution of four coupled differential equations

$$\boxed{\begin{aligned} G^R &= (E - H_0 - \Sigma^R)^{-1} \\ \Sigma^R &= G^R D^R + G^R D^< + \cancel{G^< D^R} \end{aligned}}$$

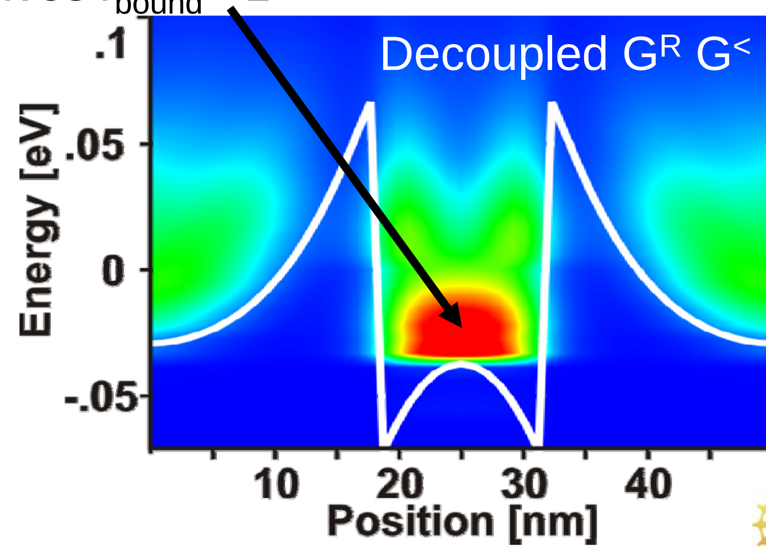
$$\boxed{\begin{aligned} G^< &= G^R \Sigma^< G^A \\ \Sigma^< &= G^< D^< \end{aligned}}$$



GaAs/$In_{.07}Ga_{.93}$As quantum well

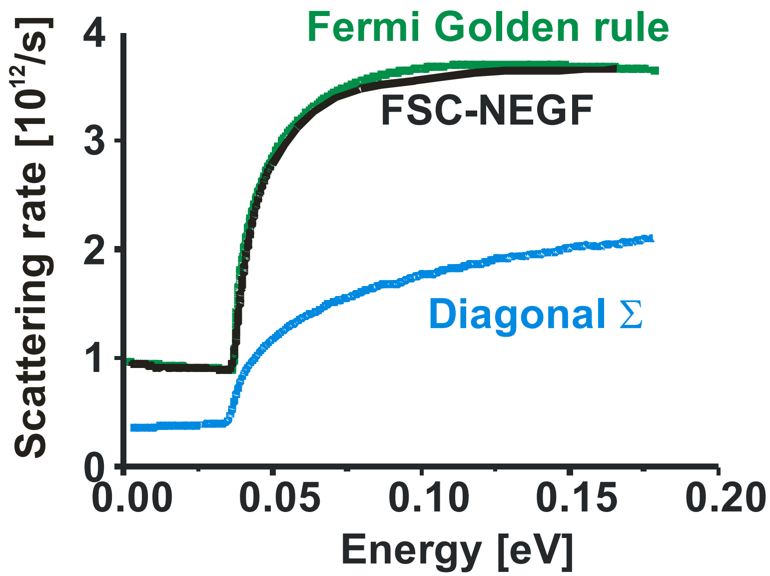


gives $f_{bound} > 1$



NEGF: Agreement with limiting cases

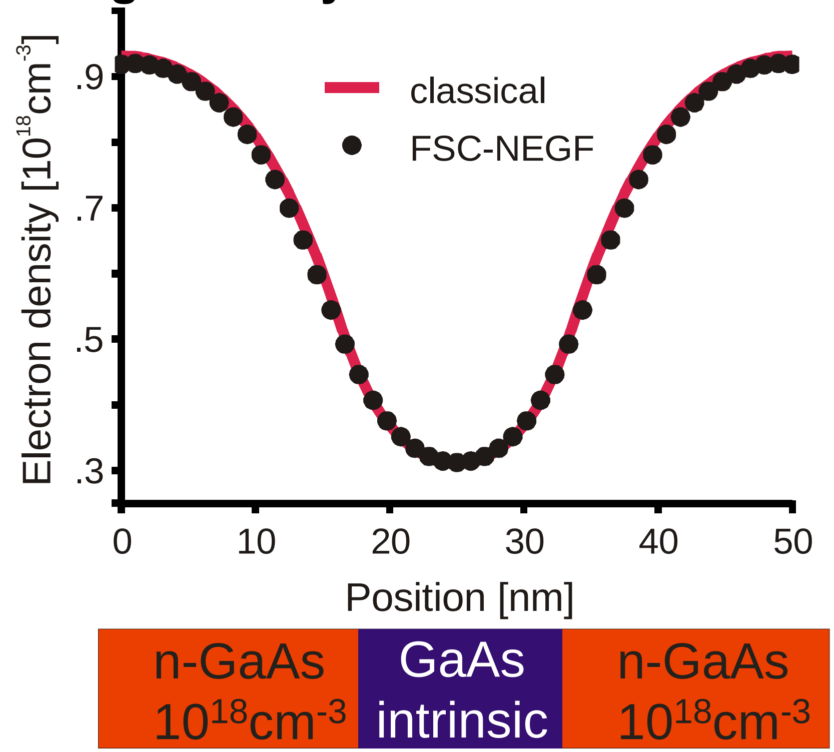
Fermi's Golden rule?
Scattering on polar optical phonons



Bulk GaAs @ 300 K
n = 10^{16} cm^{-3}, μ = -0.08 eV

NEGF agrees with Fermi's golden rule if full nonlocal scattering is included

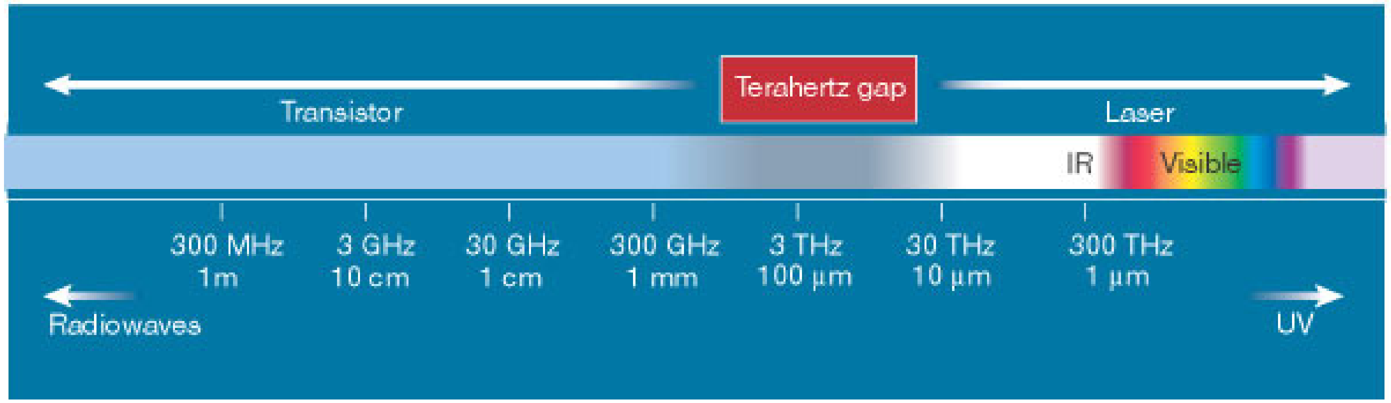
Boltzmann equation?
Charge density in GaAs n-i-n resistor



NEGF reproduces semiclassical Boltzmann equation

NEGF works fine if carefully implemented

Why THz quantum cascade lasers?

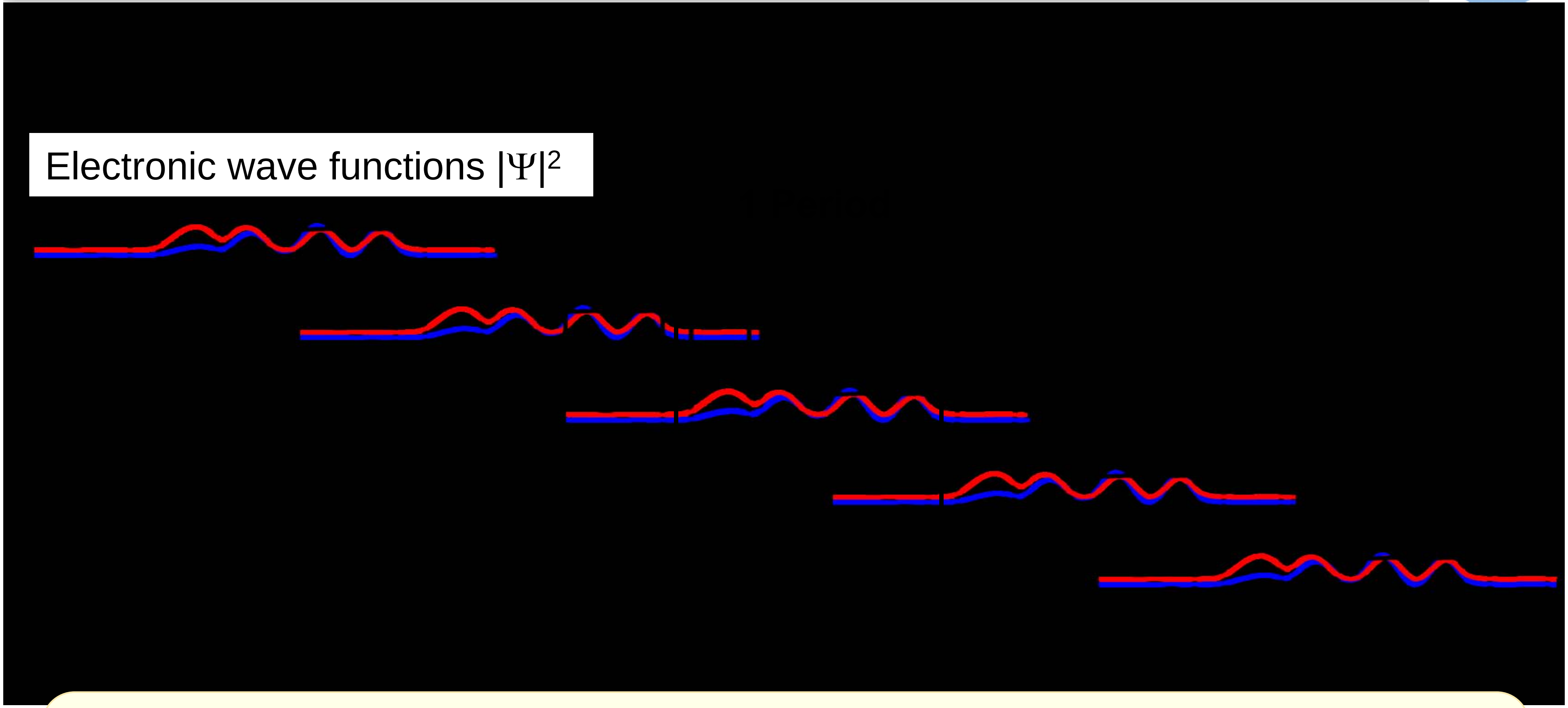


Carlo Sirtori
Nature **417**, 132(2002)

- **THz applications: Gas phase spectroscopy, telecommunication, security applications, etc.**
- **Quantum cascade lasers (QCLs) are promising candidates for high power and coherent sources of THz radiation**
- **THz-QCLs are still limited to cryogenic temperatures!**
- **Physics: Coherent transport and incoherent scattering equally important**

This talk:
Use NEGF to identify physics that limit QCL device performance

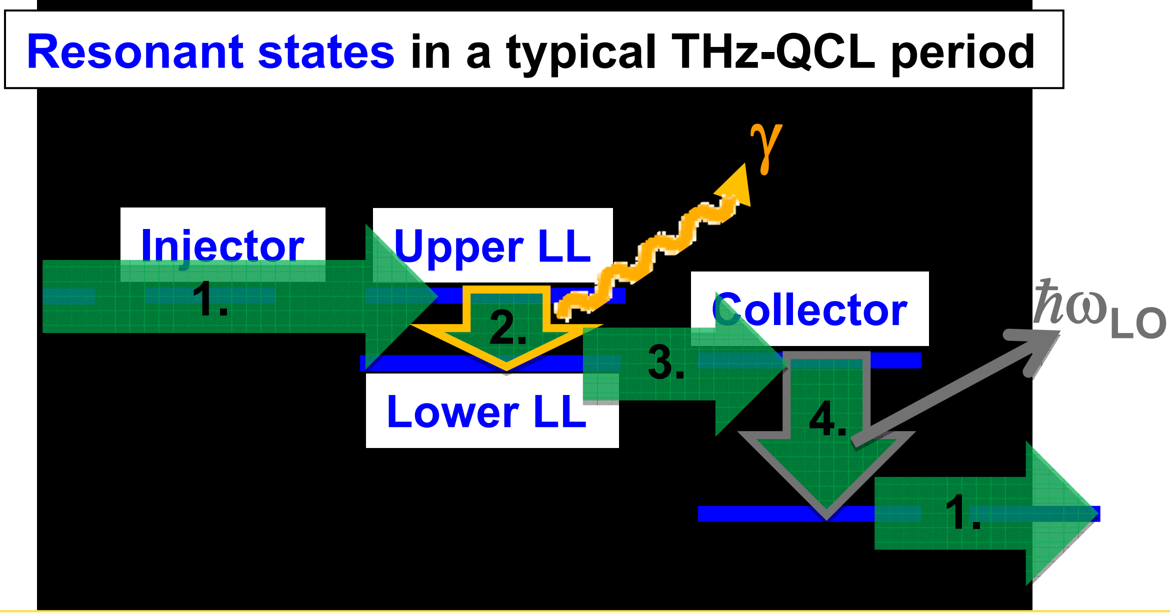
What is a quantum cascade laser?



Quantum cascade lasers…
… consist of periodically repeated quantum wells and barriers
… utilize electron transport in a single conduction band
… emit light due to electronic intersubband transitions

Typical resonant phonon THz QCL

$Al_{.15}Ga_{.85}As/GaAs$ quantum well heterostructure



Working principle:

1. Upper laser level coherently filled
2. Direct optical transition
3. Lower laser level coherently emptied
4. Electrons thermalized via 1 resonant LO-phonon emission

This NEGF implementation

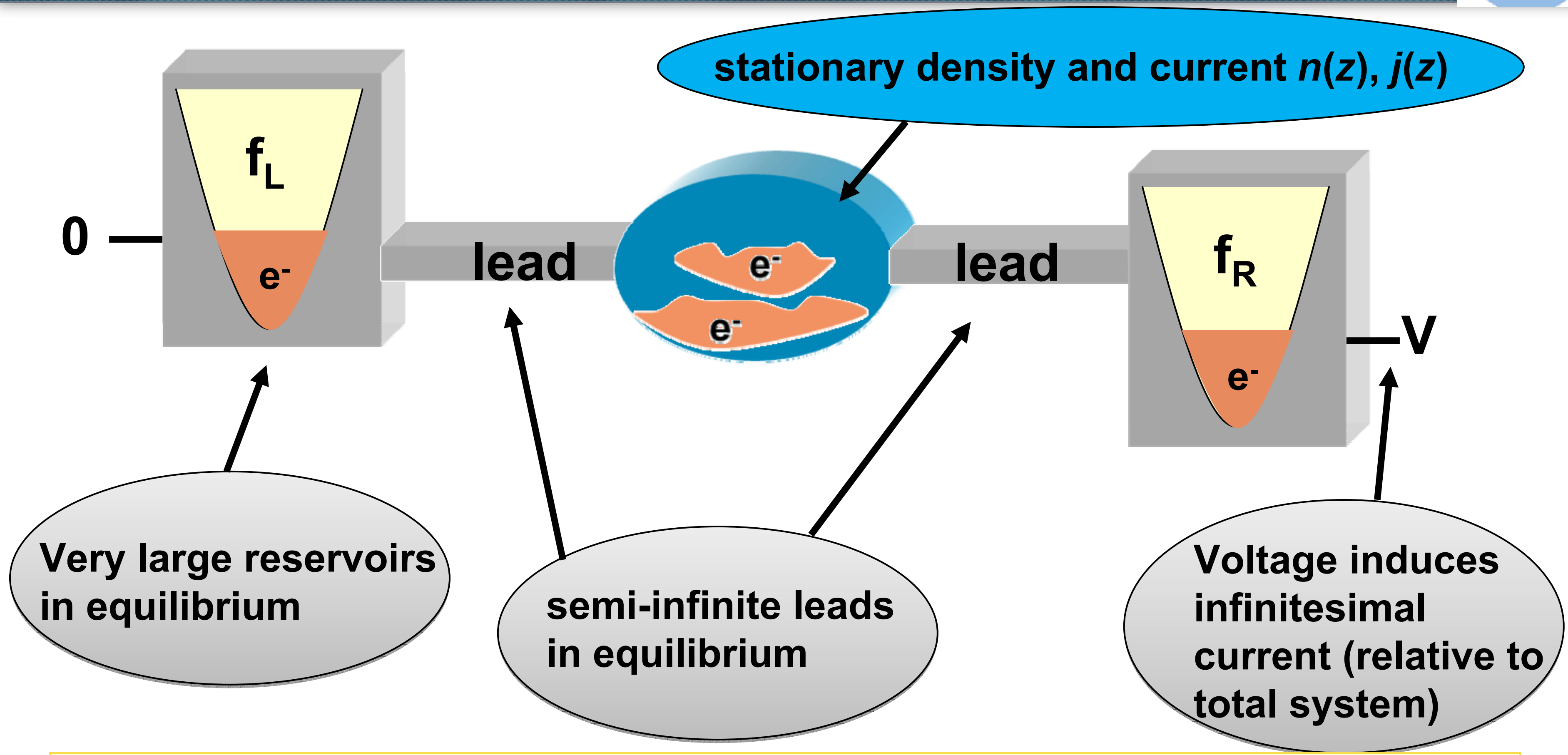
This work:

We treat the QCL as an open quantum device with semi-infinite leads

- ➢ **Fully self-consistent implementation of NEGF**
- ➢ **No periodic solutions are enforced or built-in**

- ➢ **Band structure: single non-parabolic conduction band**
- ➢ **Electron-electron interaction in Hartree (+Exchange) approximation**
- ➢ **Incoherent scattering within self-consistent Born approximation:**
- ❖ **acoustic phonons (inelastic scattering)**
- ❖ **polar optical phonons (inelastic scattering)**
- ❖ **charged impurities (elastic scattering)**
- ❖ **interface roughness (elastic scattering)**
- ❖ **alloy disorder (elastic scattering)**

Transport is a scattering problem

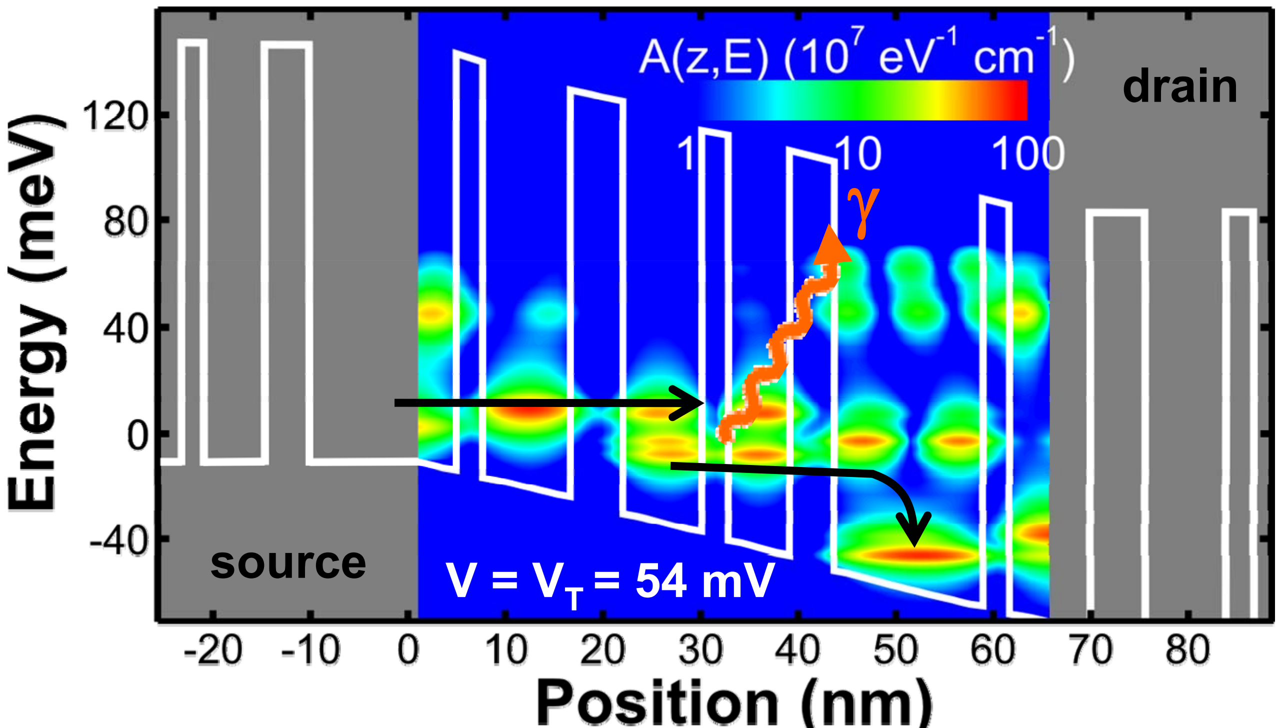


Green's functions are calculated in the scattering center (the active device)
Surroundings (boundary conditions) enter the equations as self energies

NEGF:
Complex boundary conditions can be straightforwardly implemented…
Example: THz-QCLs

Example for complex boundaries

Contour plot of spectral function in a single QCL period



Maxima of the spectral function correspond to resonant electronic states

State alignment:

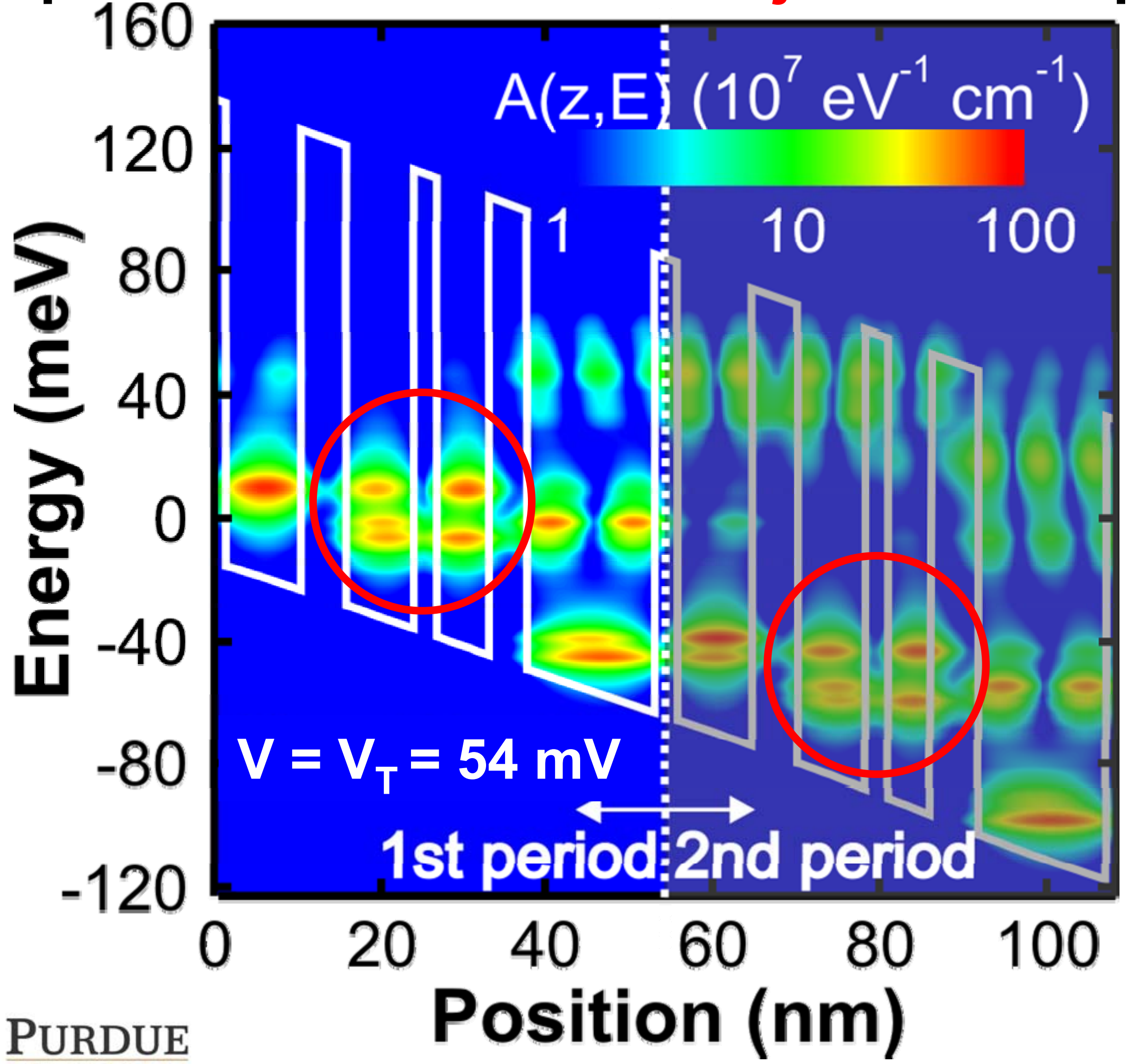
- **Upper laser state gets coherently filled**
- **Resonant emission of LO-phonons empty lower laser state**

Open boundary conditions:
Electrons within the leads are in equilibrium and travel from source to drain

Other examples for complex boundaries:
Current carrying leads, incoherent scattering in the leads…

Open, but periodic spectral function

Spectral function in two adjacent QCL periods

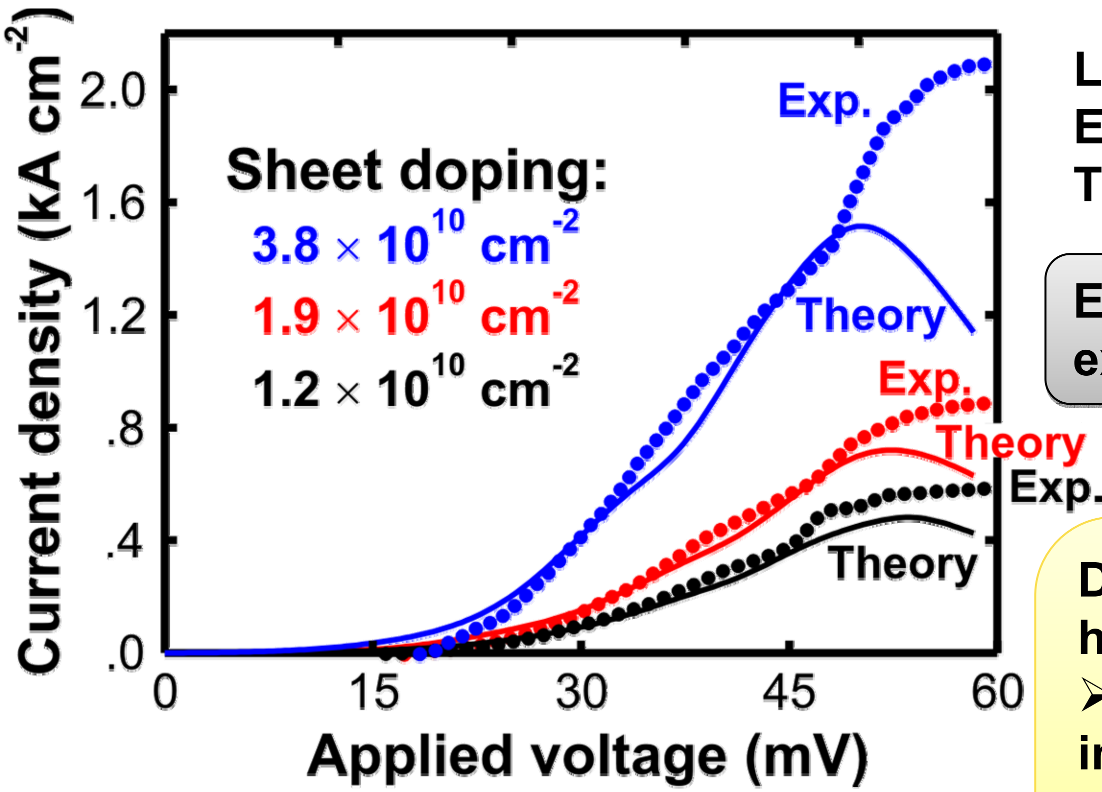


Maxima of the spectral function correspond to resonant electronic states

Density of states in two adjacent QCL periods is indeed periodic

Results: IV characteristics

Calculated and experimental DC current



Light emission at
Experiment: 2.75 THz
Theory (peak gain): 2.64 THz

Excellent agreement with experiment for various devices

GaAs/Al.15Ga.85As QCL:
(3) 9.2 (5.5) 8 (2.7) 6.6 (4.1) 15.5 (3)

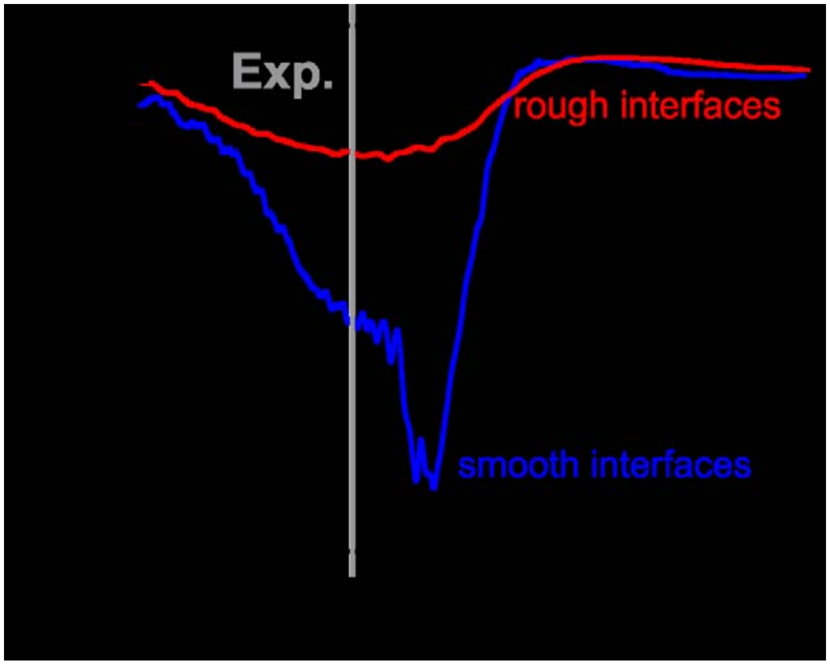
Discrepancy to experiment for higher voltages caused by:
- non-linear electron-photon interaction
- electrons at high kinetic energies (Theory: constant device temperature of 40K)

Experiment:
Benz et al. Appl. Phys. Lett. 90, 101107 (2007)

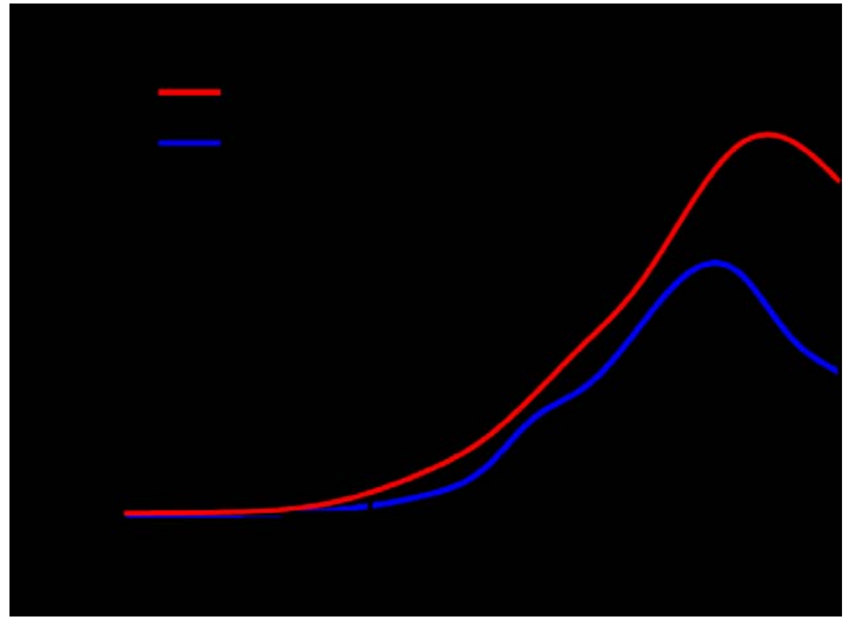
Why NEGF and not "any" method?

Example: rough interfaces in QCLs

Optical absorption coefficient



Current-voltage characteristics



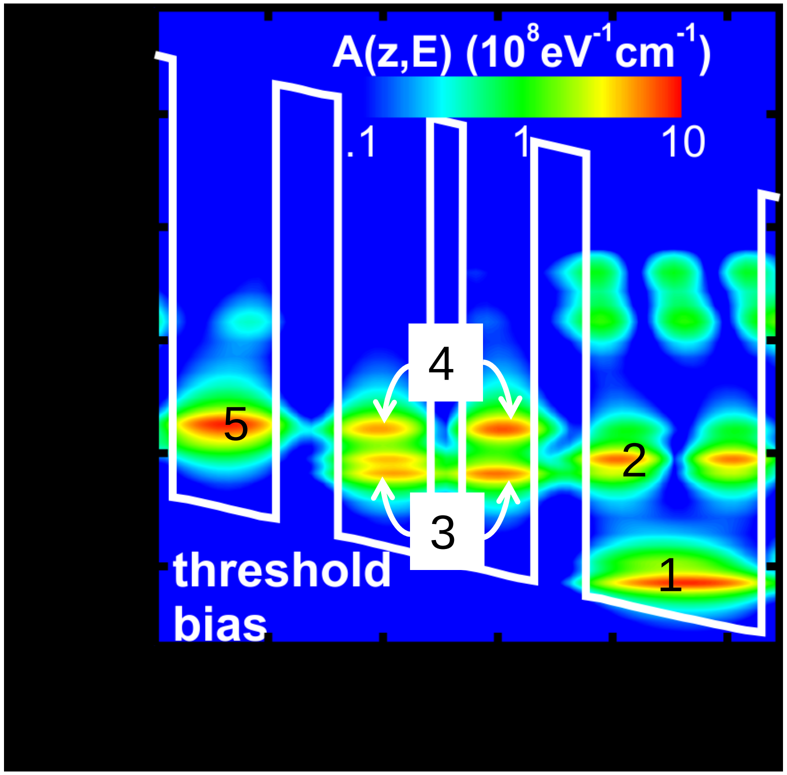
Rough interfaces

- ➢ **Dramatically reduce the optical gain by 90%**
- ➢ **Increase the DC current by up to 30%**

Energy resolved information required to explain the "Why?"

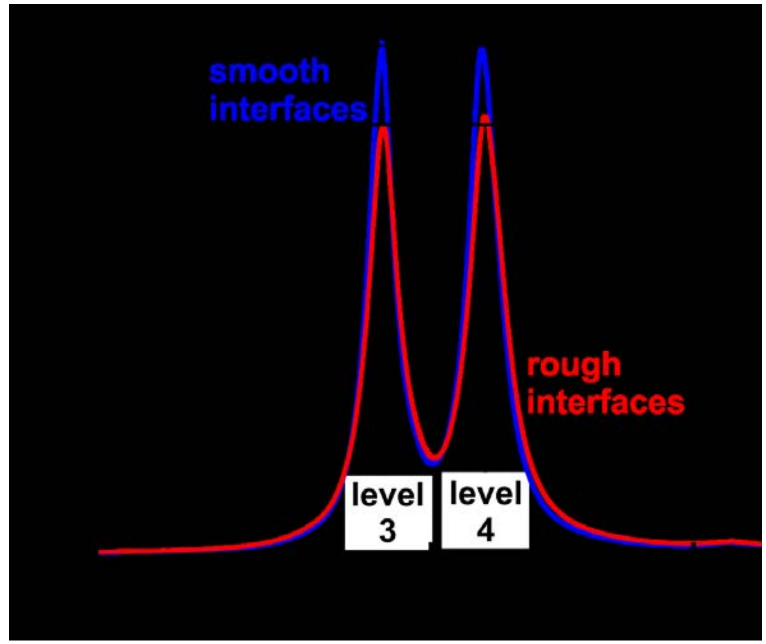
Impact of rough interfaces on QCLs

Active period of THz-QCL



Rough interfaces scattering can
- **broaden confined states**
- **change the state occupancy**

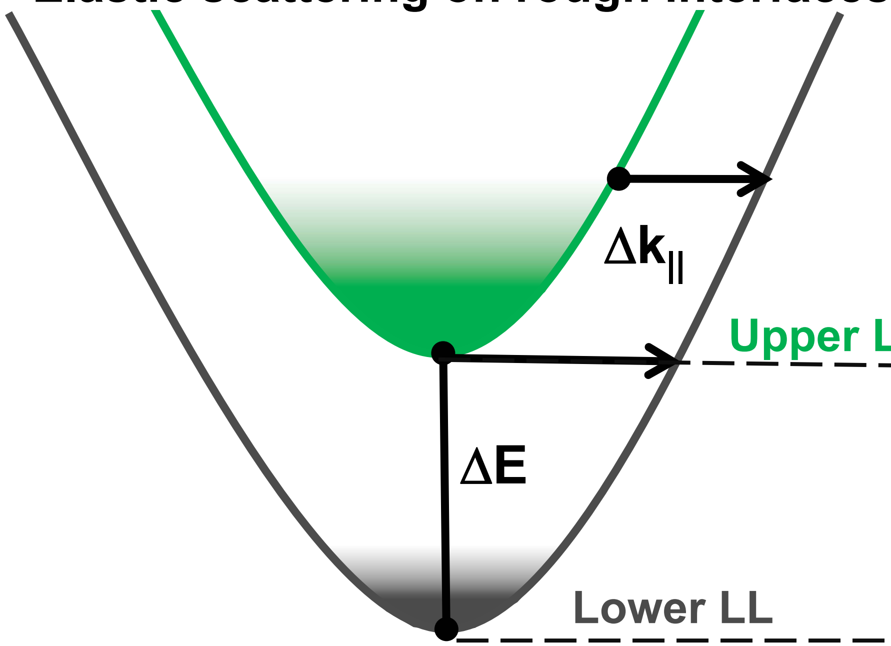
Laser state width vs. roughness

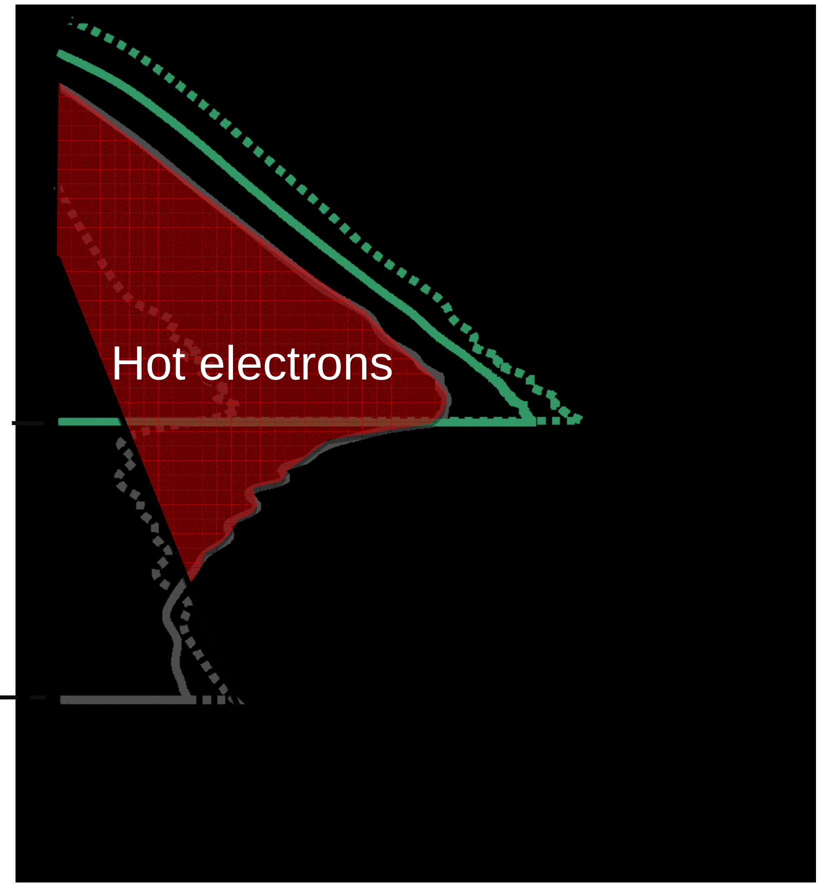


Rough interfaces broaden the laser levels only marginally

Occupation inversion & interfaces

Elastic scattering on rough interfaces

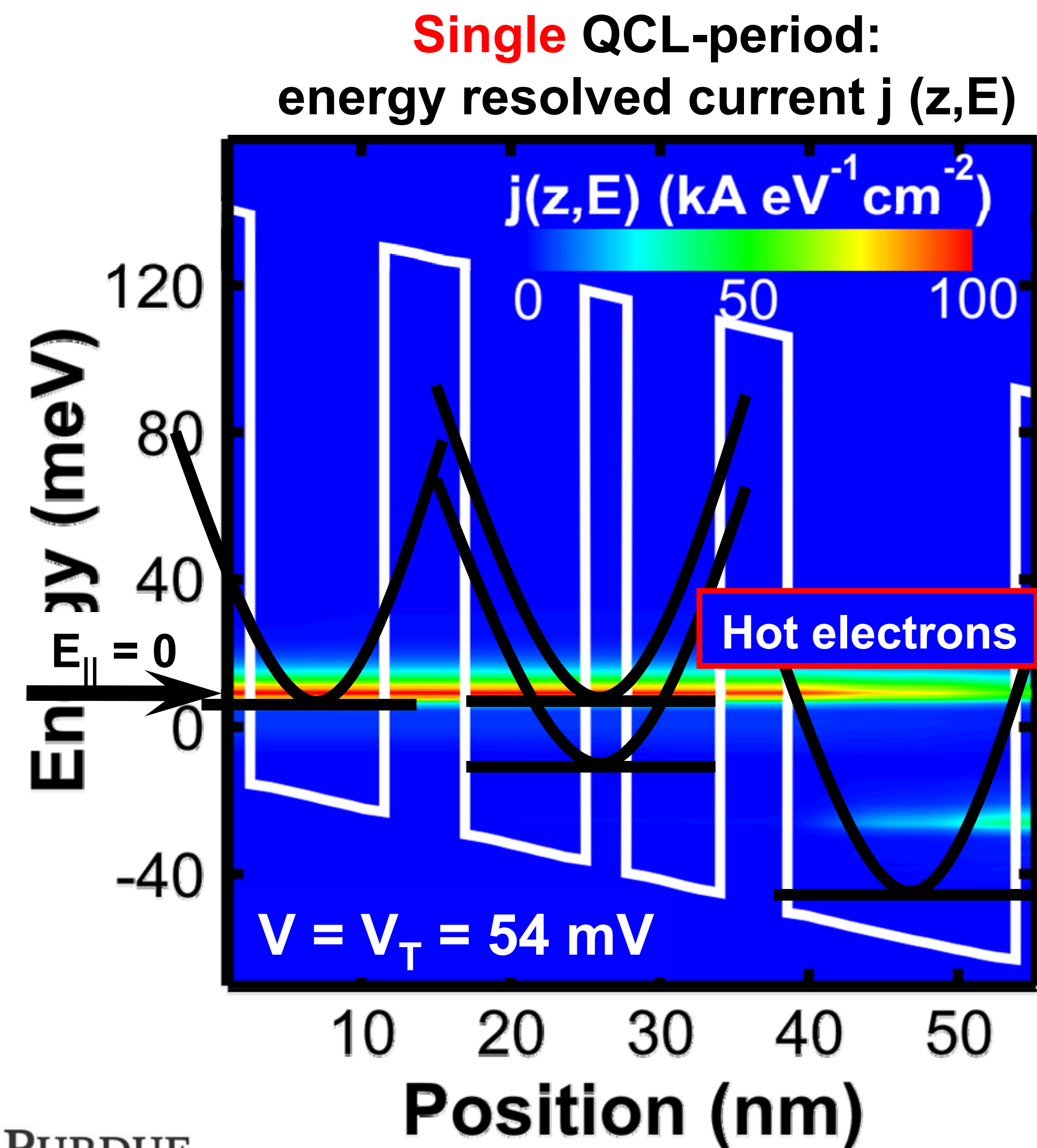




Rough interfaces
- **reduce the occupation inversion**
- **generate hot electrons in the lower laser level**

What happens with the hot electrons?
How do they affect the laser performance?

Energy resolved current density



Current density and state occupation are non-periodic

Maxima of the energy resolved current j(z,E) elucidate propagating charge carriers

Voltage drop: 54 meV
Dissipated: - 36 meV
Remaining: 18 meV

$E_{||} = 18$ meV

Roughness scattering assisted tunneling heats up the carrier distribution

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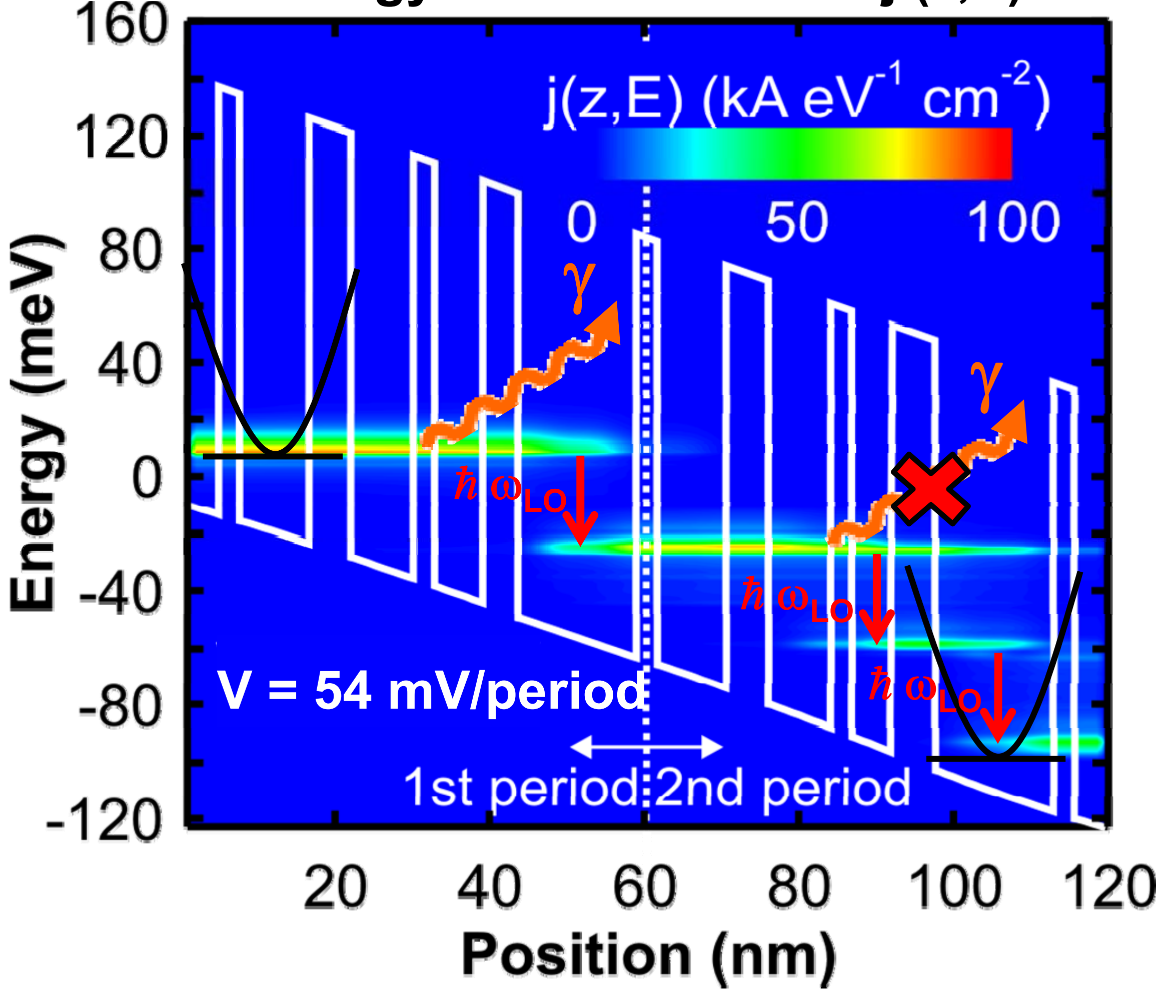
The propagation of hot electrons

Two adjacent QCL-periods: energy resolved current j (z,E)



Dominant dissipation mechanism: Resonant emission of LO-phonons (36 meV)

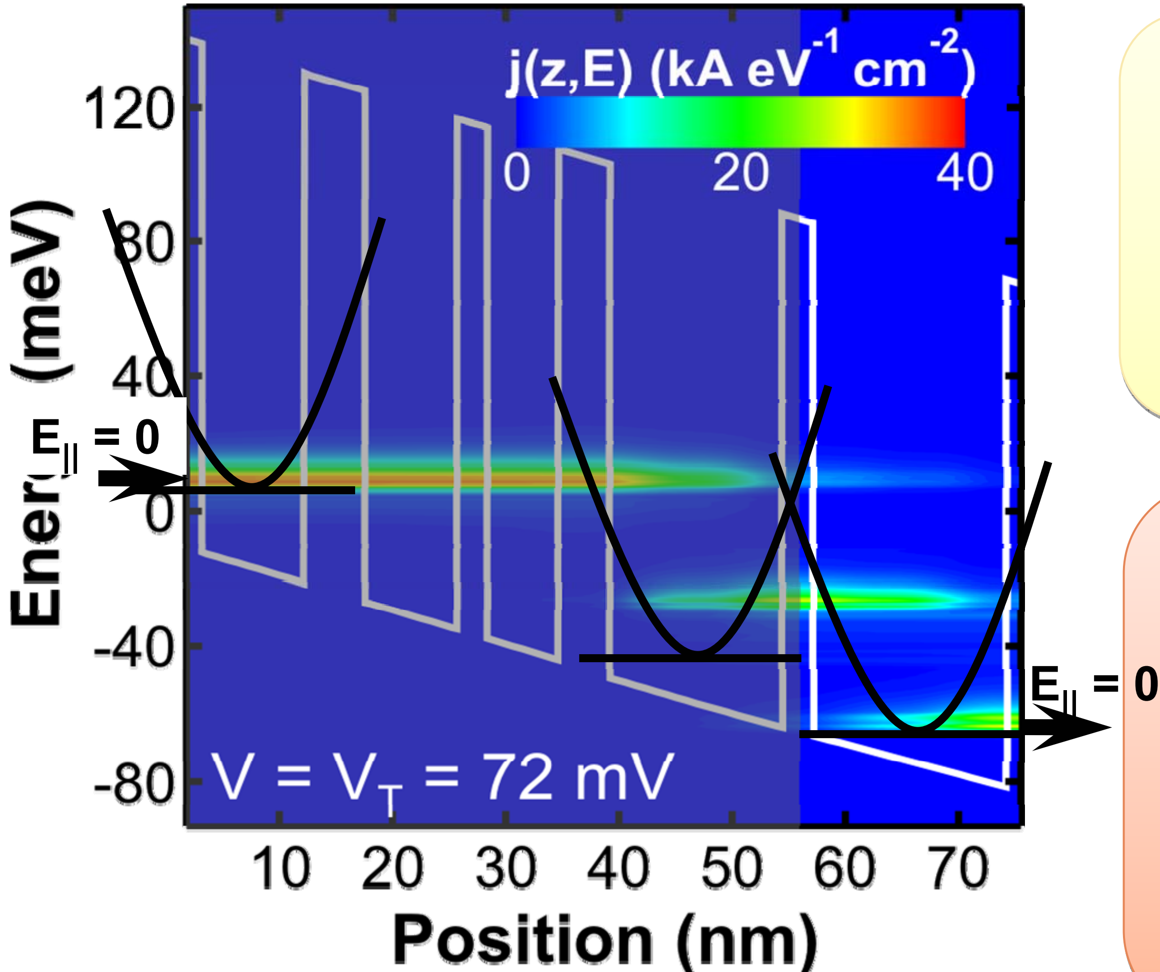
Non-periodic in-plane electron distribution

- **Nonequilibrium distribution in 2^{nd} period**
- **Non-radiative losses in 2^{nd} period (60% reduction in gain)**

Hot electrons ruin optical gain in every 2^{nd} period

How to restore QCL periodicity ?

j(z,E) in a single period at threshold bias



Propose novel design with additional quantum well:
- Suppresses coherent leakage
- Allows second resonant LO-phonon emission

At threshold voltage:
- Electrons are thermalized within each period
- Nonradiative transitions suppressed
- Electron distribution pinned to the QCL geometry

GaAs/Al.15Ga.85As QCL:
(3) 9.2 (5.5) 8 (2.7) 6.6 (4.1) <u>15.5</u> (3) 17.1 (3)

Conclusion

Non-equilibrium Green's functions formalism (NEGF)

- Describes coherent and incoherent effects simultaneously
- Allows straightforward implementation of complex boundary conditions
- Has to be carefully implemented to avoid artifacts

NEGF applied on THz-QCLs:

- A very good agreement of the calculated I-V characteristics and optical gain with experiment
- The full information of a NEGF calculation (inaccessible by experiments or many other models) is vital for a thorough device analysis
- Rough interfaces generate hot electrons and nonperiodic effects in state of the art THz-QCLs

Thank you!