# Density matrix description of transport and gain in quantum cascade lasers in a magnetic field

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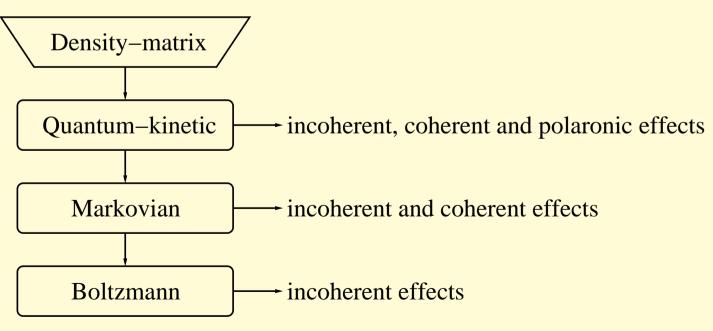
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# **Objectives**

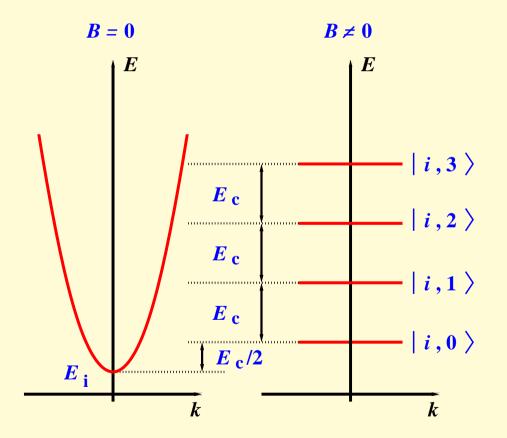
- To investigate quantum-mechanical (coherent and polaronic) effects in QCLs in a magnetic field and their influence on:
  - Electron populations.
  - Output characteristics.
- To develop a quantum-mechanical theory of transport and optical properties of QCLs in a magnetic field.





#### QCLs in a magnetic field

- Discrete electronic structure (Landau levels).
- Scattering rates are significantly enhanced or reduced, depending on the Landau level (LL) configuration.
- Reduced scattering rates  $\Rightarrow$  improved performance:
  - Lower threshold current.
  - Larger population inversion and optical gain.



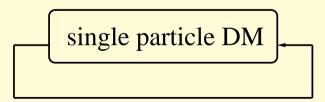
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# **Electron transport in a cascade - density-matrix approach**

- Single particle electron density matrices  $f_{i_1i_2,k} = \left\langle \hat{c}_{i_1,k}^{\dagger} \hat{c}_{i_2,k} \right\rangle$ ,  $n_{i_1i_2} = \sum_{k'} f_{i_1i_2,k'} / L_x L_y$ :
  - The diagonal elements the occupation probabilities of LLs.
  - The non-diagonal elements the quantum-mechanical coherence between LLs.
- The Hamiltonian:  $\hat{H} = \hat{H}_0 + \hat{H}_{el} + \hat{H}_{ep}$  (non-interacting electrons, the electron-light interaction, the electron-LO phonon interaction).
- Non-interacting electrons:

$$\frac{d}{dt}n_{i_1i_2}\Big|_{\hat{H}_0} = \frac{1}{i\hbar}(E_{i_2} - E_{i_1})n_{i_1i_2}.$$

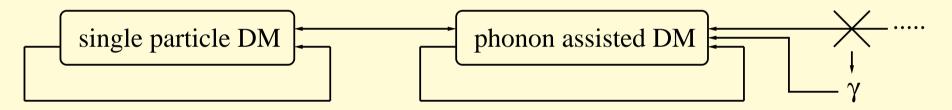
• Interaction of electrons with *z*-polarized light: Landau index conserved.



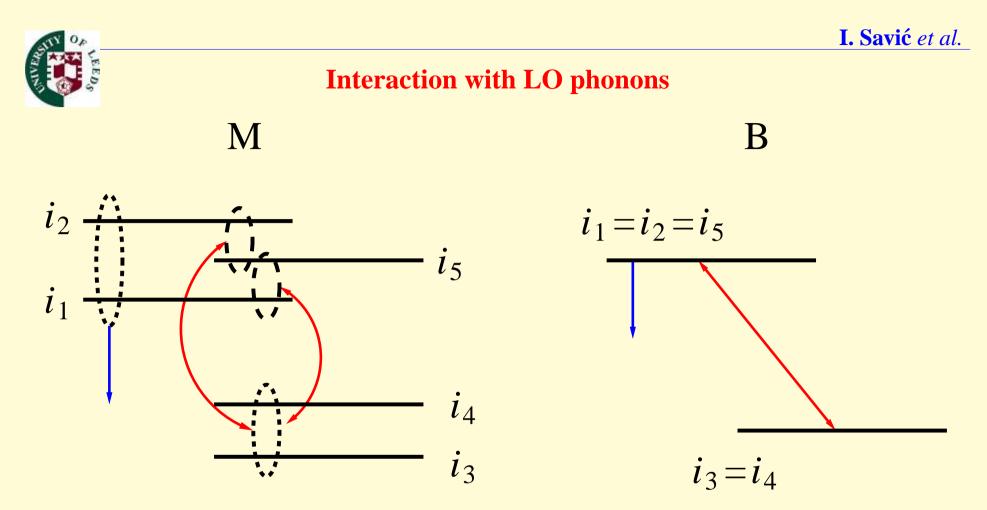


# **Interaction with LO phonons**

- Quantum-kinetic (non-Markovian) description:
  - Phonon-assisted matrices  $s_{k,\mathbf{q},k'}^{i_1i_2} = \left\langle \hat{c}_{i_1,k}^{\dagger} \hat{b}_{\mathbf{q}} \hat{c}_{i_2,k'} \right\rangle$ .



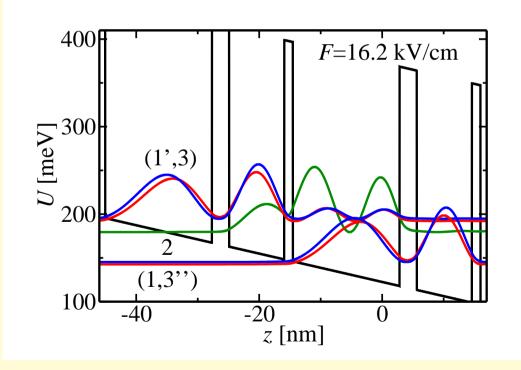
- Broadening of LLs represented by a phenomenological damping constant  $\gamma$ .
- Markovian description:
  - Adiabatic elimination of phonon-assisted matrices  $\Rightarrow$  the quantum-kinetic equations reduce to the Markovian equations.
  - Broadening of LLs a Lorentzian with the FWHM of  $2\hbar\gamma$ .



- The semiclassical limit (non-diagonal matrix elements neglected) ⇒ the Markovian equations reduce to the Boltzmann equations.
- The tight-binding description and the periodicity of the quantities involved were used in all three approaches.



- Three-level scheme, LO phonon depopulation of the lower laser level, no injector.
- THz GaAs/Al<sub>0.3</sub>Ga<sub>0.7</sub>As, laser transition  $\sim 15.2$  meV.
- Dominant influence of the electron-LO phonon interaction on the populations.

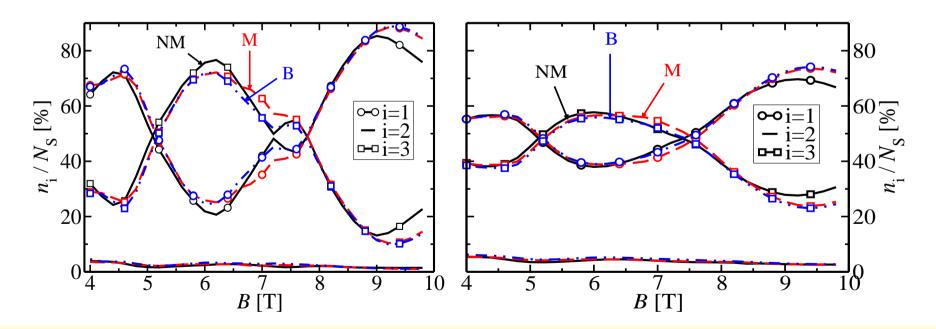


The conduction band profile of the QCL.



# **Populations**

- Similar values of populations and their dependence on *B* from all three approaches.
- The differences due to coupling between populations and polarizations in the Markovian approach (among populations, polarizations and phonon-assisted matrices in the non-Markovian approach).

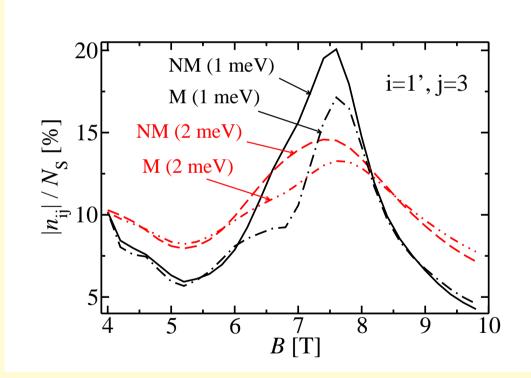


The electron population over QCL states (all Landau levels) vs magnetic field. Left:  $\hbar \gamma = 1$  meV. Right:  $\hbar \gamma = 2$  meV.



# **Polarizations**

- Finite values of polarizations in the steady state.
- The largest polarization  $\sim 10\%$ .



The electron polarization between the ground state of the preceding period and the upper laser level (all Landau levels) vs magnetic field.



#### **Nature of electron transport - coherent vs incoherent**

• Quantum-mechanical (Markovian and non-Markovian) interpretation - coherent current.

$$J = -\frac{e}{d} \sum_{i_1, i_2=1}^{N} \left[ v_{i_1 i_2} n_{i_2 i_1} + v_{i_1 (i_2+N)} n_{(i_2+N) i_1} + v_{(i_2+N) i_1} n_{i_1 (i_2+N)} \right]$$
$$v_{i_1 i_2} = \frac{i}{\hbar} \langle i_1 | [\hat{H}, \hat{z}] | i_2 \rangle = \frac{i}{\hbar} (E_{i_1} - E_{i_2}) z_{i_1 i_2} + \frac{1}{m^*} e A_R \delta_{i_1, i_2}.$$

• Semiclassical interpretation - incoherent current.

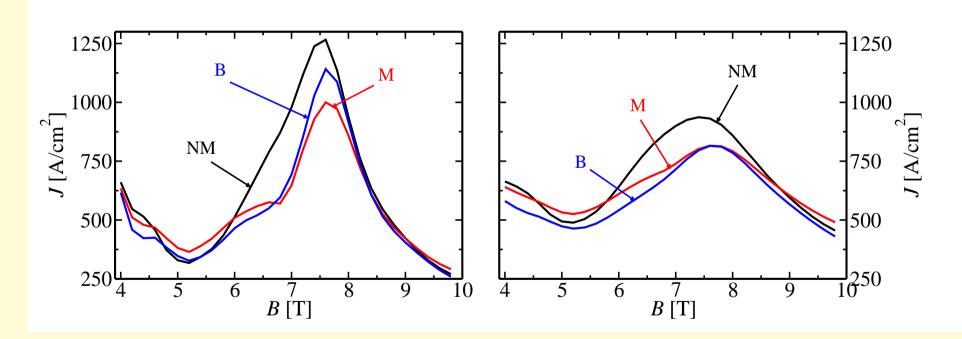
$$J = \frac{e}{d} \left[ \sum_{\substack{i=1 \ i < f}}^{N} \sum_{\substack{f=1 \ (i < f)}}^{2N} (z_f - z_i) \left[ n_i W_{if} (1 - \alpha_B n_f) - n_f W_{fi} (1 - \alpha_B n_i) \right] \right].$$

Ref.: S. C. Lee, F. Banit, M. Woerner, and A. Wacker, Phys. Rev. B 73, 245320 (2006).



#### Current

- Similar values of the current and its dependence on *B* in all three approaches.
- Relatively small coherences in the steady state.

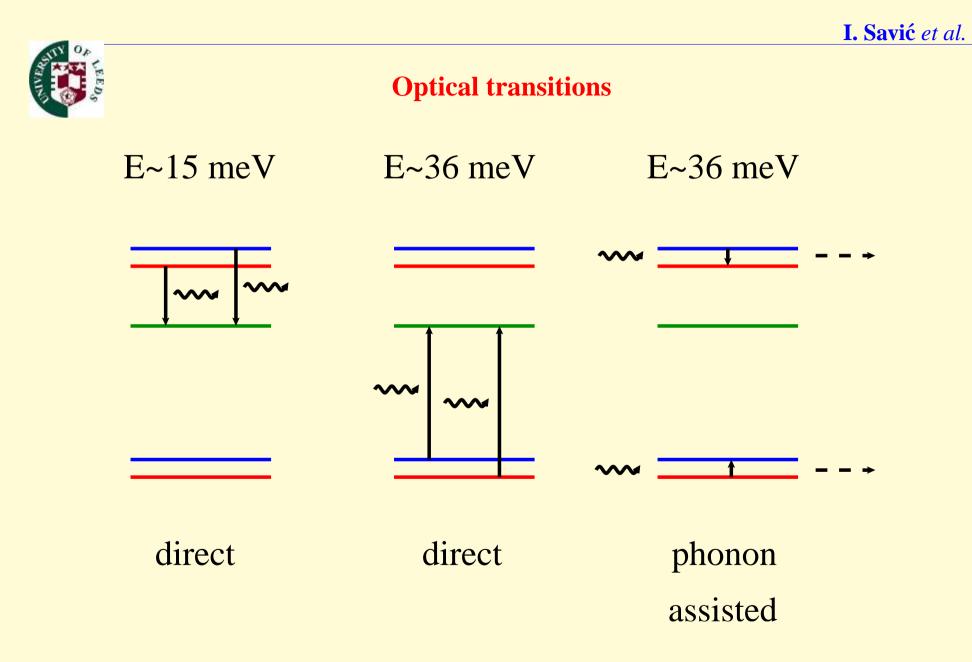


Current density vs magnetic field dependence. Left:  $\hbar \gamma = 1$  meV. Right:  $\hbar \gamma = 2$  meV.



# **Optical gain - general considerations**

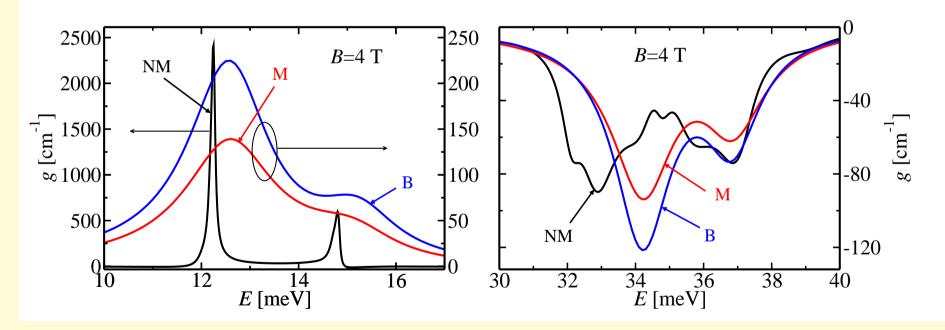
- Quantum-mechanical description:  $g(\omega) \sim \text{Im}[\chi(\omega)] \sim \text{Im}[J(\omega)]$ .
  - Non-Markovian approach:
    - \* Direct optical transitions the gain linewidth determined by coupling to the LO phonon assisted transitions.
    - \* LO phonon assisted optical transitions  $\sim \frac{1}{E_{i_2} \pm \hbar \omega_{\text{LO}} E_{i_1} \pm \hbar \omega i\hbar \gamma}$  the linewidth is of the order of  $\sim 2\hbar \gamma$ .
  - Markovian approach:
    - \* Direct optical transitions  $\sim \frac{1}{E_{i_2} \pm \hbar \omega_{\text{LO}} E_{i_1} i\hbar \gamma}$  the linewidth determined by the scattering processes.
- Semiclassical description: Fermi's golden rule.
  - Direct optical transitions the linewidth taken to be  $2\hbar\gamma$ .





# **Optical gain - non-Markovian case**

- The gain linewidth for the energies corresponding to the laser transitions is considerably smaller than for the energies around one LO phonon energy.
- Signatures of the polaron shift.

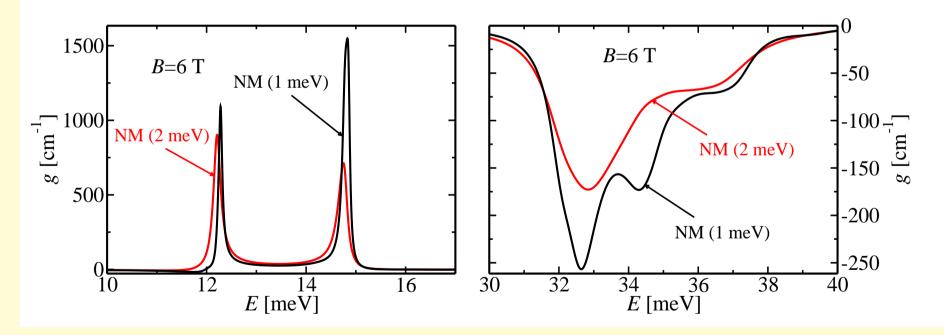


Optical gain vs energy for a magnetic field of 4 T and  $\hbar\gamma = 1$  meV. Left: The energy range is in the vicinity of the optical transition energies. Right: The energy range is in the vicinity of one longitudinal optical phonon energy.



# **Optical gain - non-Markovian case**

- Additional peaks for energies close to one LO phonon energy.
- A non-trivial interplay between the resonant LO phonon assisted transitions and resonant direct optical transitions for energies close to LO phonon energy.



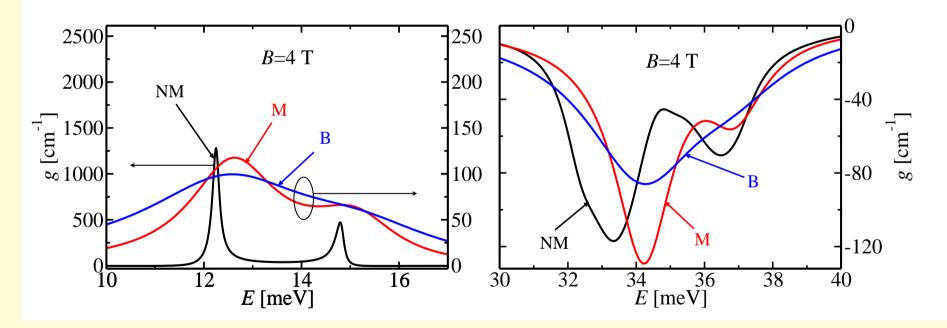
Optical gain vs energy for a magnetic field of 6 T. Left: The energy range is in the vicinity of the optical transition energies. Right: The energy range is in the vicinity of one longitudinal optical phonon energy.



# **Optical gain - Markovian case**

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- Resonant scattering terms present throughout the energy range of interest.
- Large linewidth for the energies corresponding to the laser transitions and the energies around one LO phonon energy.



Optical gain vs energy for a magnetic field of 4 T and  $\hbar\gamma = 2$  meV. Left: The energy range is in the vicinity of the optical transition energies. Right: The energy range is in the vicinity of one longitudinal optical phonon energy.



#### Summary

- Quantum-mechanical theory of gain and electron transport in QCLs in a magnetic field based on the density-matrix formalism:
  - Non-Markovian.
  - Markovian.
  - Boltzmann.
- Similar populations.
- Finite, but relatively small coherences.
- Comparable values of the current densities, despite different interpretations of the origin of the transport processes.
- Narrow linewidths for laser transitions and evidence of polaron formation in the non-Markovian treatment, in contrast to the Markovian and Boltzmann predictions.

Ref.: I. Savić, N. Vukmirović, Z. Ikonić, D. Indjin, R. W. Kelsall, P. Harrison, and V. Milanović, cond-mat/0702508, accepted for publication in Phys. Rev. B.