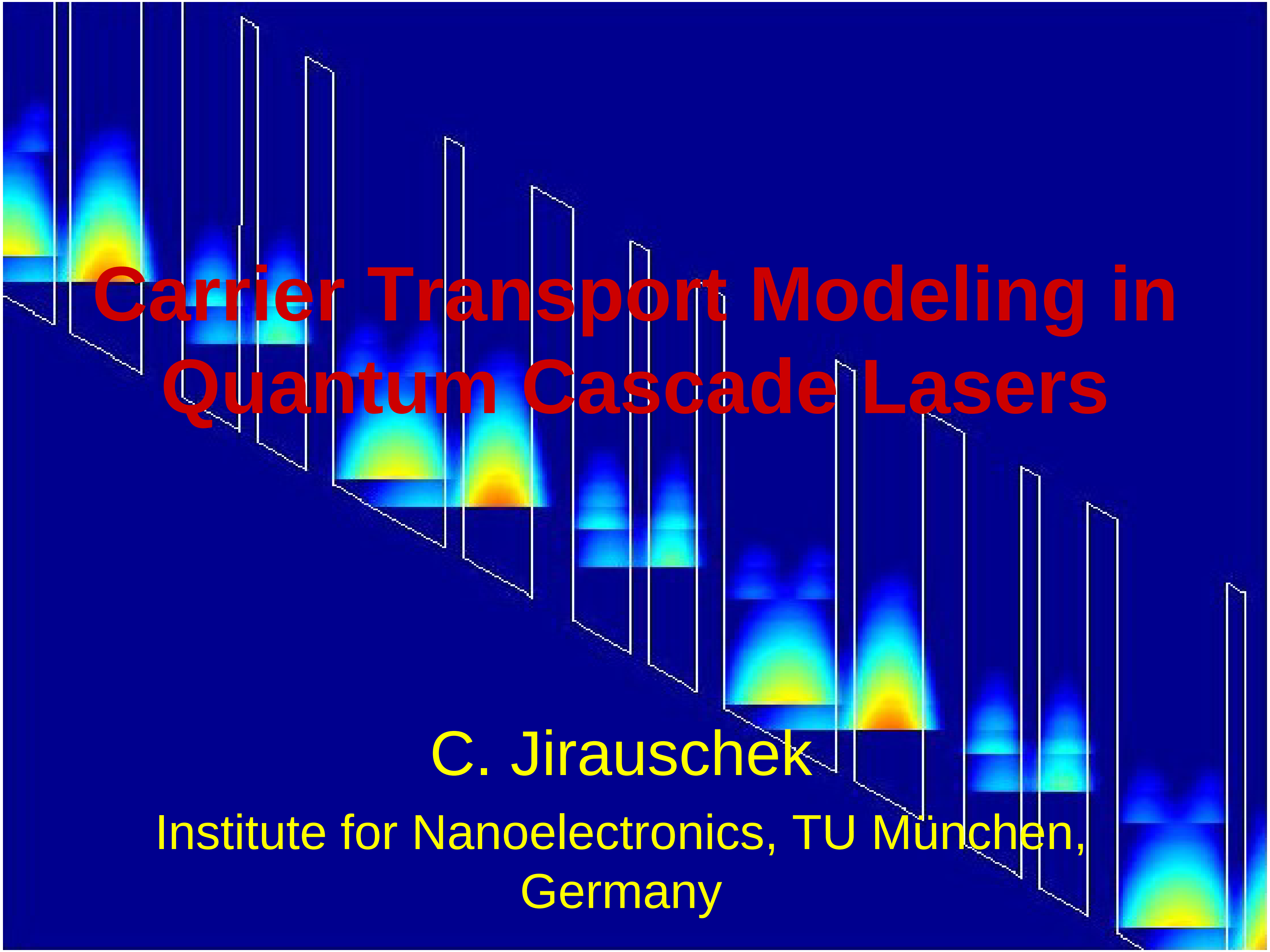

Carrier Transport Modeling in Quantum Cascade Lasers

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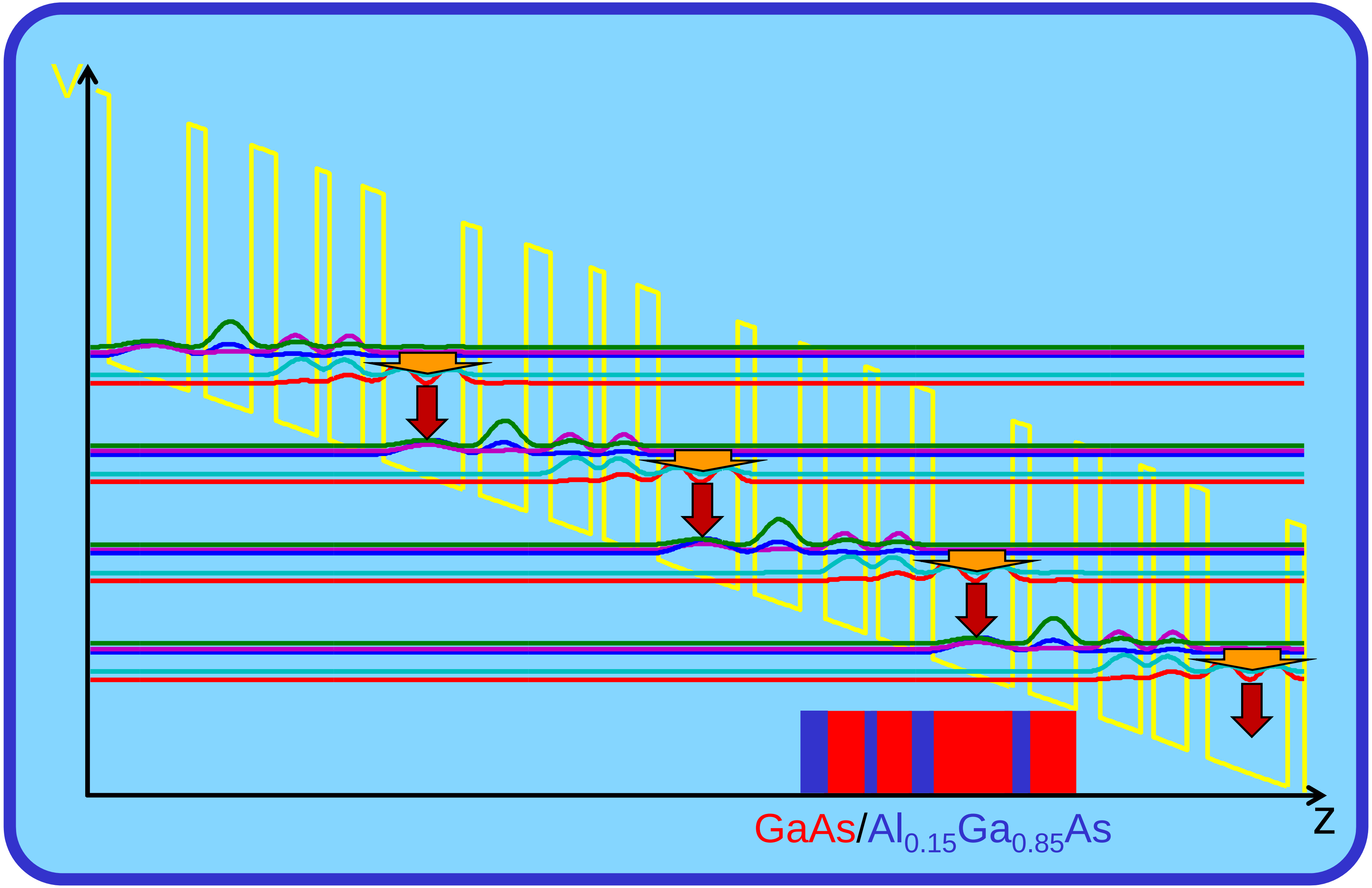
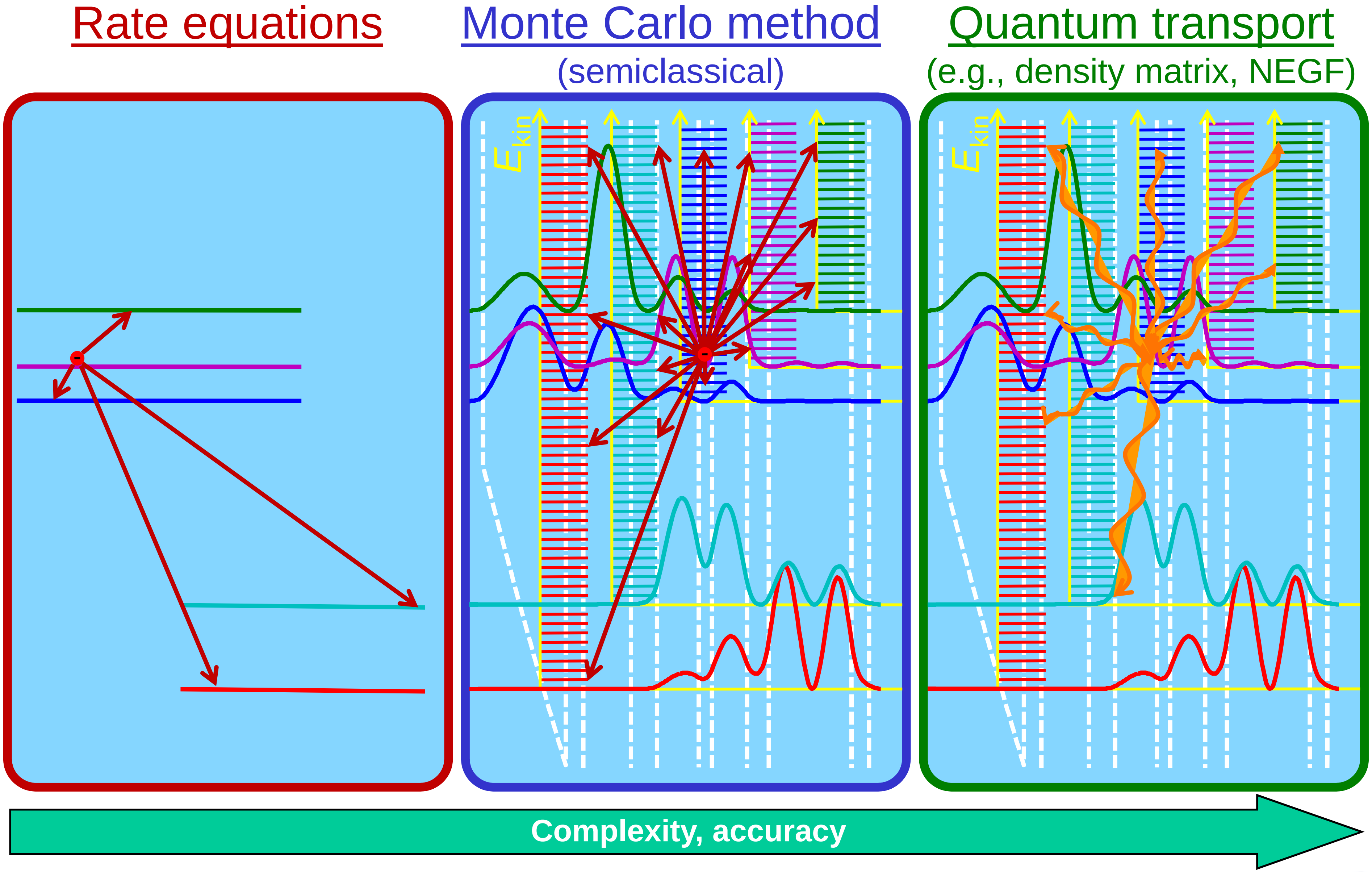
Overview

- Methods overview
- Open two-level model
- Monte Carlo simulation
- Quantum transport

Typical QCL Structure



Carrier Transport Simulation Methods



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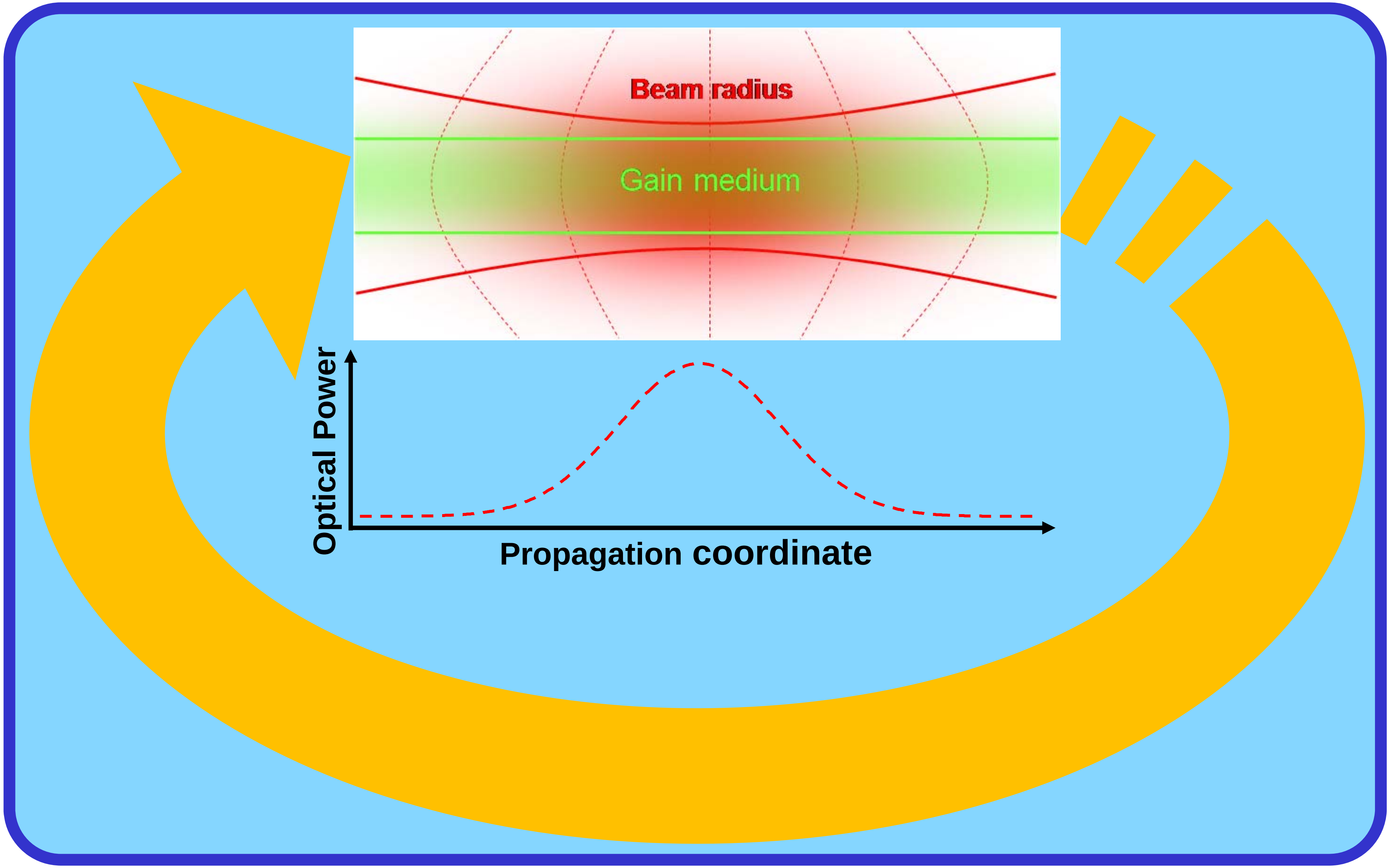
Quantum Cascade Ring Laser



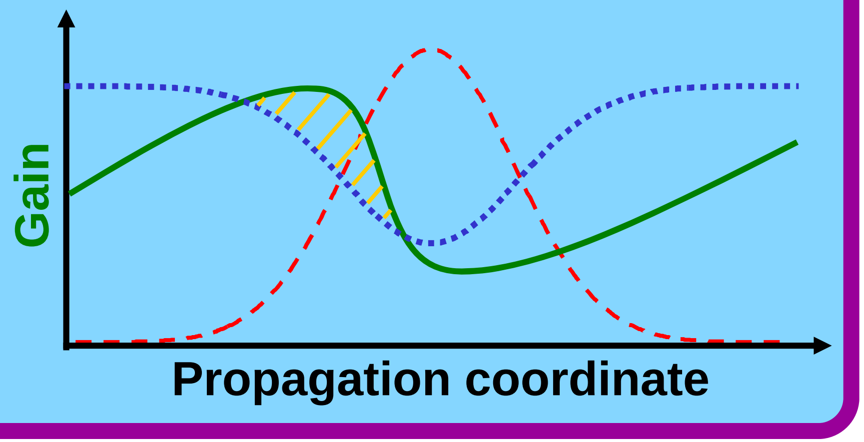
Extended Maxwell-Bloch Equations

Field: $$\frac{n}{c}\partial_t E = -\partial_z E - \mathrm{i}\frac{kN\mu\Gamma}{2\epsilon_0 n^2}\eta - \boxed{\frac{1}{2}\ell\left(E\right)E}$$

Polarization: $$\partial_t \eta = \frac{\mathrm{i}\mu}{2\hbar}E\Delta - \frac{\eta}{T_2}$$

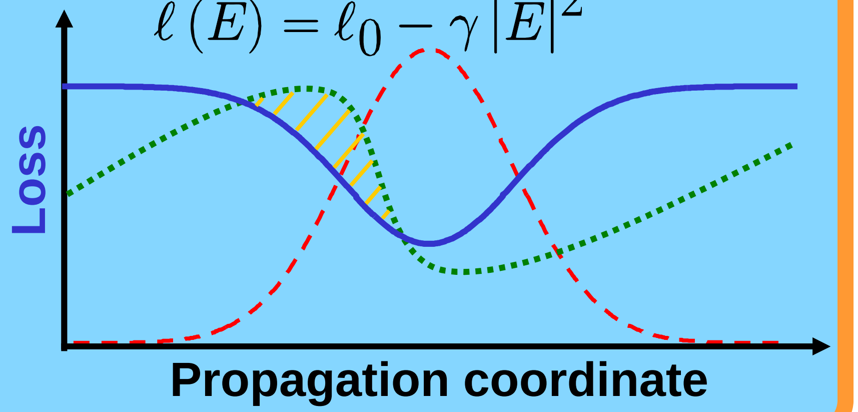
Inversion: $$\partial_t \Delta = \boxed{\frac{\Delta_p - \Delta}{T_1}} + \frac{\mathrm{i}\mu}{\hbar}\left(E^*\eta - c.c.\right)$$

Gain recovery



Saturable absorption

$$\ell\left(E\right) = \ell_0 - \gamma\left|E\right|^2$$

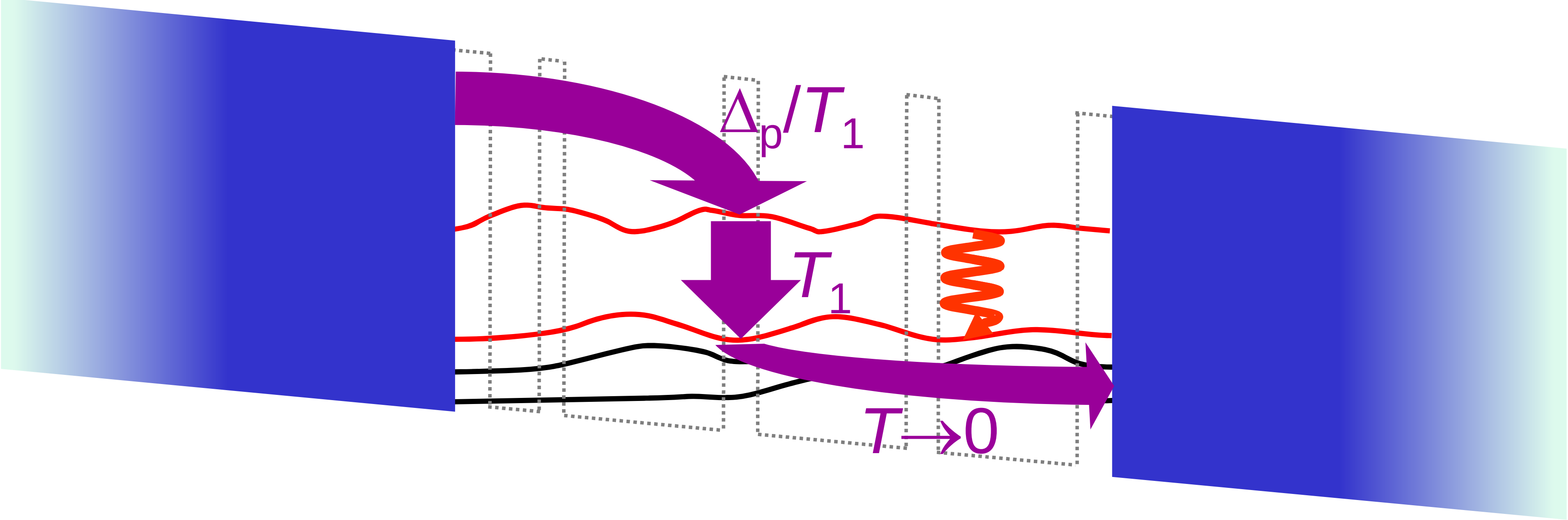


Rate Equations

Field: $$\frac{n}{c}\partial_t E = -\partial_z E - \mathrm{i}\frac{kN\mu\Gamma}{2\epsilon_0 n^2}\eta - \frac{1}{2}\ell\left(E\right)E$$

Polarization: $$\partial_t \eta = \frac{\mathrm{i}\mu}{2\hbar}E\Delta - \frac{\eta}{T_2}$$

Inversion: $$\partial_t \Delta = \frac{\Delta_p - \Delta}{T_1} + \frac{\mathrm{i}\mu}{\hbar}\left(E^*\eta - c.c.\right)$$



Coherent Effects

Field: $$\frac{n}{c}\partial_t E = -\partial_z E - \mathrm{i}\frac{kN\mu\Gamma}{2\epsilon_0 n^2}\eta - \frac{1}{2}\ell\left(E\right)E$$

Polarization: $$\partial_t \eta = \frac{\mathrm{i}\mu}{2\hbar}E\Delta - \frac{\eta}{T_2}$$

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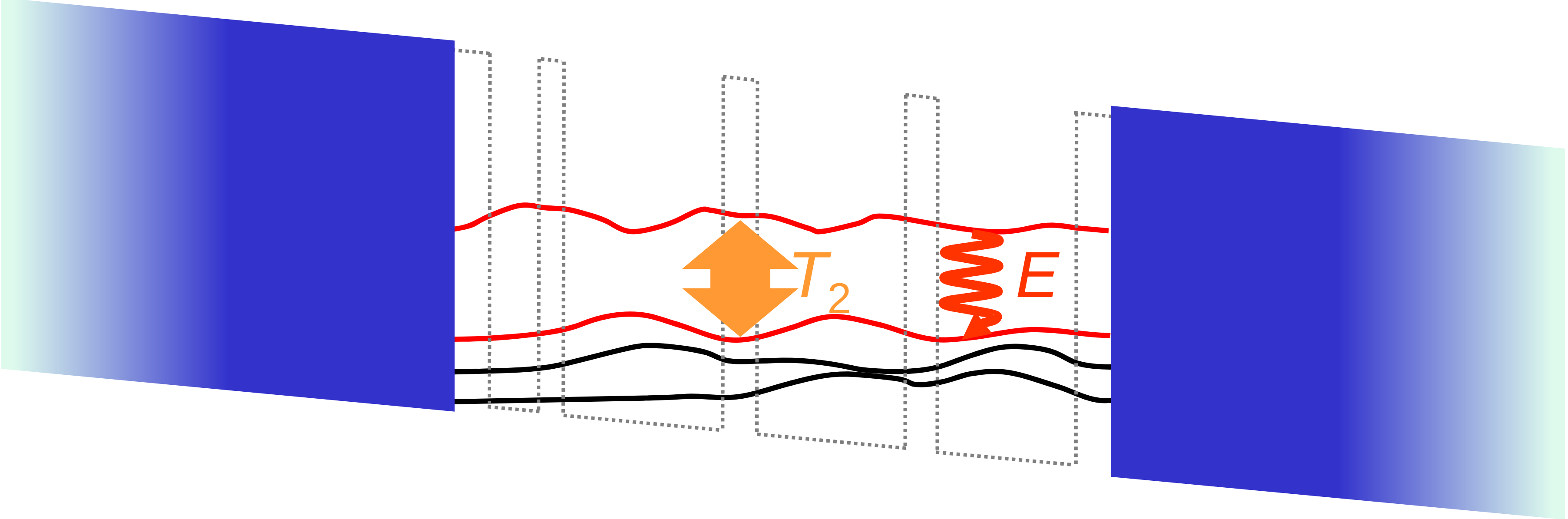
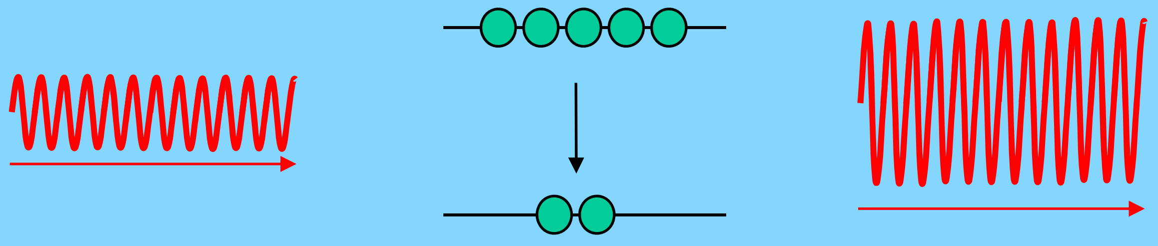
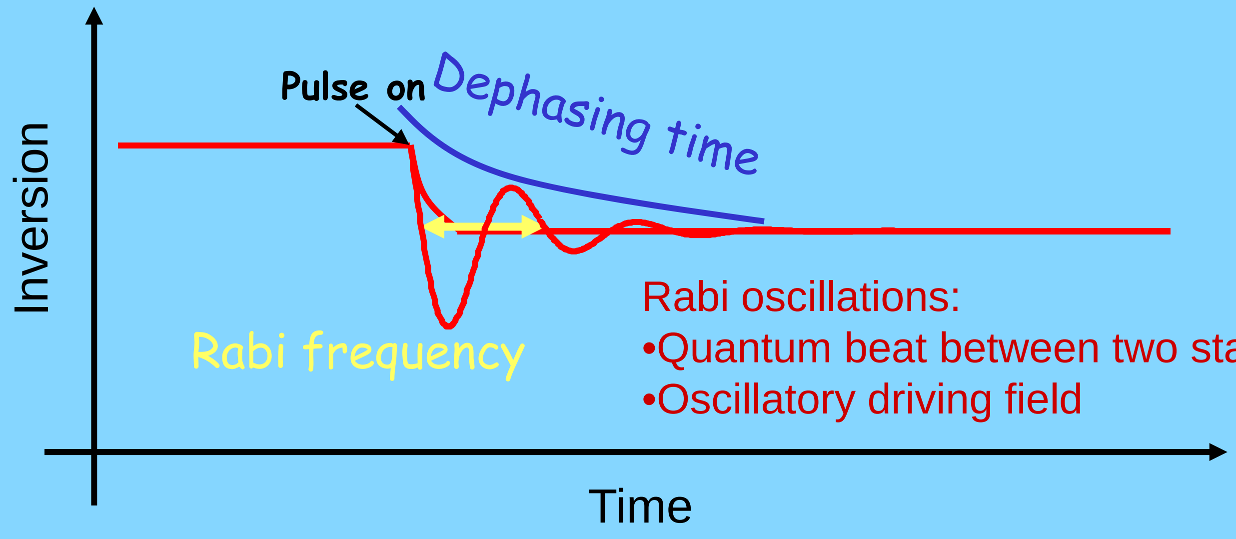


Coherent Effects

Standard amplification: Rate equations

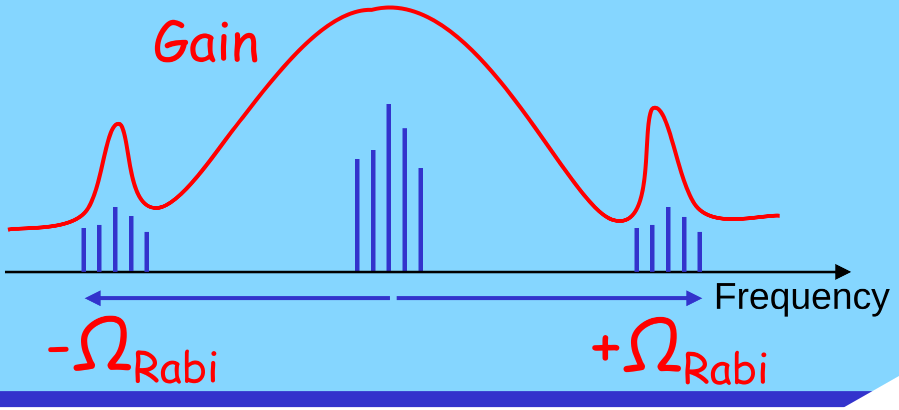


Coherent effects (Maxwell-Bloch equations)



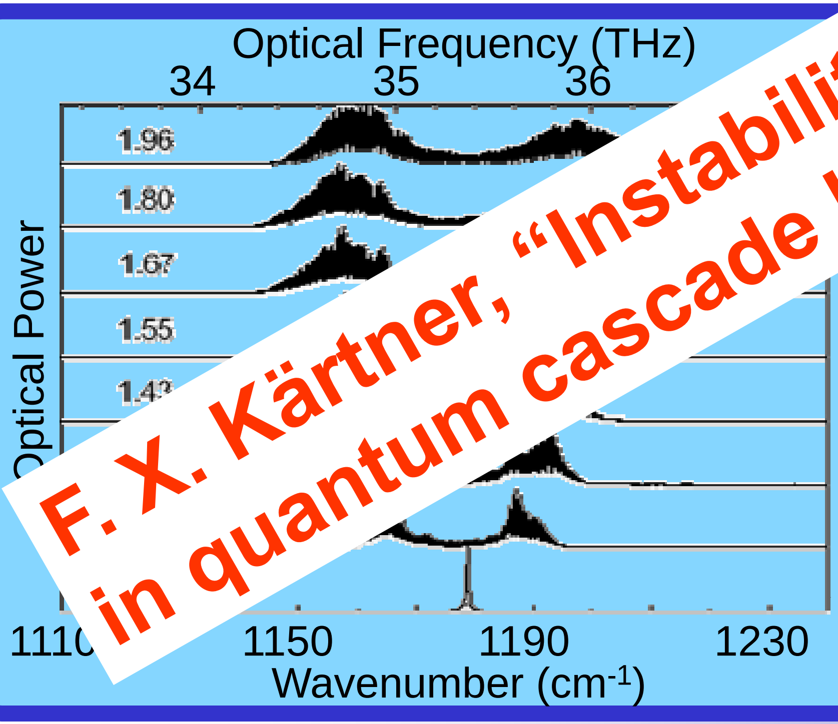
Rabi oscillations:
- Quantum beat between two states
- Oscillatory driving field

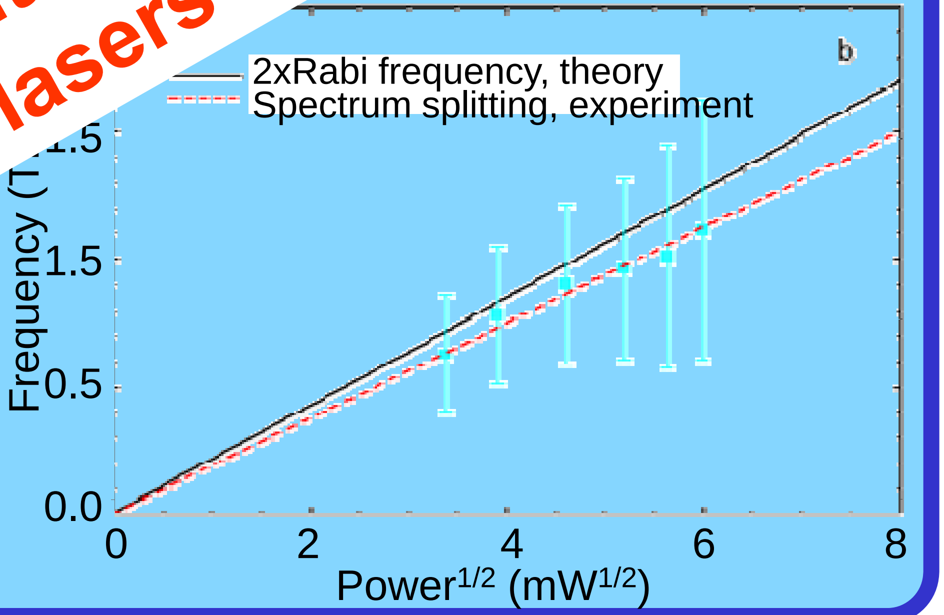
Coherent instability = Rabi splitting



Slow gain	Mode lockin Q swit
Fast gai	C y urning]

F. X. Kärtner, “Instabilities and mode-locking in quantum cascade lasers”, IQCLSW 2008





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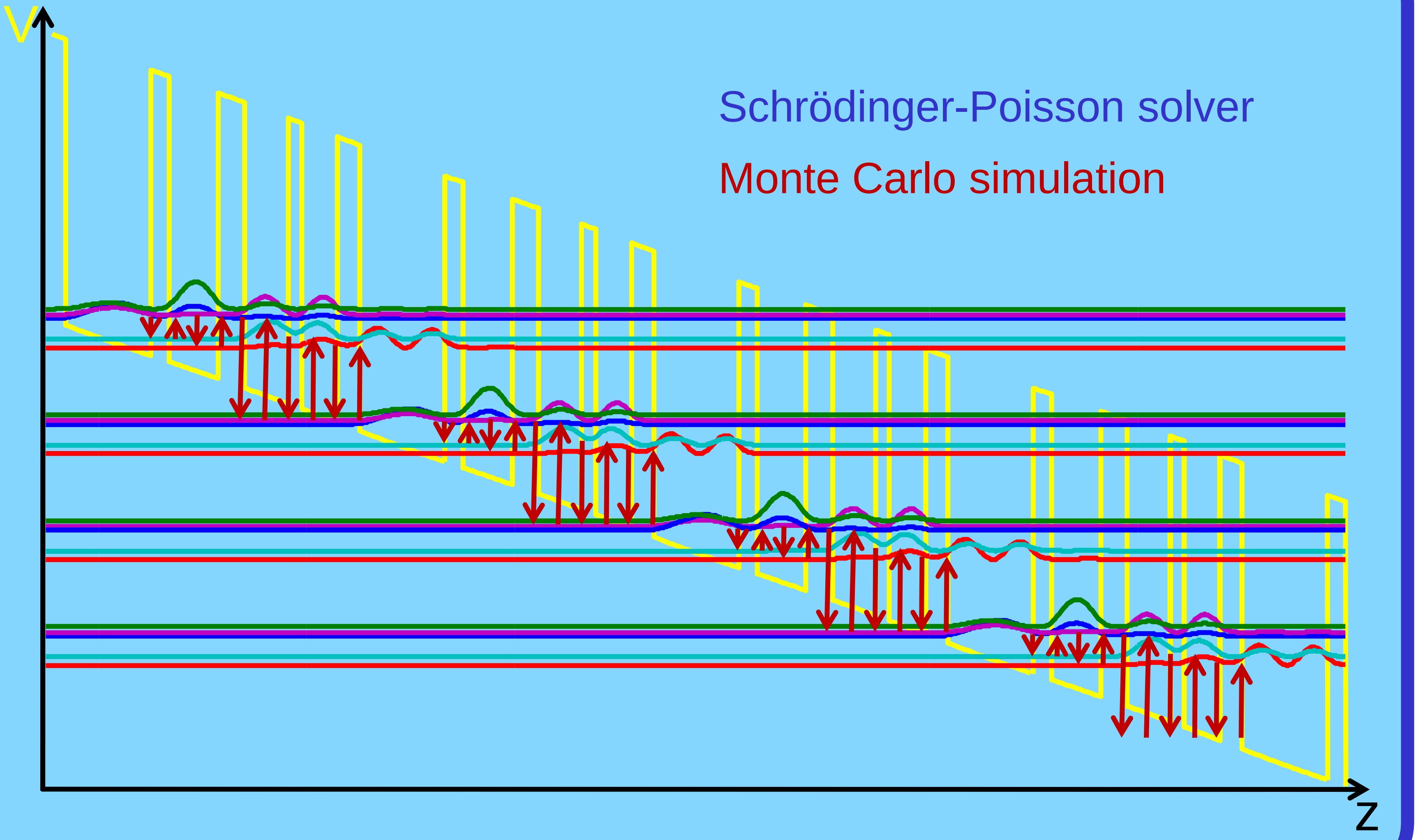
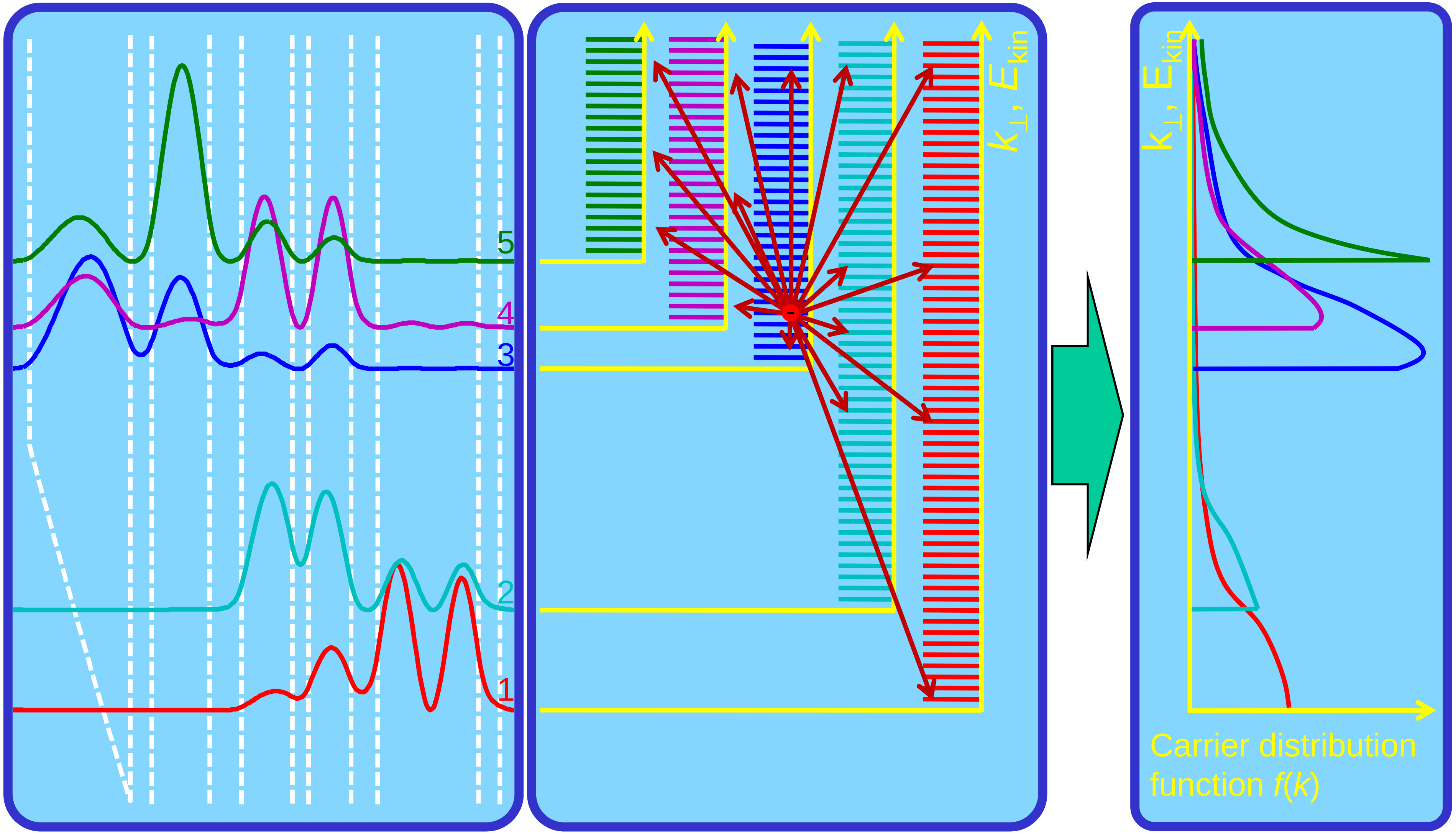
Simulation



Schrödinger-Poisson solver

Monte Carlo simulation

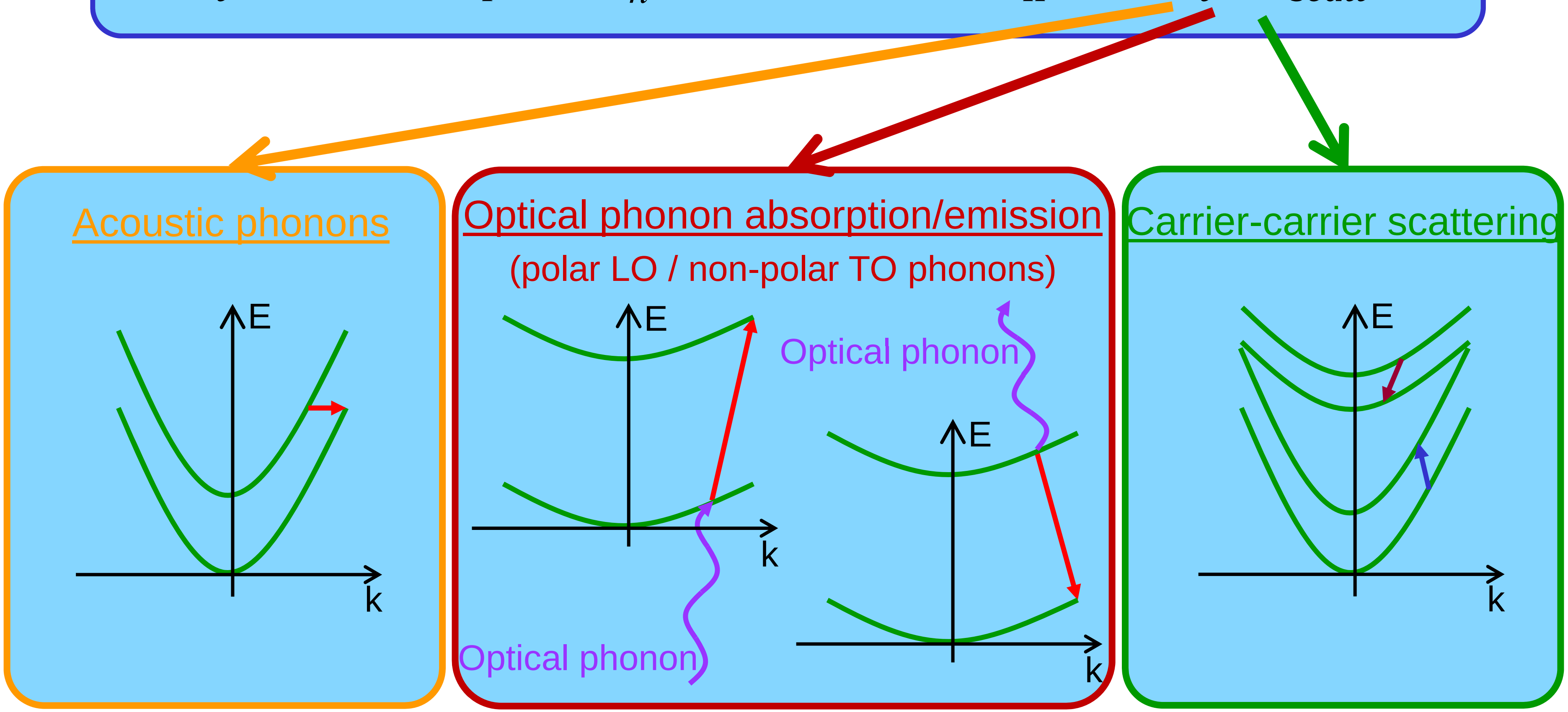
Monte Carlo Solver



Boltzmann equation

carrier distribution function f(**r**,**k**,t)

$$\partial_t f = -\mathbf{v}\nabla_{\mathbf{r}} f - \tfrac{q_c}{\hbar}(\mathbf{E}+\mathbf{v}\times\mathbf{B})\nabla_{\mathbf{k}} f + \partial_t f\,|_{scatt}$$



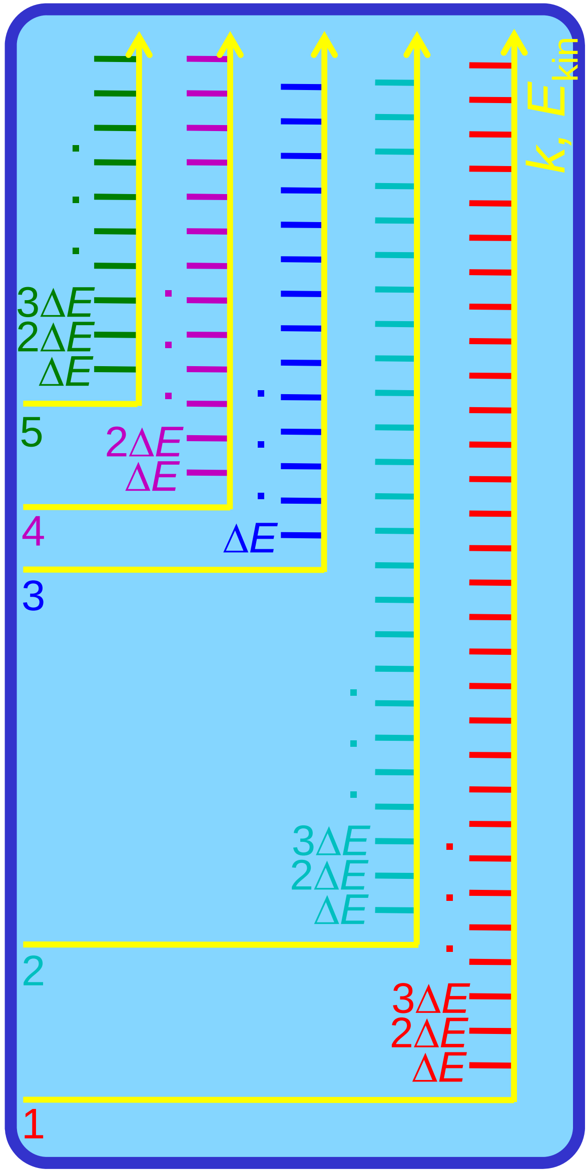
Acoustic phonons

Optical phonon absorption/emission

(polar LO / non-polar TO phonons)

Carrier-carrier scattering

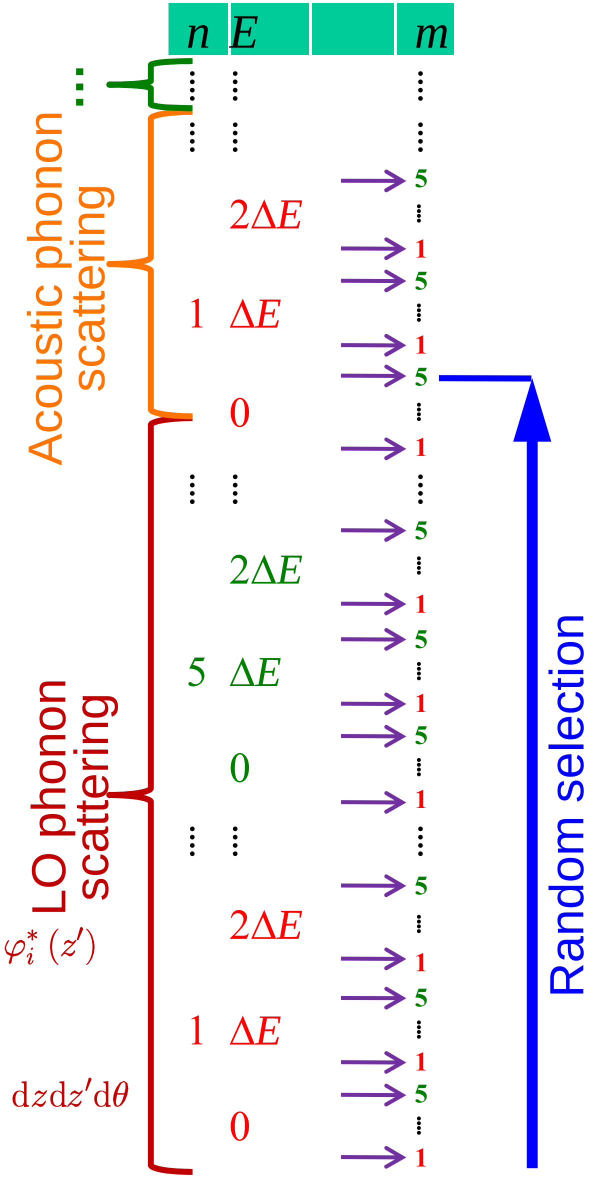
Evaluation of Scattering Rates



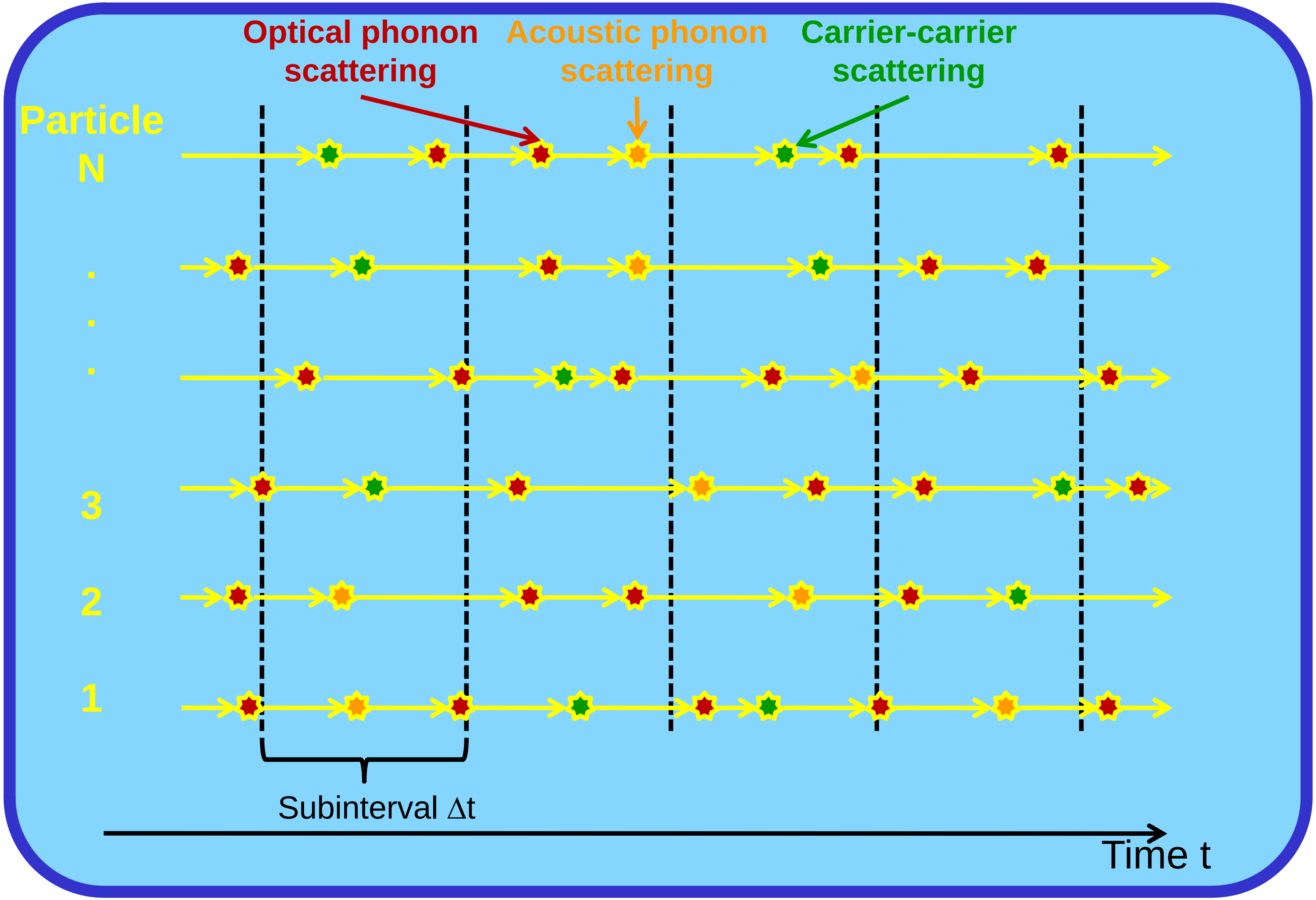
Tabulate scattering rates

$$W_{ik\to f}=\Xi^2\frac{k_BTm_f^*}{\rho v_s^2\hbar^3}\times\int_{-\infty}^{\infty}\left|\varphi_f\left(z\right)\right|^2\left|\varphi_i\left(z\right)\right|^2\mathrm{d}z$$

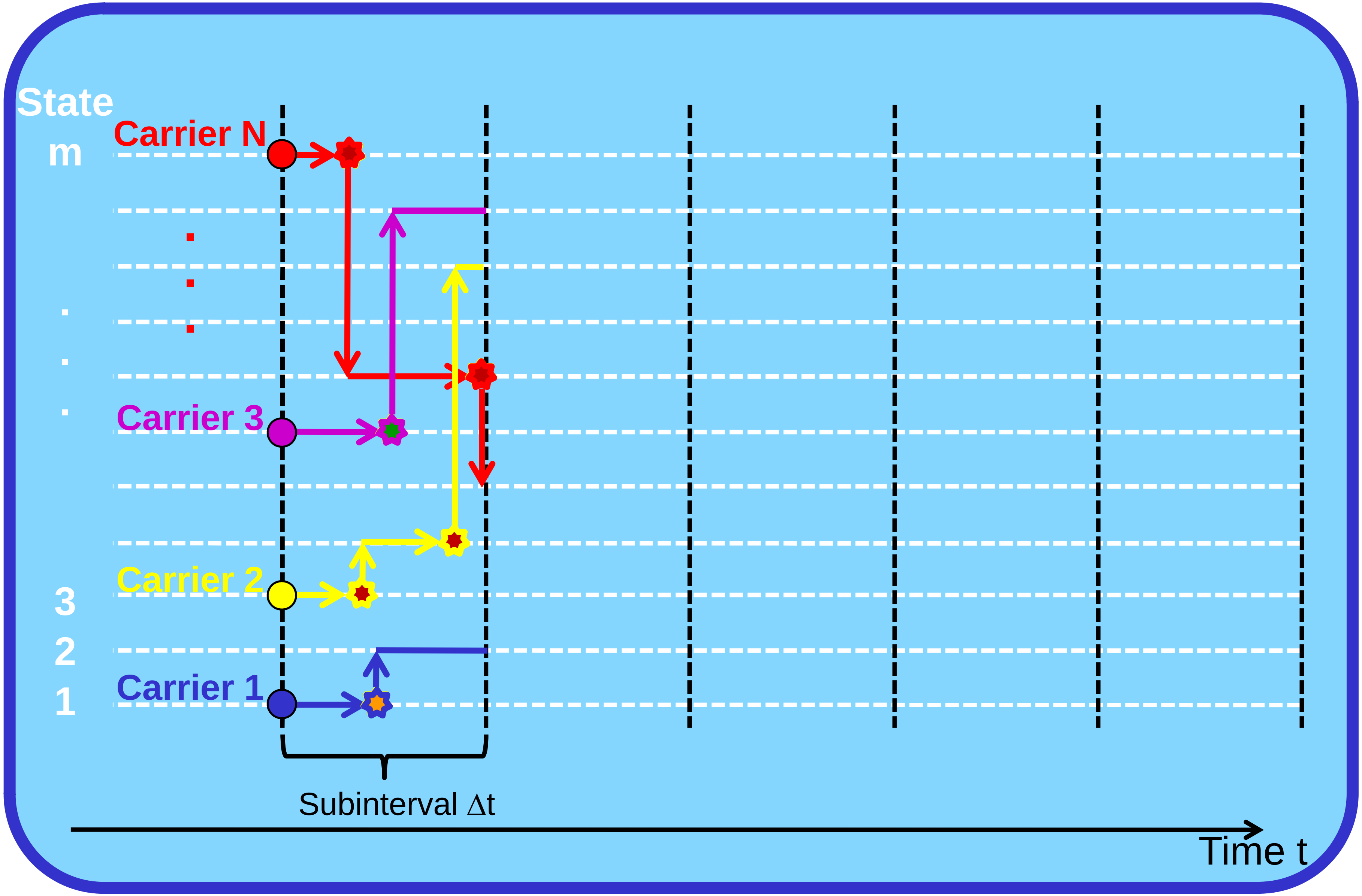
$$W_{ik\to f}^{e,a}=\frac{m_f^*\omega_{LO}e^2}{8\pi^2\hbar^2}\varepsilon_0^{-1}\left(\varepsilon_{r,\infty}^{-1}-\varepsilon_{r,0}^{-1}\right)\times\left(N_{Ph}+\frac{1}{2}\pm\frac{1}{2}\right)\times\int\limits_0^{2\pi}\iint\limits_{-\infty}^{\infty}\left[\varphi_f^*\left(z\right)\varphi_f\left(z'\right)\varphi_i\left(z\right)\varphi_i^*\left(z'\right)\times\int\limits_{-\infty}^{\infty}\frac{\left(q_z^2+q_\parallel^2\right)e^{\pm\mathrm{i}q_z(z-z')}}{\left(q_z^2+q_\parallel^2+q_s^2\right)^2}\mathrm{d}q_z\right]\mathrm{d}z\mathrm{d}z'\mathrm{d}\theta$$



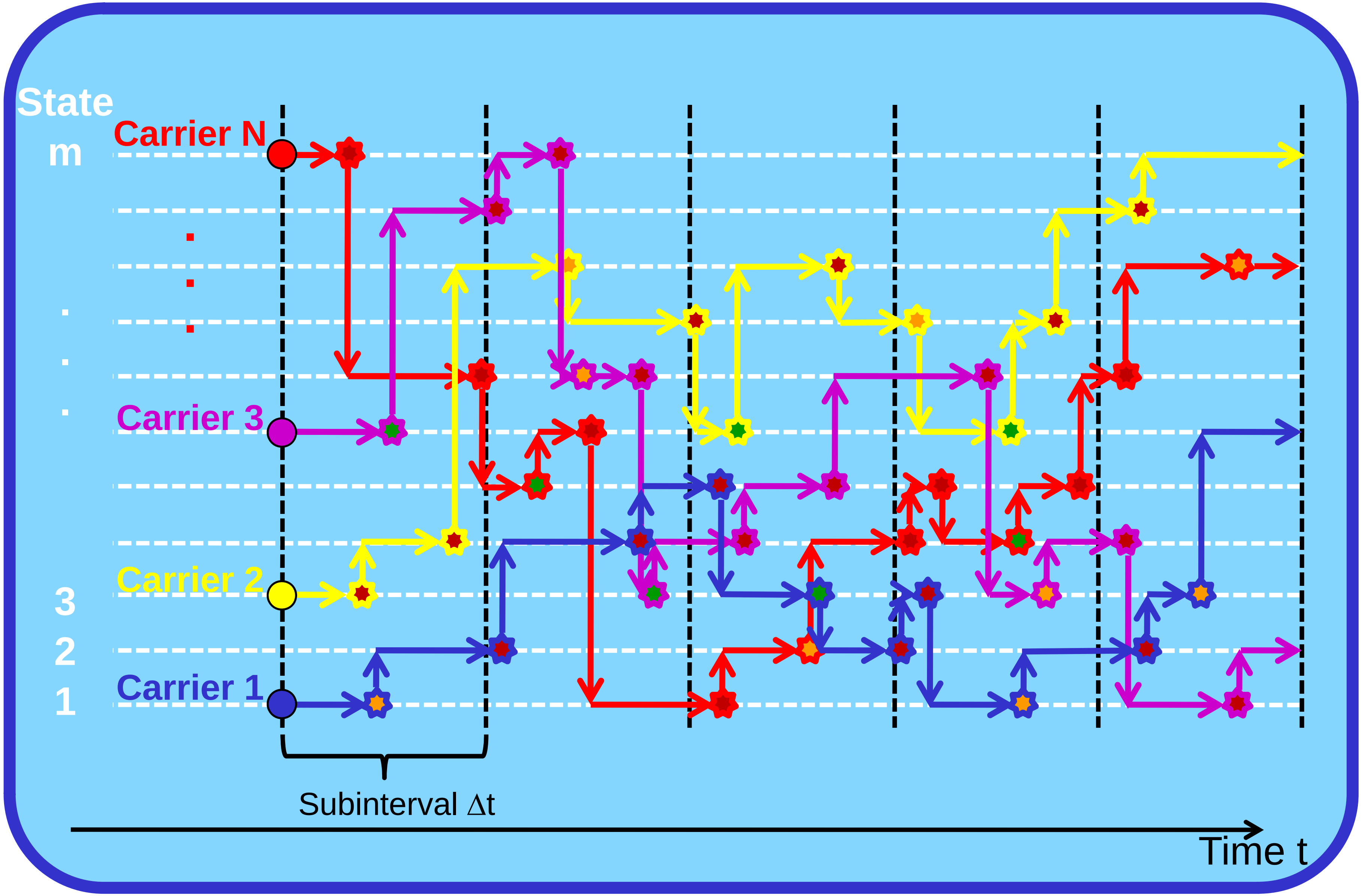
Ensemble Monte Carlo Method



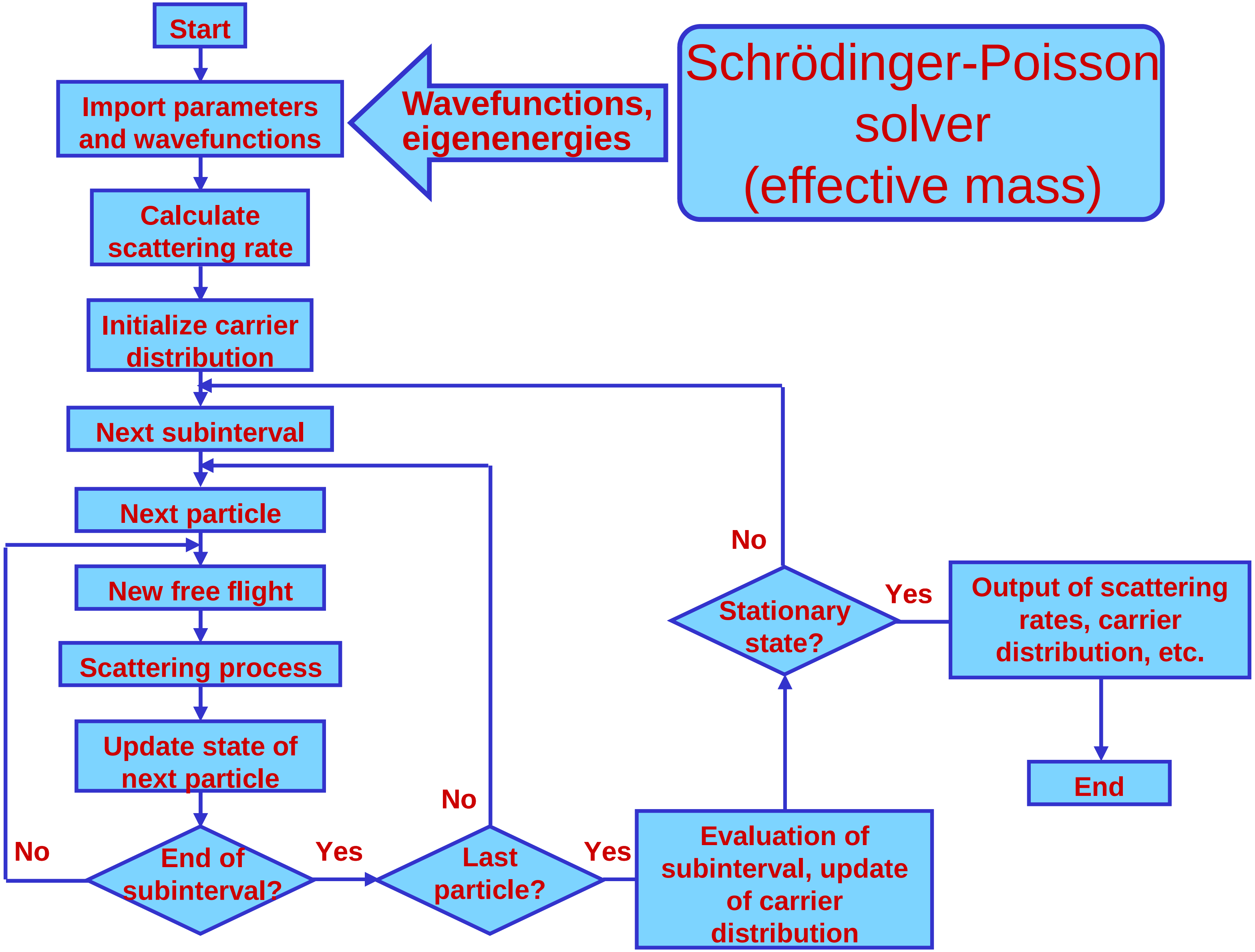
Ensemble Monte Carlo Method



Ensemble Monte Carlo Method



Monte Carlo Solver



Start

Import parameters and wavefunctions

Wavefunctions, eigenenergies

Schrödinger-Poisson solver (effective mass)

Calculate scattering rate

Initialize carrier distribution

Next subinterval

Next particle

New free flight

Scattering process

Update state of next particle

End of subinterval?

No

Yes

Last particle?

No

Yes

Evaluation of subinterval, update of carrier distribution

Stationary state?

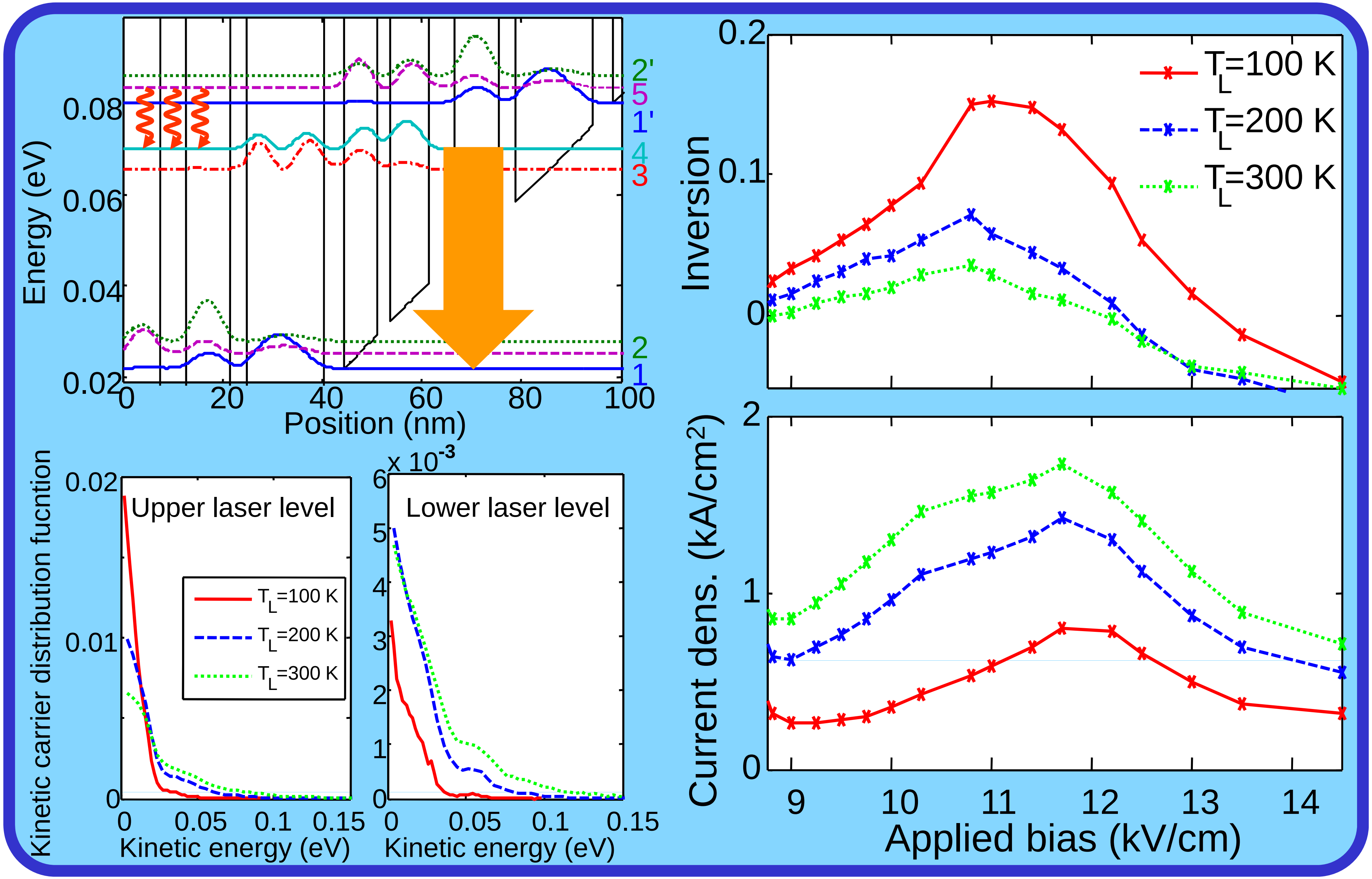
No

Yes

Output of scattering rates, carrier distribution, etc.

End

Monte Carlo Simulation - Example THz QCLs



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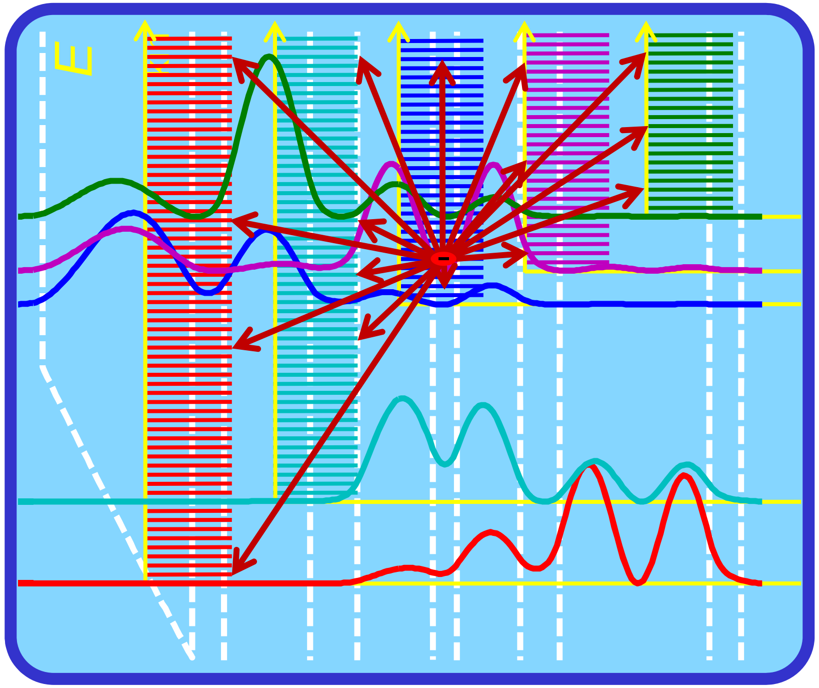
Carrier Transport Simulation Methods

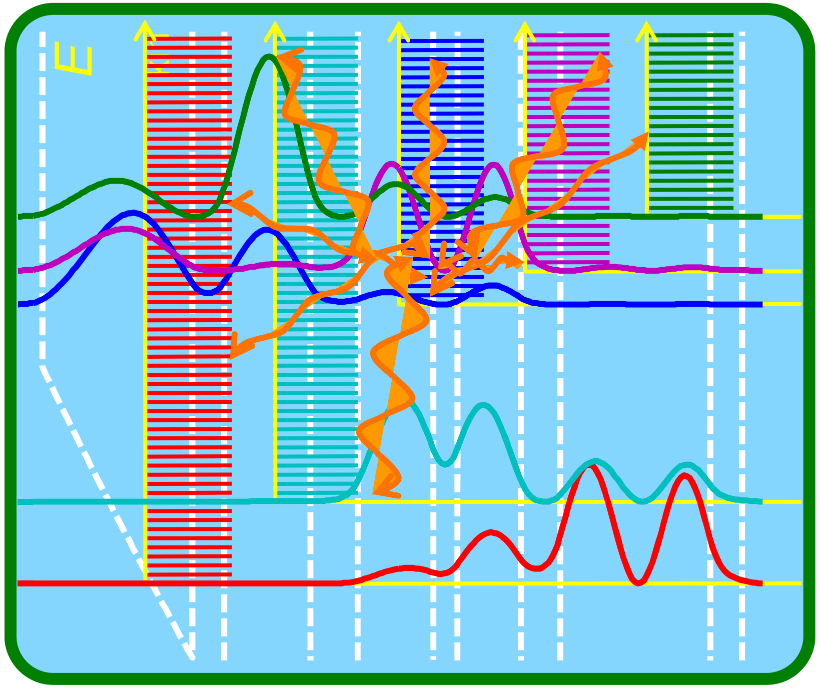
Monte Carlo method



semiclassical; no quantum correlations (e.g., dephasing)

modest computational effort

Non-equilibrium Green's function method (NEGF)

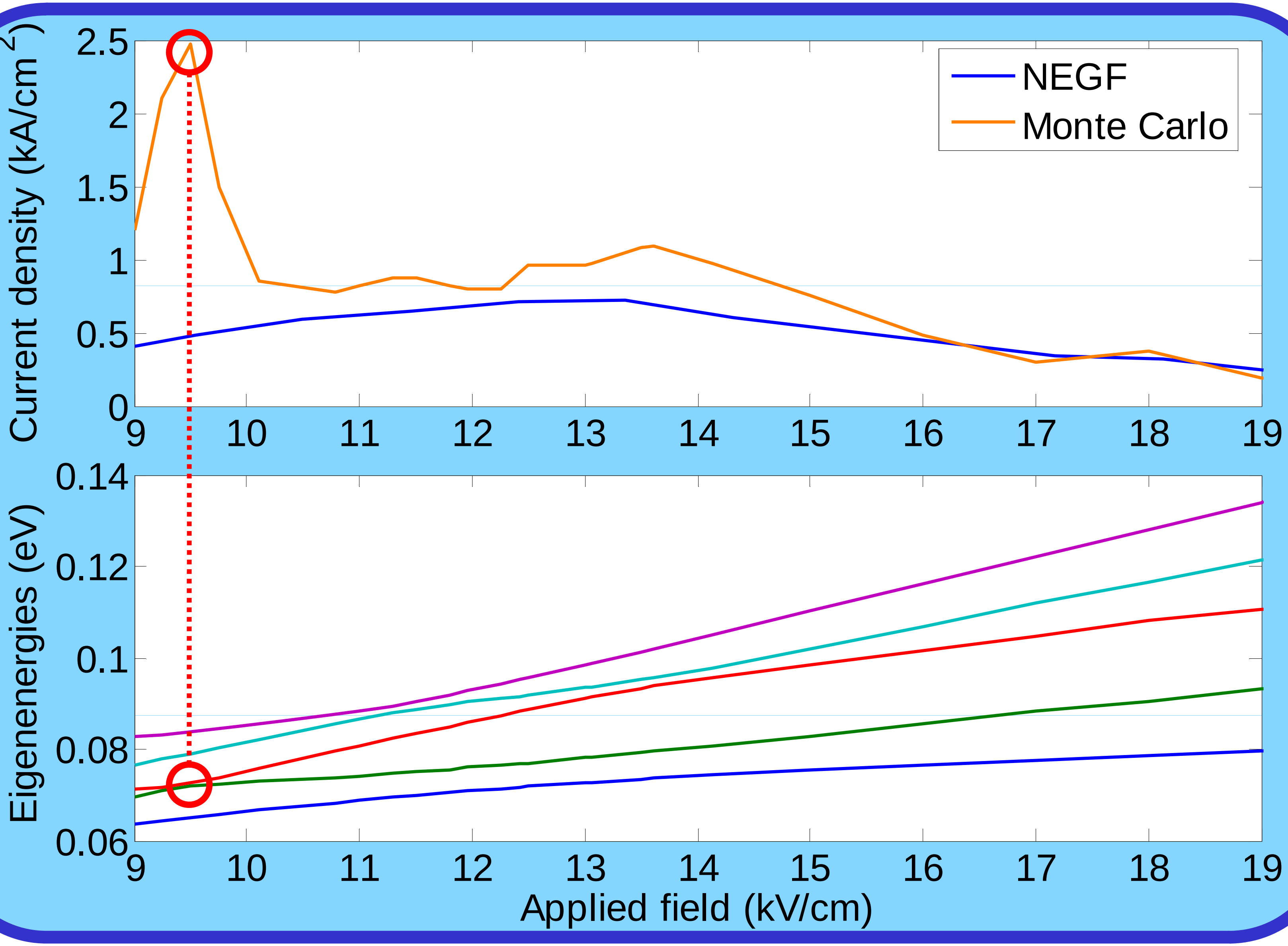


most general scheme for incoherent quantum transport

huge computational effort

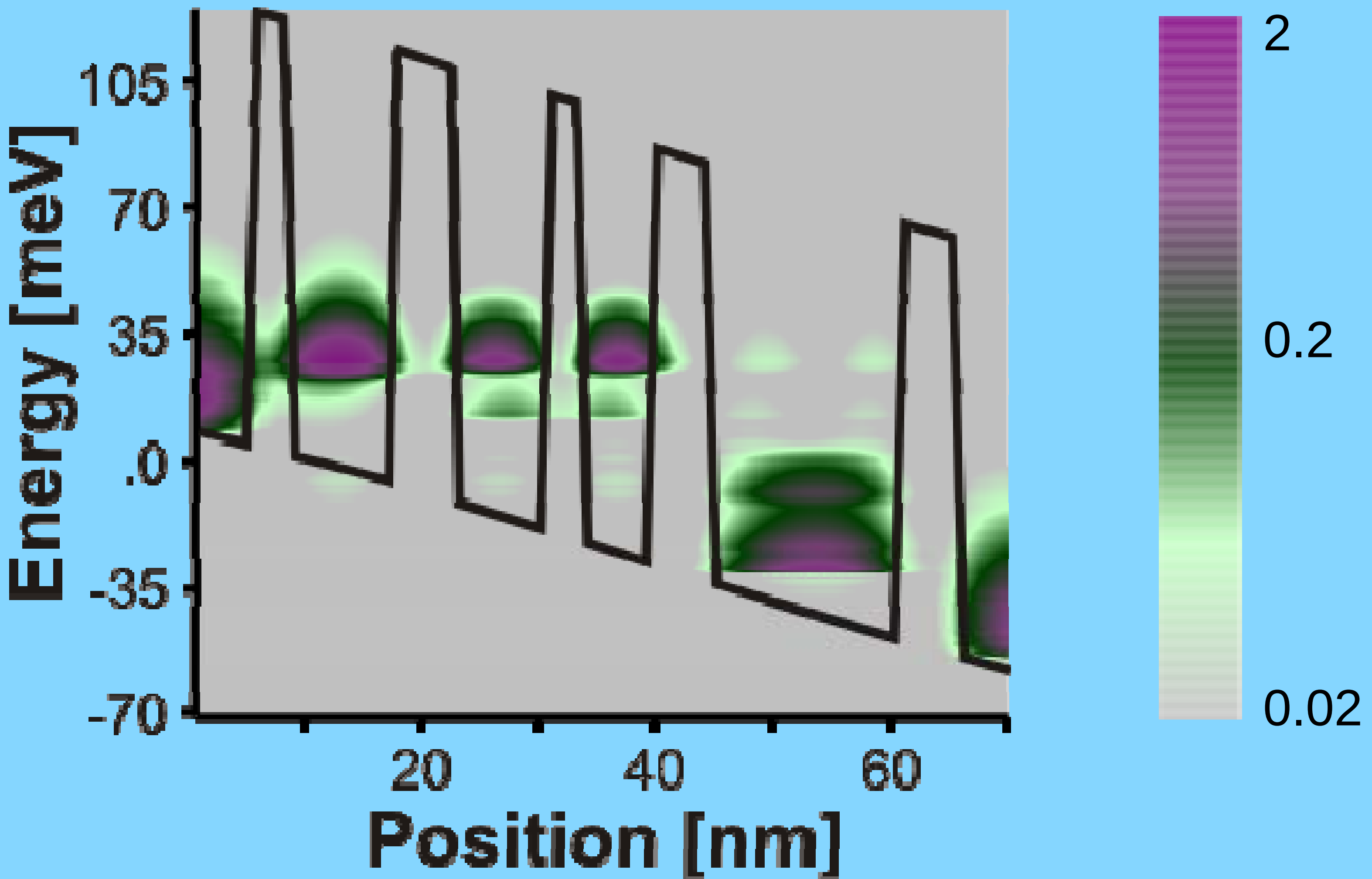
⇒ neglect e-e scattering,…

Current Density for 3.4 THz Structure (100 K)



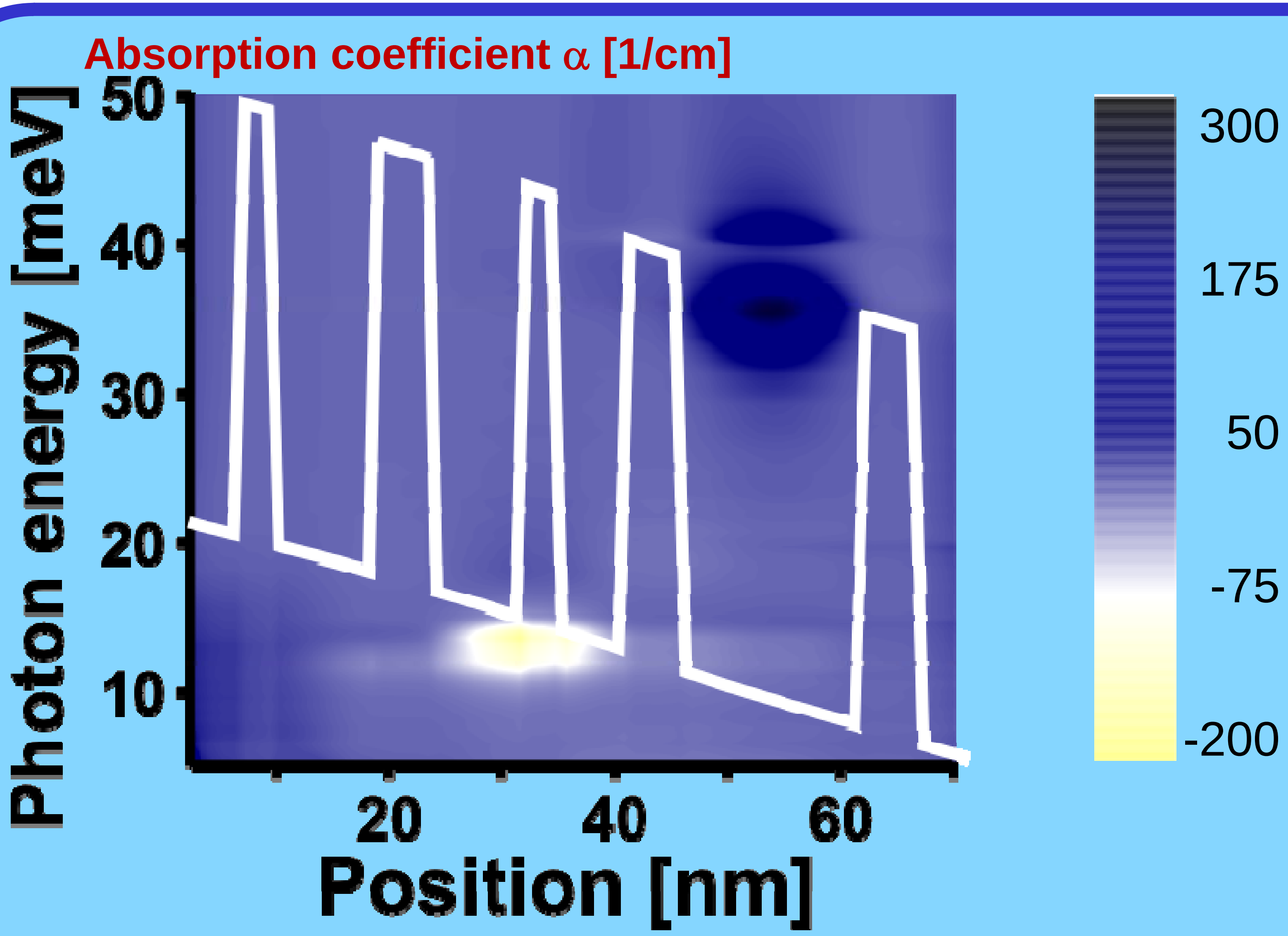
Electron Resolved Density of States

Energy resolved electron density [10^{18} cm^{-3}eV^{-1}]



T. Kubis et al., phys. stat. sol. (c) **5**, 232 (2008)

Optical Gain at Current Peak



Results (Summary)

Open two-level model

- Includes rate equation elements and quantum effects
- Description of optical instabilities/mode-locking in QCLs

C. Y. Wang et al., Phys. Rev. A **75**, 031802(R) (2007).

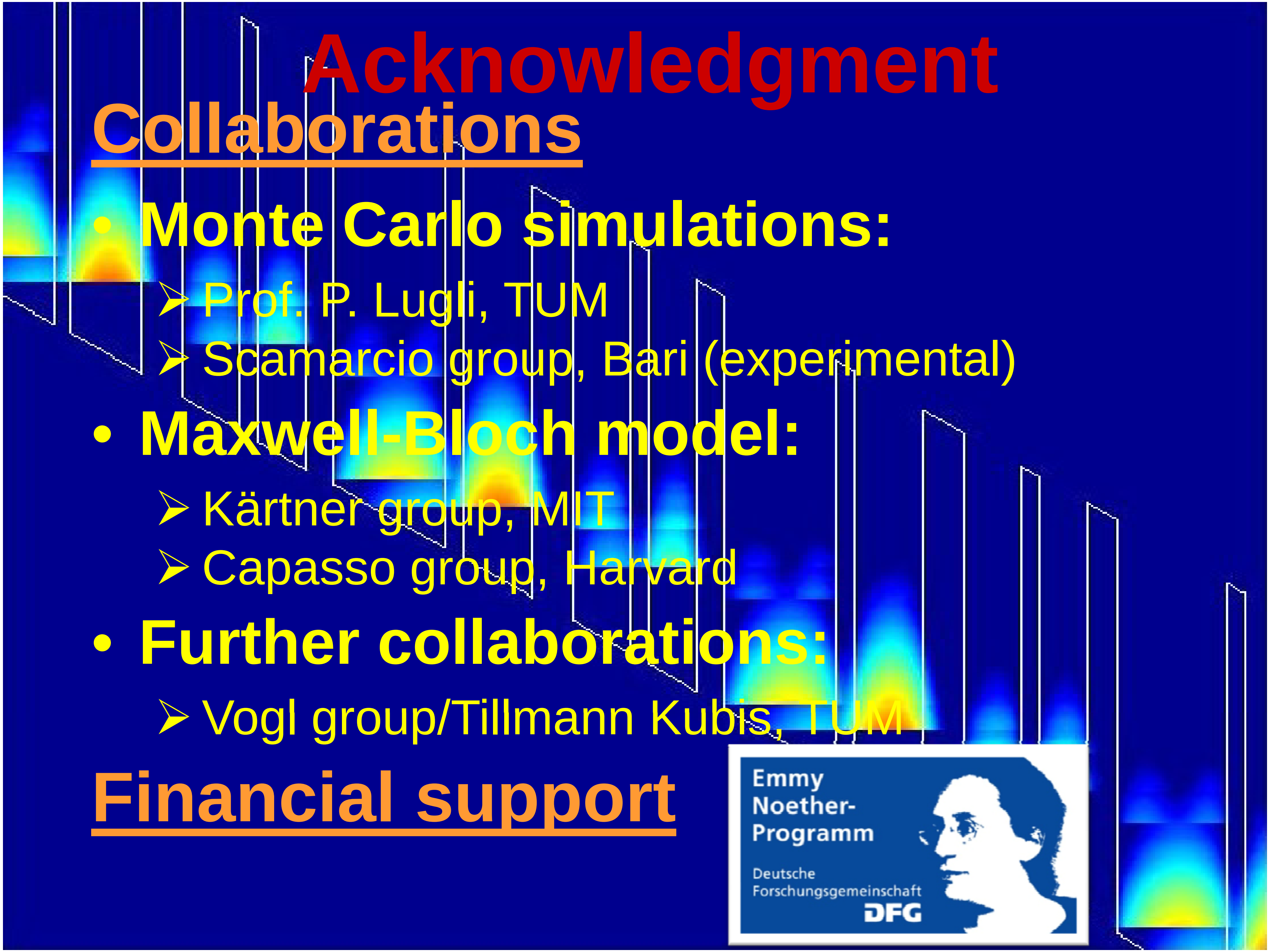
Monte Carlo simulation of QCLs

- Takes into account kinetic electron distribution
- Analysis of experimental results

C. Jirauschek et al., J. Appl. Phys. **101**, 086109 (2007);
C. Jirauschek and P. Lugli, phys. stat. sol. (c) **5**, 221 (2008);
C. Jirauschek and P. Lugli, J. Comput. Electron. **7**, 436 (2008).

Quantum transport

- Includes quantum correlations/dephasing
- Allows for simulation of spectral gain



Acknowledgment

Collaborations

- **Monte Carlo simulations:**
  - ➢ Prof. P. Lugli, TUM
  - ➢ Scamarcio group, Bari (experimental)
- **Maxwell-Bloch model:**
  - ➢ Kärtner group, MIT
  - ➢ Capasso group, Harvard
- **Further collaborations:**
  - ➢ Vogl group/Tillmann Kubis, TUM

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