



Electron-phonon interaction. Can dispersionless phonons provide relaxation?

P. Gartner , J. Seebeck, F. Jahnke

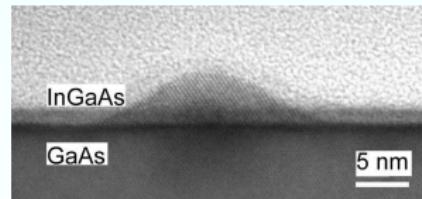
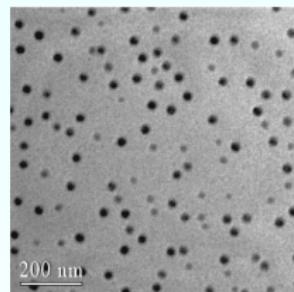
Institute for Theoretical Physics
University of Bremen

Kiel, 2010



Introduction

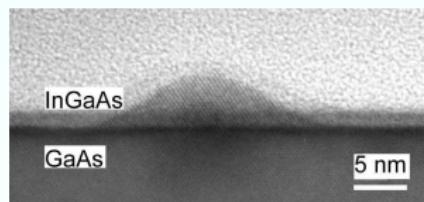
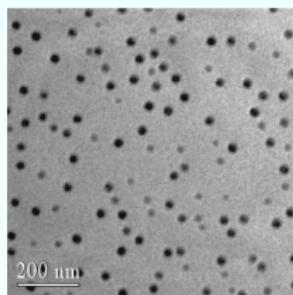
Self-assembled quantum dots



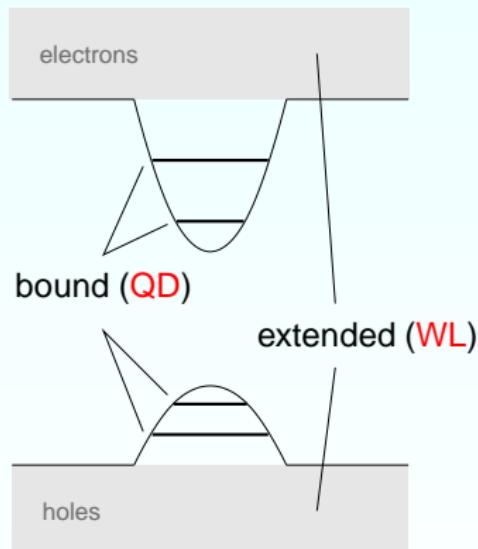
S. Anders et al., Phys. Rev. B **66**, 125309 (2002)

Introduction

Self-assembled quantum dots



Energy spectrum



S. Anders et al., Phys. Rev. B **66**, 125309 (2002)

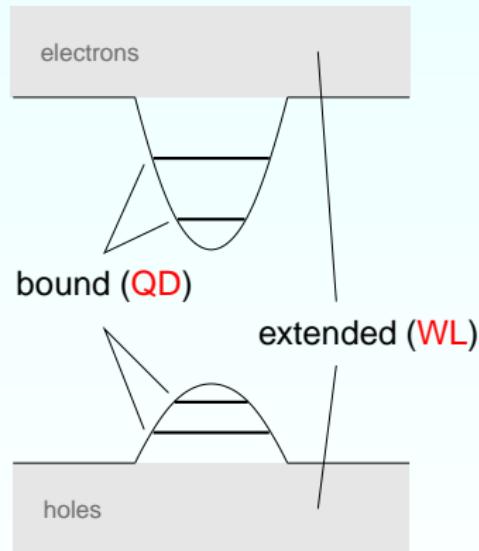
Introduction

Discrete spectrum

- important for optoelectronics
- controlled by quantum dot geometry

Carrier kinetics

Energy spectrum



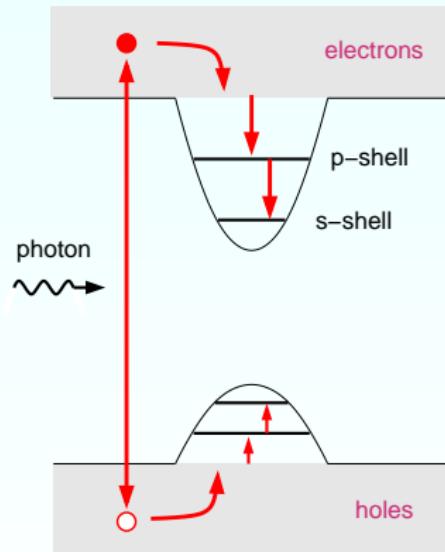
Introduction

Discrete spectrum

- important for optoelectronics
- controlled by quantum dot geometry

Carrier kinetics

Capture and relaxation



Introduction

Low carrier densities

- carrier-carrier scattering negligible
- carrier-LO-phonon interaction dominant

Perturbation theory:

- capture and relaxation prevented
phonon bottleneck

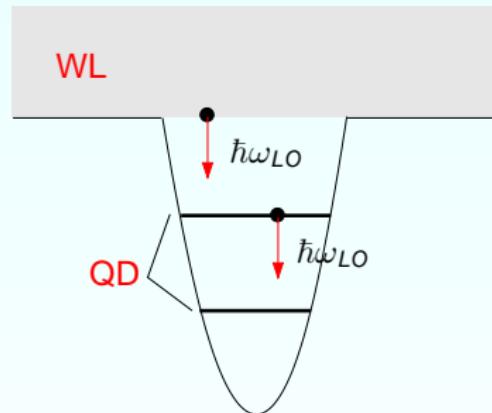
Introduction

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phonon bottleneck



U.Bockelmann, G. Bastard, PRB **42**, 8947 (1990)

H. Benisty *et al.*, PRB **44**, 10945 (1991)

Introduction

Experiment:

fast (ps) capture and relaxation

Introduction

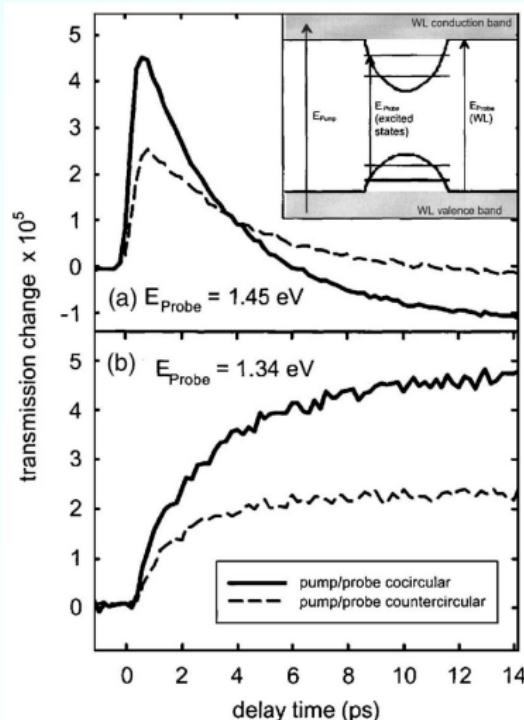
Experiment:

fast (ps) capture and relaxation

Example:

S. Trumm et al. APL **87**, 153113 (2005)

- rapid relaxation inside wetting layer
- rapid transfer to bound states
- characteristic times (ps) independent of excitation power



Outline

- Boltzmann kinetics
 - relaxation properties, in general and with dispersionless LO-phonons
- Carrier-phonon system in equilibrium
 - carrier renormalization \implies the polaron
- Quantum kinetics
 - 2-time quantum kinetics
 - 1-time approximation
- Results (QWs and QDs)
- Numerical difficulties

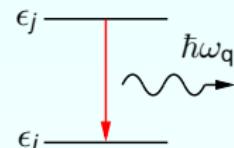
Boltzmann kinetics

Carrier-phonon Hamiltonian:

$$H = \sum_i \epsilon_i a_i^\dagger a_i + \sum_{\mathbf{q}} \hbar \omega_{\mathbf{q}} b_{\mathbf{q}}^\dagger b_{\mathbf{q}} + \sum_{i,j,\mathbf{q}} M_{i,j}(\mathbf{q}) a_i^\dagger a_j (b_{\mathbf{q}} + b_{-\mathbf{q}}^\dagger)$$

$$\omega_{\mathbf{q}} = \omega_{LO}, \quad M_{i,j}(\mathbf{q}) = g_{\mathbf{q}} \langle \varphi_i | e^{i\mathbf{q}\mathbf{r}} | \varphi_j \rangle$$

$$g_q^2 \propto \alpha \frac{1}{q^2} \quad \text{Fröhlich coupling}$$



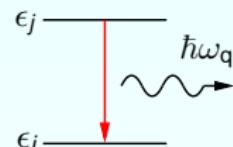
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Time evolution of population $f_i = \langle a_i^\dagger a_i \rangle$:

$$\frac{\partial f_i}{\partial t} = \sum_j \{ W_{i,j}(1-f_i)f_j - W_{j,i}(1-f_j)f_i \}$$

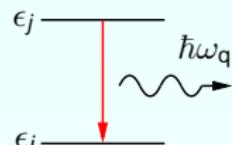
Boltzmann kinetics

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Time evolution of population $f_i = \langle a_i^\dagger a_i \rangle$:

$$\frac{\partial f_i}{\partial t} = \sum_j \{ W_{i,j}(1 - f_j) f_j - W_{j,i}(1 - f_i) f_i \}$$

$W_{i,j}$ = **Golden Rule** transition rate $j \longrightarrow i$:

$$W_{i,j} = \frac{2\pi}{\hbar} \sum_{\mathbf{q}} |M_{i,j}(\mathbf{q})|^2 \{ N_{\mathbf{q}} \delta(\epsilon_i - \epsilon_j - \hbar\omega_{\mathbf{q}}) + (N_{\mathbf{q}} + 1) \delta(\epsilon_i - \epsilon_j + \hbar\omega_{\mathbf{q}}) \}$$

Boltzmann kinetics

Relaxation properties (analytic):

- conserves positivity:

$$f_i(0) \geq 0 \implies f_i(t) \geq 0$$

- stationary solution:

$$f_i(t) = 1/[e^{\beta(\epsilon_i - \mu)} + 1] = F(\epsilon_i)$$

- for any $f_i(0) \geq 0$

$$f_i(t) \longrightarrow F(\epsilon_i) \quad \text{as} \quad t \longrightarrow \infty$$

provided all states can be connected using paths with nonzero transition rates.

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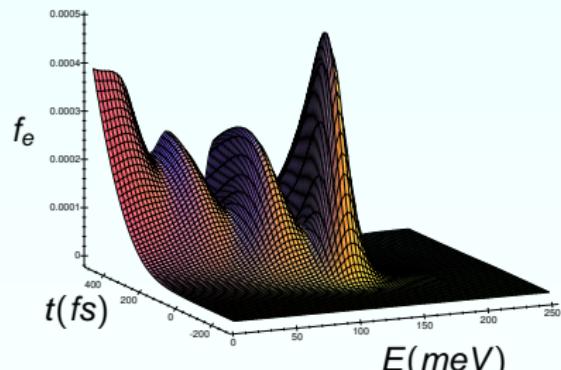
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LO-phonons + continuous spectrum (QW)



phonon cascade

Boltzmann kinetics

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$$f_i(0) \geq 0 \implies f_i(t) \geq 0$$

- stationary solution:

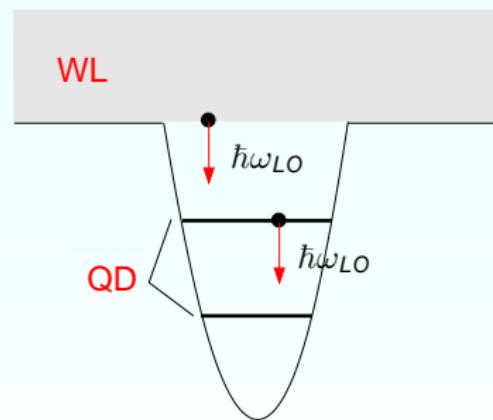
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LO-phonons in quantum dots



phonon bottleneck

Boltzmann kinetics

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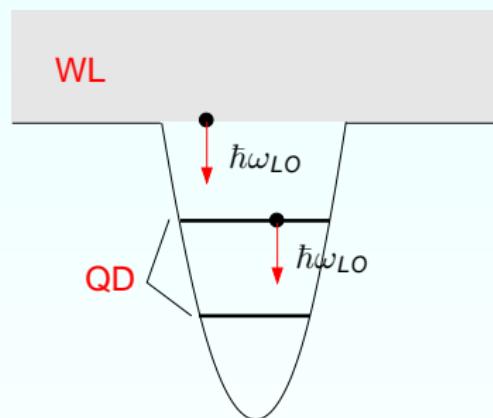
$$f_i(t) \longrightarrow F(\epsilon_i) \quad \text{as} \quad t \longrightarrow \infty$$

provided all states can be connected using paths with nonzero transition rates.

Proposed solutions:

- LO+LA: T.Inoshita, H.Sakaki, PRB.**46**, 7260 (1992)
- LO+LO: A. Knorr group (Berlin) in press

LO-phonons in quantum dots



phonon bottleneck

Boltzmann vs. quantum kinetics

Experiment: fast capture and relaxation (ps)

Boltzmann kinetics:

- weak coupling
- slow evolution
- long time
- no memory (Markovian)

Boltzmann vs. quantum kinetics

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Quantum kinetics:

- strong coupling
- fast evolution
- both early and later times
- memory effects included

Boltzmann vs. quantum kinetics

Experiment: fast capture and relaxation (ps)

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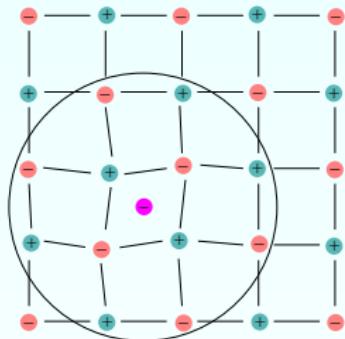
Quantum kinetics:

- strong coupling
- fast evolution
- both early and later times
- memory effects included

Relaxation properties (numeric)

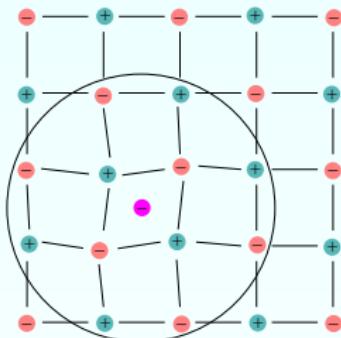
- is a steady state reached ?
- steady state = thermal equilibrium ?

Polarons



electron polarizes crystal

Polarons



free carrier retarded GF

$$G_{\alpha}^R(t) = \frac{\theta(t)}{i\hbar} e^{-\frac{i}{\hbar}\epsilon_{\alpha}t}$$

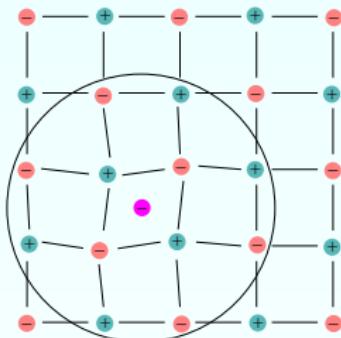
$$G_{\alpha}^R(\omega) = \frac{1}{\hbar\omega - \epsilon_{\alpha} + i\delta}$$

electron polarizes crystal

spectral function

$$\begin{aligned}\hat{G}_{\alpha}(\omega) &= -2\text{Im } G_{\alpha}^R(\omega) \\ &= 2\pi \delta(\hbar\omega - \epsilon_{\alpha})\end{aligned}$$

Polarons



electron polarizes crystal

free carrier retarded GF

$$G_{\alpha}^R(t) = \frac{\theta(t)}{i\hbar} e^{-\frac{i}{\hbar}\epsilon_{\alpha}t}$$

polaron retarded GF

$$G_{\alpha}^R(\omega) = \frac{1}{\hbar\omega - \epsilon_{\alpha} + \Sigma_{\alpha}^R(\omega)}$$

$$G_{\alpha}^R(\omega) = \frac{1}{\hbar\omega - \epsilon_{\alpha} + i\delta}$$

$\Sigma_{\alpha}^R(\omega)$ self-energy for carrier-phonon interaction

spectral function

$$\hat{G}_{\alpha}(\omega) = ?$$

$$\begin{aligned}\hat{G}_{\alpha}(\omega) &= -2\text{Im } G_{\alpha}^R(\omega) \\ &= 2\pi \delta(\hbar\omega - \epsilon_{\alpha})\end{aligned}$$

Quantum well polaron

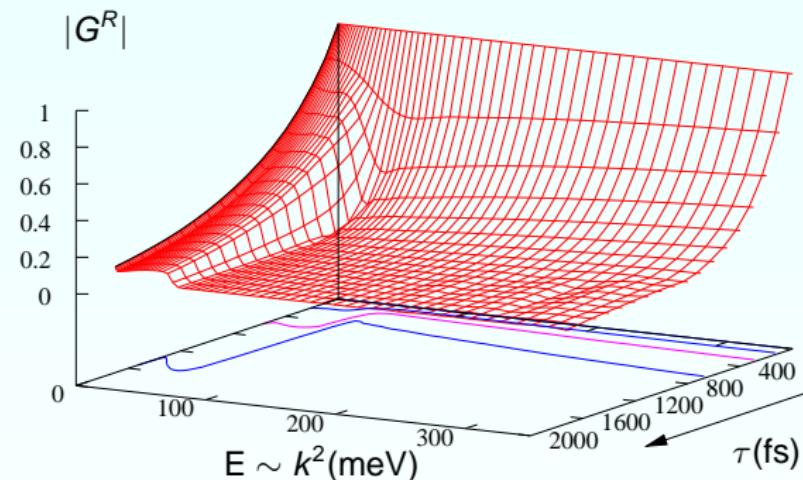
Self-consistent Random Phase Approximation

$$\left\{ i\hbar \frac{\partial}{\partial \tau} - \epsilon_k \right\} G_k^R(\tau) =$$

$$= \int_0^\tau d\tau' \Sigma_k^R(\tau') G_k^R(\tau - \tau')$$

$$\Sigma = \begin{array}{c} \text{dashed arc} \\ \text{--- real axis} \end{array}$$

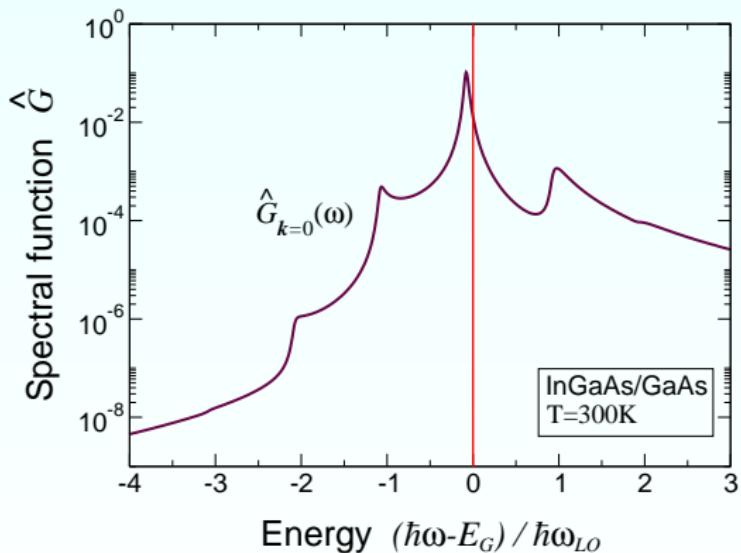
- ☞ arbitrary order in α
- ☞ multi-phonon processes



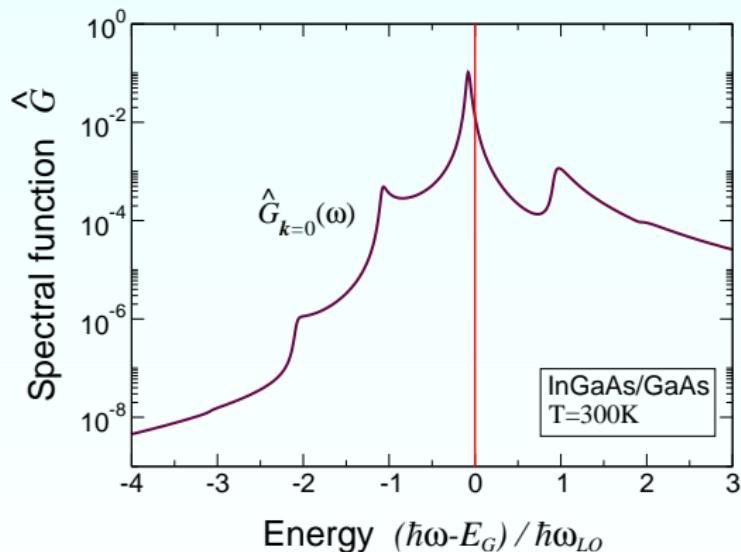
GaAs at $T = 300K$

$$\alpha = 0.06, \quad \hbar\omega_{LO} = 36 \text{ meV}$$

Quantum well polaron



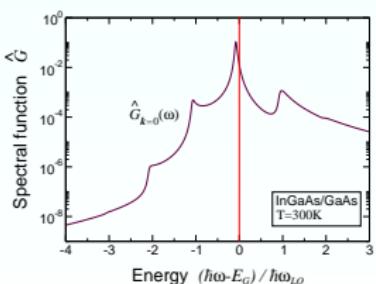
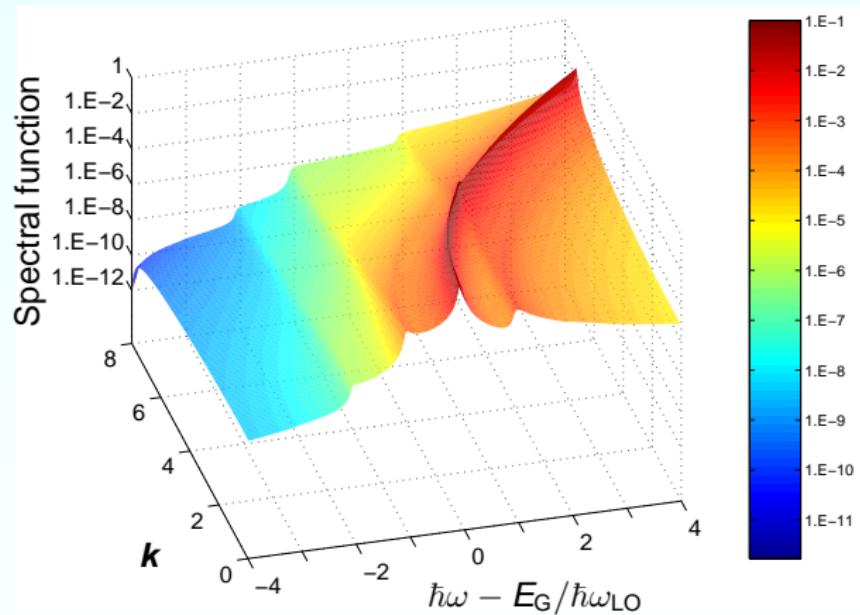
Quantum well polaron



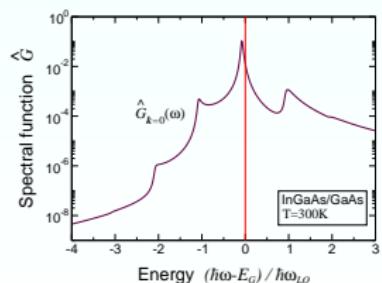
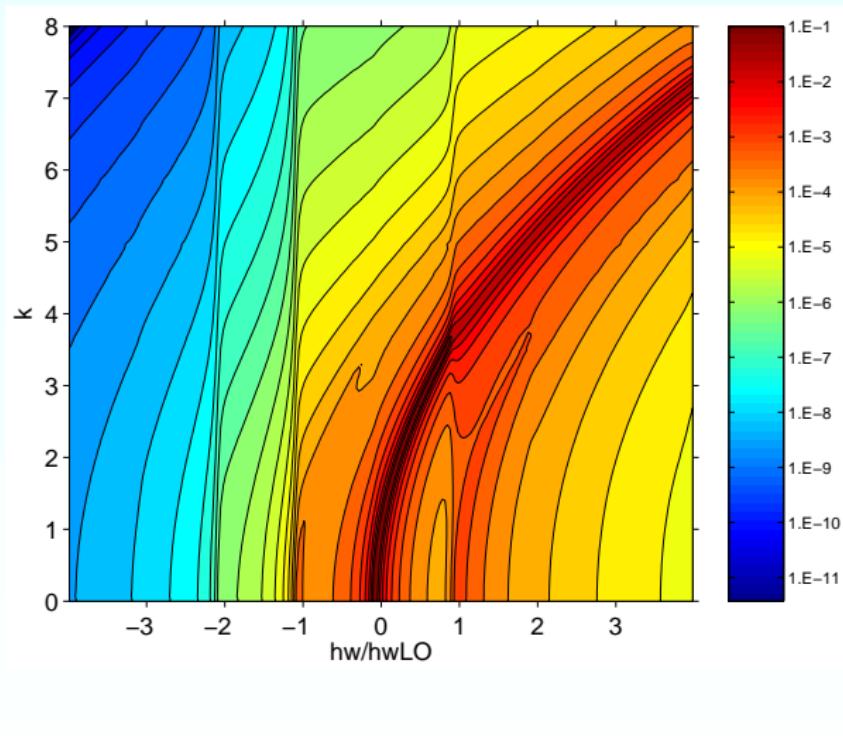
polaron shift
energy broadening
phonon satellites

J. Seebeck, T.R. Nielsen, P. Gartner, F. Jahnke, Phys. Rev. B **71**, 125327 (2005)

Quantum well polaron



Quantum well polaron



Quantum dot polaron

LO-phonons + quantum dot states only

- Self-consistent Random Phase Approximation

- T.Inoshita, H.Sakaki, PRB **56**, 2061 (1998)
- K.Král, Z.Khás, PRB **57**, 4355 (1998)

- finite number of phonons \implies diagonalization

- O.Verzelen, R.Fereira, G.Bastard, PRB **62**, 4809 (2000)
- T.Stauber, R.Zimmermann, H. Castella, PRB **62**, 7336 (2000)

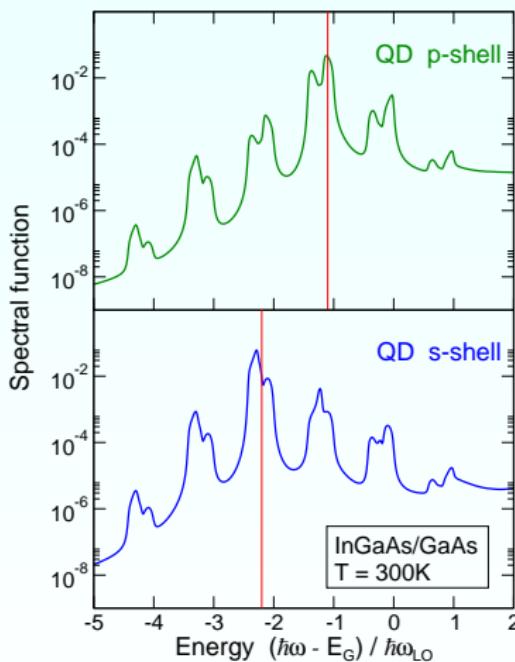
BUT wetting layer states important for both kinetics and spectrum

Quantum dot polaron

LO-phonons + quantum dot + wetting layer states

Quantum dot polaron

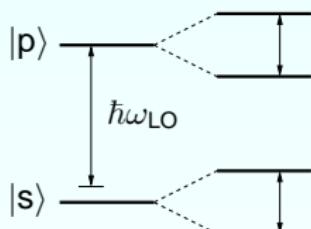
LO-phonons + quantum dot + wetting layer states



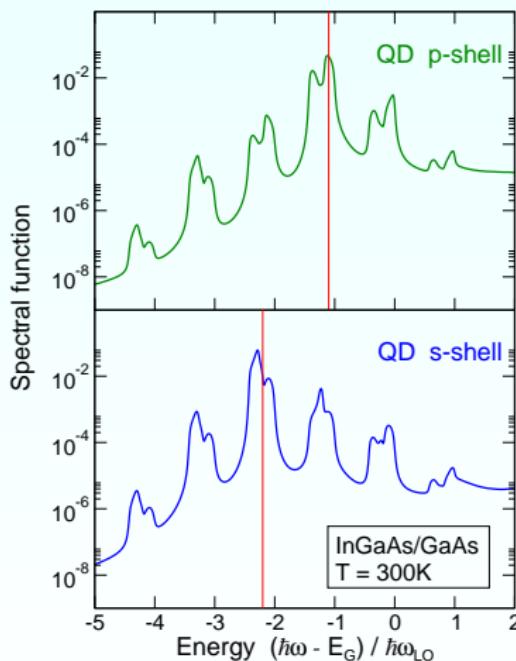
$$\Delta E = 1.1 \hbar\omega_{LO}$$

Quantum dot polaron

LO-phonons + quantum dot + wetting layer states



Hybridization



$$\Delta E = 1.1 \hbar\omega_{\text{LO}}$$

Quantum kinetics

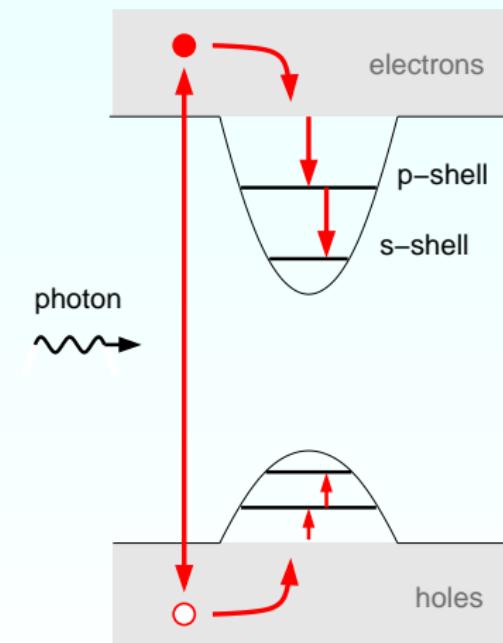
Quantity of interest:

$$\rho_\alpha(t) = \begin{pmatrix} f_\alpha^e(t) & \psi_\alpha(t) \\ \psi_\alpha^*(t) & 1 - f_\alpha^h(t) \end{pmatrix} = -i\hbar G_\alpha^<(t, t)$$

2x2 matrix in the band index, $\alpha = \mathbf{k}, s, p$

Methods:

- Equation of Motion **X**
 - hierarchy problem
- Nonequilibrium Green's Functions **✓**
 - polaronic effects
 - **2-time** quantities



Quantum kinetics

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Methods:

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Nonequilibrium Green's Functions

Closed Equations for

$$G(\mathbf{t}_1, \mathbf{t}_2) = \frac{1}{i\hbar} \left\langle T \left[\psi(\mathbf{t}_1) \psi^\dagger(\mathbf{t}_2) \right] \right\rangle$$

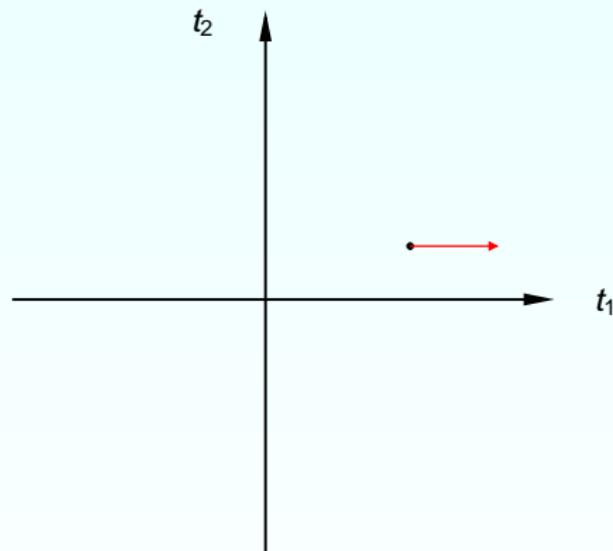
Procedure:

- solve for $G_\alpha(\mathbf{t}_1, \mathbf{t}_2)$
- recover physical data from the **time-diagonal** $\mathbf{t}_1 = \mathbf{t}_2$

Quantum kinetics 2-time

Kadanoff-Baym equations:

$$\left\{ i\hbar \frac{\partial}{\partial t_1} - H_0(1) \right\} G_\alpha(t_1, t_2) = \\ = \{\Sigma \cdot G\}_\alpha(t_1, t_2)$$



Quantum kinetics 2-time

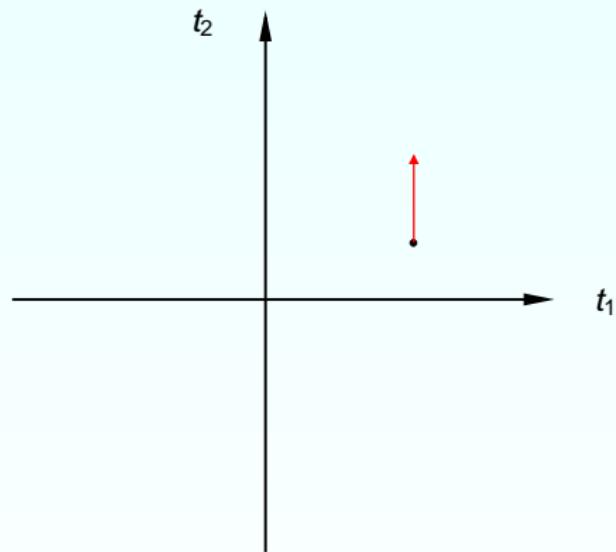
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$$= \{\Sigma \cdot G\}_\alpha(t_1, t_2)$$

$$\left\{ i\hbar \frac{\partial}{\partial t_2} + H_0(2) \right\} G_\alpha(t_1, t_2) =$$

$$= -\{G \cdot \Sigma\}_\alpha(t_1, t_2)$$



Quantum kinetics 2-time

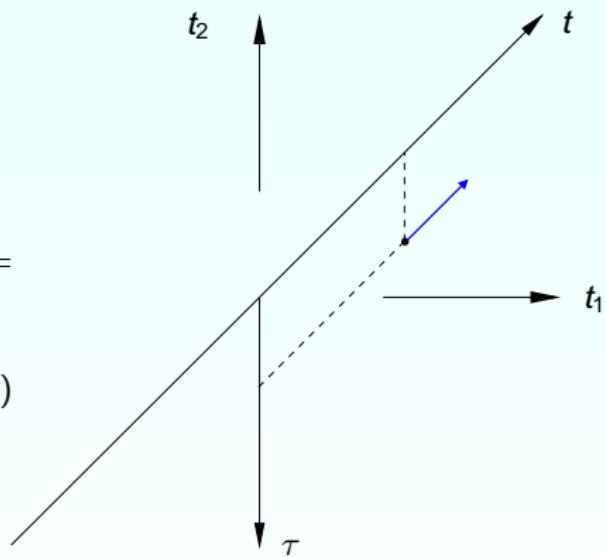
Reparametrize:

$$(t_1, t_2) = (t, t - \tau)$$

t - main time τ - relative time

$$\left\{ i\hbar \frac{\partial}{\partial t} - H_0(1) + H_0(2) \right\} G_\alpha(t, t - \tau) =$$

$$= \{\Sigma \cdot G\}_\alpha(t, t - \tau) - \{G \cdot \Sigma\}_\alpha(t, t - \tau)$$

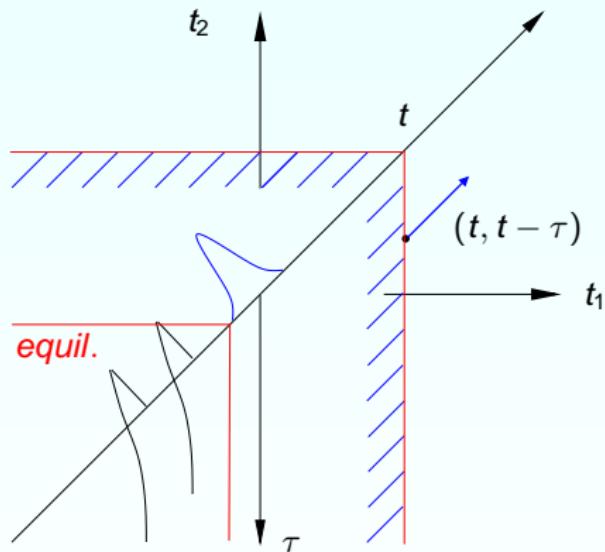


Quantum kinetics 2-time

Polaronic Green's Function:

$$G_{\alpha}^R(t, t - \tau) = G_{\alpha}^R(\tau)$$

- “initial” condition
- natural memory cutoff



Quantum kinetics 2-time

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} G_{\mathbf{k}}^{R,<}(t, t - \tau) &= \Sigma_{\mathbf{k}}^{\delta}(t) G_{\mathbf{k}}^{R,<}(t, t - \tau) - G_{\mathbf{k}}^{R,<}(t, t - \tau) \Sigma_{\mathbf{k}}^{\delta}(t - \tau) + \\ &\quad + i\hbar \frac{\partial}{\partial t} G_{\mathbf{k}}^{R,<}(t, t - \tau) \Big|_{coll} ; \quad \tau \geq 0 \end{aligned}$$

Instantaneous self-energy:

$$\Sigma_{\mathbf{k}}^{\delta}(t) = \begin{pmatrix} \epsilon_{\mathbf{k}}^c & -\mathbf{d}_{cv} \cdot \mathbf{E}(t) \\ -\mathbf{d}_{vc} \cdot \mathbf{E}(t) & \epsilon_{\mathbf{k}}^v \end{pmatrix}$$

The optical excitation connects the two bands.

Quantum kinetics 2-time

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} G_{\mathbf{k}}^{R,<} (t, t - \tau) &= \Sigma_{\mathbf{k}}^{\delta}(t) G_{\mathbf{k}}^{R,<} (t, t - \tau) - G_{\mathbf{k}}^{R,<} (t, t - \tau) \Sigma_{\mathbf{k}}^{\delta}(t - \tau) + \\ &\quad + i\hbar \frac{\partial}{\partial t} G_{\mathbf{k}}^{R,<} (t, t - \tau) \Big|_{coll} ; \quad \tau \geq 0 \end{aligned}$$

RPA self-energies:



$$\Sigma_{\mathbf{k}}^R(t, t') = i\hbar \sum_{\mathbf{q}} g_{\mathbf{q}}^2 \left[D^>(t - t') G_{\mathbf{k}-\mathbf{q}}^R(t, t') + D^R(t - t') G_{\mathbf{k}-\mathbf{q}}^<(t, t') \right]$$

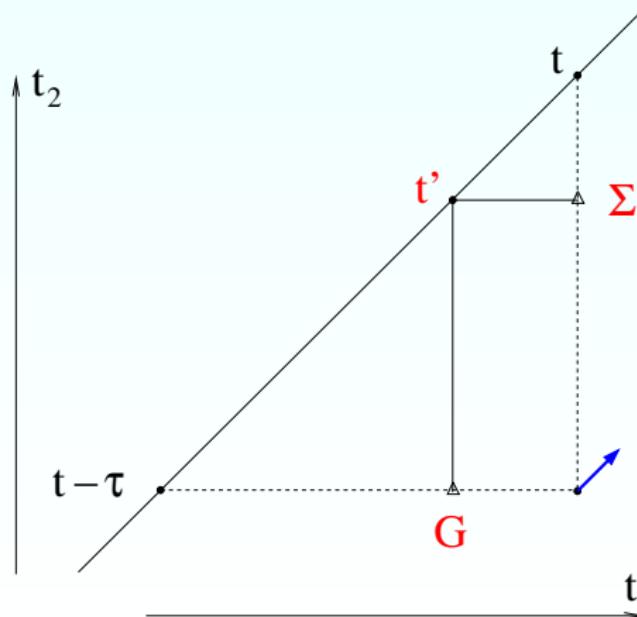
$$\Sigma_{\mathbf{k}}^<(t, t') = i\hbar \sum_{\mathbf{q}} g_{\mathbf{q}}^2 D^<(t - t') G_{\mathbf{k}-\mathbf{q}}^<(t, t')$$

$$i\hbar D^>(\tau) = (N_{LO} + 1) e^{-i\hbar\omega_{LO}\tau} + N_{LO} e^{i\hbar\omega_{LO}\tau} = i\hbar D^<(-\tau)$$

Quantum kinetics 2-time

Collision terms for G^R :

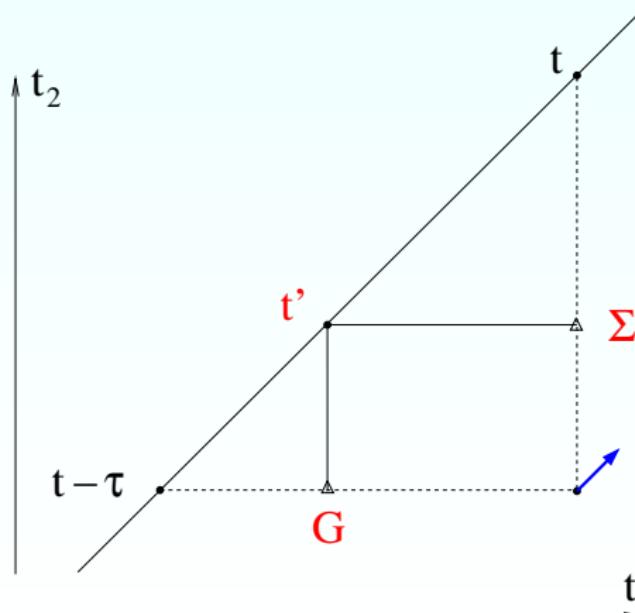
$$i\hbar \frac{\partial}{\partial t} G_{\mathbf{k}}^R(t, t - \tau) \Big|_{coll} = \int_{t-\tau}^t dt' \left[\Sigma_{\mathbf{k}}^R(t, t') G_{\mathbf{k}}^R(t', t - \tau) - G_{\mathbf{k}}^R(t, t') \Sigma_{\mathbf{k}}^R(t', t - \tau) \right]$$



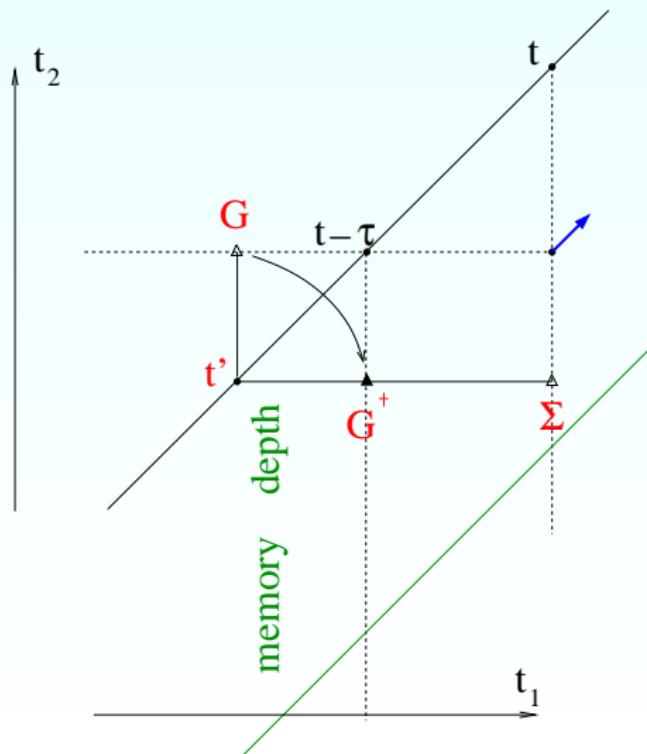
Quantum kinetics 2-time

Collision terms for G^R :

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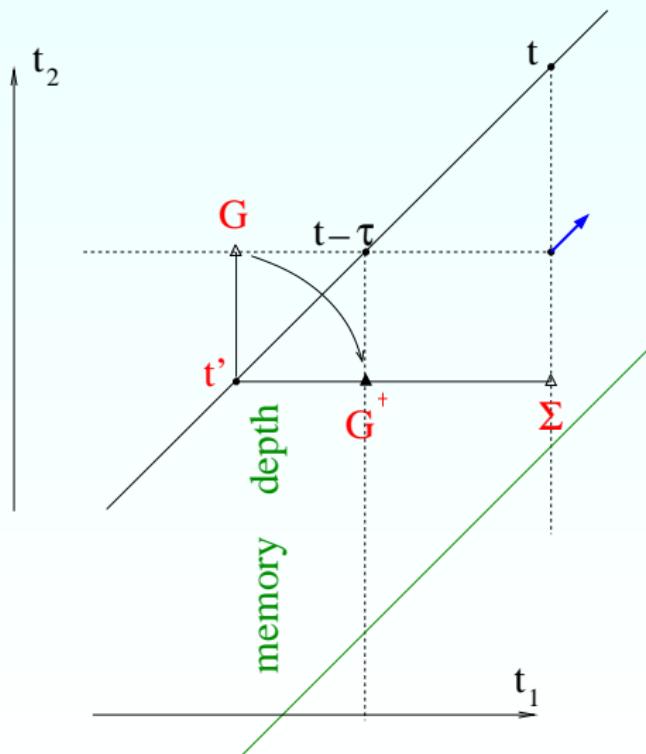


Quantum kinetics 2-time

Collision terms for $G^<$:

$$\left. i\hbar \frac{\partial}{\partial t} G_{\mathbf{k}}^<(t, t - \tau) \right|_{coll} = \int_{-\infty}^t dt' \left[\Sigma_{\mathbf{k}}^R(t, t') G_{\mathbf{k}}^<(t', t - \tau) \right. \\ \left. + \Sigma^< G^A - G^R \Sigma^< - G^<(t, t') \Sigma^A \right]$$

Quantum kinetics 2-time

Collision terms for $G^<$:

$$i\hbar \frac{\partial}{\partial t} G_{\mathbf{k}}^<(t, t - \tau) \Big|_{coll} = \int_{-\infty}^t dt' \left[\Sigma_{\mathbf{k}}^R(t, t') G_{\mathbf{k}}^<(t', t - \tau) + \Sigma^< G^A - G^R \Sigma^< - G^<(t, t') \Sigma^A \right]$$

$$\begin{aligned} G^<(t_1, t_2) &= -[G^<(t_2, t_1)]^\dagger \\ G^A(t_2, t_1) &= [G^R(t_1, t_2)]^\dagger \end{aligned}$$

Quantum kinetics 2-time

Initial conditions - the polaron

Before the pulse \Rightarrow equilibrium

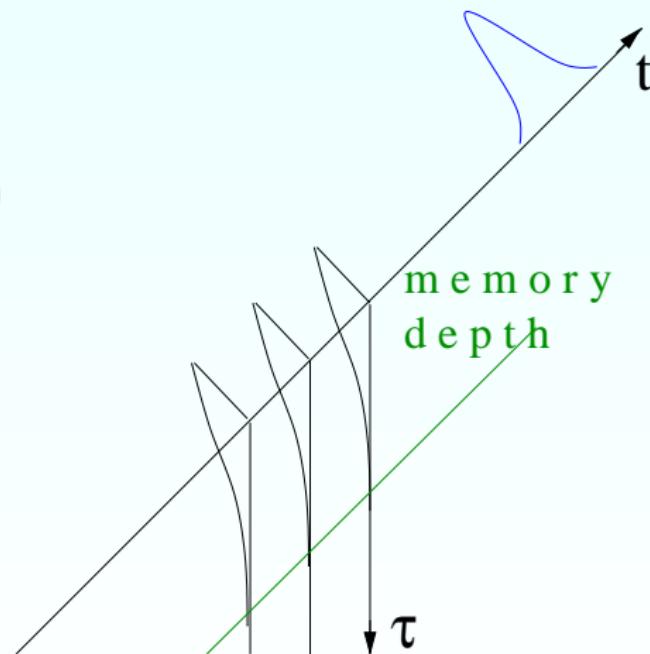
$$G^R(t, t - \tau) = \begin{pmatrix} g_c^R(\tau) & 0 \\ 0 & g_v^R(\tau) \end{pmatrix}$$

$$G^<(t, t - \tau) = \begin{pmatrix} 0 & 0 \\ 0 & -g_v^R(\tau) \end{pmatrix}$$

$$g_c^<(\tau) = 0$$

$$g_v^>(\tau) = 0$$

$$g_v^R(\tau) = g_v^>(\tau) - g_v^<(\tau)$$



Quantum kinetics 2-time

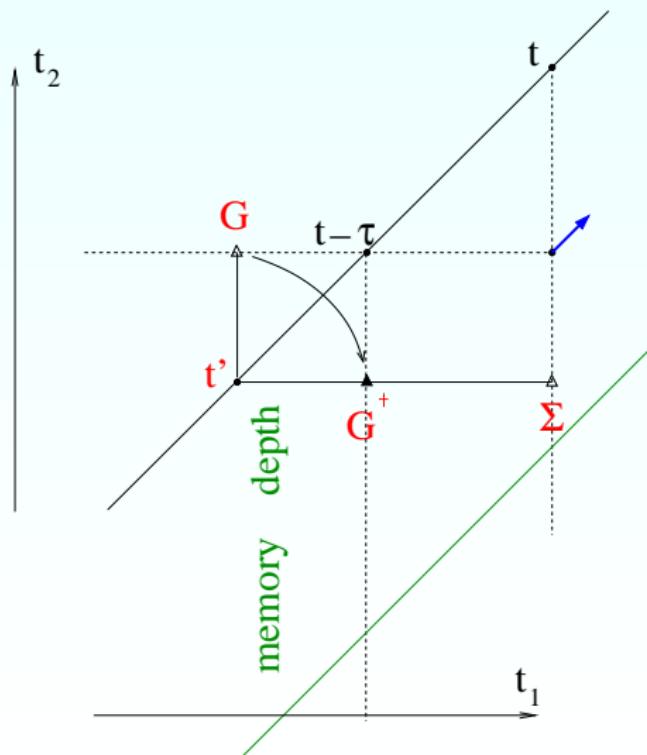
No t-evolution before excitation:

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} G_{\mathbf{k}}^{R,<}(t, t - \tau) &= \Sigma_{\mathbf{k}}^{\delta}(t) G_{\mathbf{k}}^{R,<}(t, t - \tau) - G_{\mathbf{k}}^{R,<}(t, t - \tau) \Sigma_{\mathbf{k}}^{\delta}(t - \tau) + \\ &\quad + i\hbar \frac{\partial}{\partial t} G_{\mathbf{k}}^{R,<}(t, t - \tau) \Big|_{coll} ; \quad \tau \geq 0 \end{aligned}$$

$$\Sigma_{\mathbf{k}}^{\delta}(t) = \begin{pmatrix} \epsilon_{\mathbf{k}}^c & \mathbf{0} \\ \mathbf{0} & \epsilon_{\mathbf{k}}^v \end{pmatrix}$$

$$\Sigma_{\mathbf{k}}^{\delta} G_{\mathbf{k}}^{R,<}(t, t - \tau) - G_{\mathbf{k}}^{R,<}(t, t - \tau) \Sigma_{\mathbf{k}}^{\delta} = 0$$

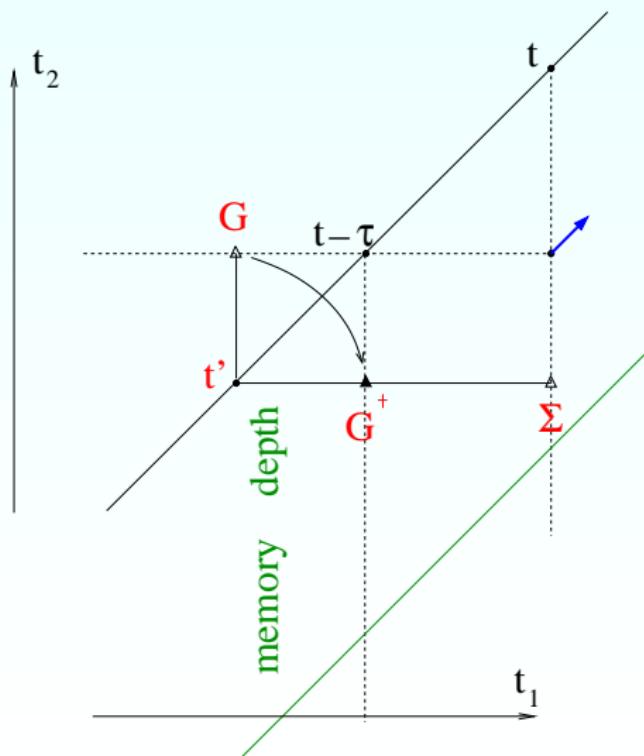
Quantum kinetics 2-time

No t-evolution before excitation:

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} G_{\mathbf{k}}^{<}(t, t - \tau) \Big|_{coll} = \\ \int_{-\infty}^t dt' \left[\Sigma_{\mathbf{k}}^R(t, t') G_{\mathbf{k}}^{<}(t', t - \tau) \right. \\ \left. + \Sigma^{<} G^A - G^R \Sigma^{<} - G^{<}(t, t') \Sigma^A \right] \end{aligned}$$

Quantum kinetics 2-time

No t-evolution before excitation:



$$\left. i\hbar \frac{\partial}{\partial t} G_{\mathbf{k}}^{<}(t, t - \tau) \right|_{coll} = \int_{-\infty}^t dt' \left[\Sigma_{\mathbf{k}}^R(t, t') G_{\mathbf{k}}^{<}(t', t - \tau) + \Sigma^{<} G^A - G^R \Sigma^{<} - G^{<}(t, t') \Sigma^A \right]$$

$$G^R(t, t - \tau) = \begin{pmatrix} g_c^R(\tau) & 0 \\ 0 & g_v^R(\tau) \end{pmatrix}$$

$$G^{<}(t, t - \tau) = \begin{pmatrix} 0 & 0 \\ 0 & -g_v^R(\tau) \end{pmatrix}$$

Quantum kinetics 1-time

- Generalized Kadanoff-Baym ansatz (GKBA)

$$G_{\alpha}^{\lessgtr}(t, t') \approx i\hbar G_{\alpha}^R(t - t') G_{\alpha}^{\lessgtr}(t', t') \quad t > t'$$

$$\begin{aligned} \frac{d}{dt} f_{\alpha}(t) = & 2\text{Re} \int_{-\infty}^t dt' \sum_{\beta q} |M_{\alpha,\beta}(q)|^2 G_{\beta}^R(t-t') [G_{\alpha}^R(t-t')]^* \\ & \times \left\{ -f_{\alpha}(\textcolor{red}{t'}) [1 - f_{\beta}(\textcolor{red}{t'})] D_q^>(t-t') \right. \\ & \left. + [1 - f_{\alpha}(\textcolor{red}{t'})] f_{\beta}(\textcolor{red}{t'}) D_q^<(t-t') \right\} \end{aligned}$$

$$D_q^{\lessgtr}(t) = N_{LO} e^{\mp i\omega_{LO} t} + (1 + N_{LO}) e^{\pm i\omega_{LO} t}$$

- renormalized quasiparticles (polarons)
- beyond Markov approximation (memory effects)

Quantum kinetics 1-time

- Generalized Kadanoff-Baym ansatz (GKBA)

$$G_{\alpha}^{\lessgtr}(t, t') \approx i\hbar G_{\alpha}^R(t - t') G_{\alpha}^{\lessgtr}(t', t') \quad t > t'$$

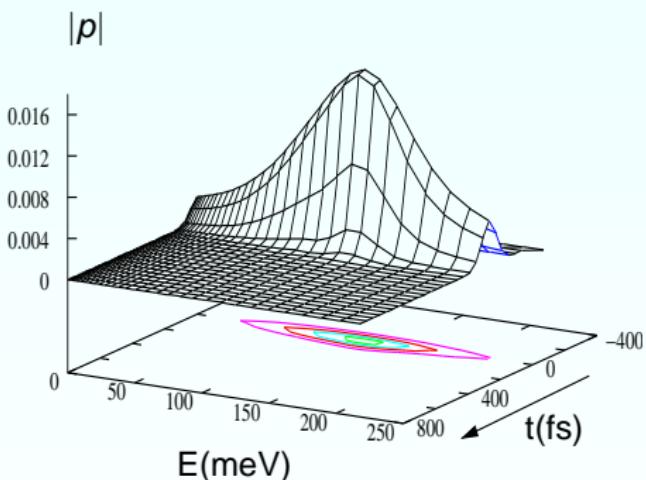
$$\begin{aligned} \frac{d}{dt} f_{\alpha}(t) = 2\text{Re} \int_{-\infty}^t dt' \sum_{\beta q} |M_{\alpha,\beta}(q)|^2 e^{-i\epsilon_{\beta}(t-t')} [e^{-i\epsilon_{\alpha}(t-t')}]^* \\ \times \left\{ -f_{\alpha}(\textcolor{red}{t}) [1 - f_{\beta}(\textcolor{red}{t})] D_q^>(t - t') \right. \\ \left. + [1 - f_{\alpha}(\textcolor{red}{t})] f_{\beta}(\textcolor{red}{t}) D_q^<(t - t') \right\} \end{aligned}$$

$$D_q^{\lessgtr}(t) = N_{LO} e^{\mp i\omega_{LO}t} + (1 + N_{LO}) e^{\pm i\omega_{LO}t}$$

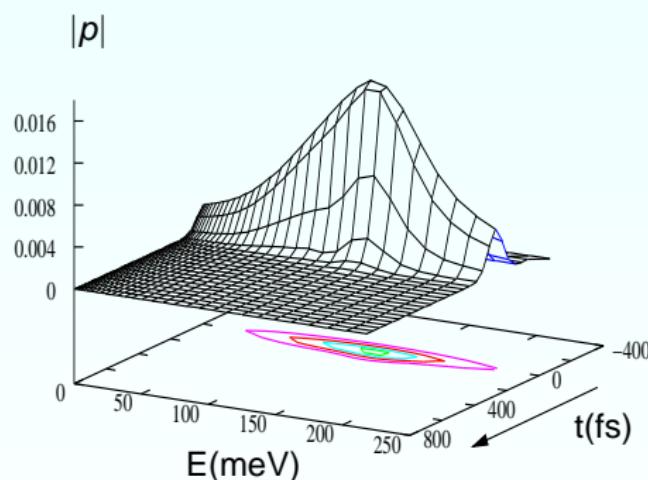
- bare particles
- Markov approximation (no memory effects)

Quantum well results: polarization

CdTe $\alpha = 0.31$ T = 300K



2-time

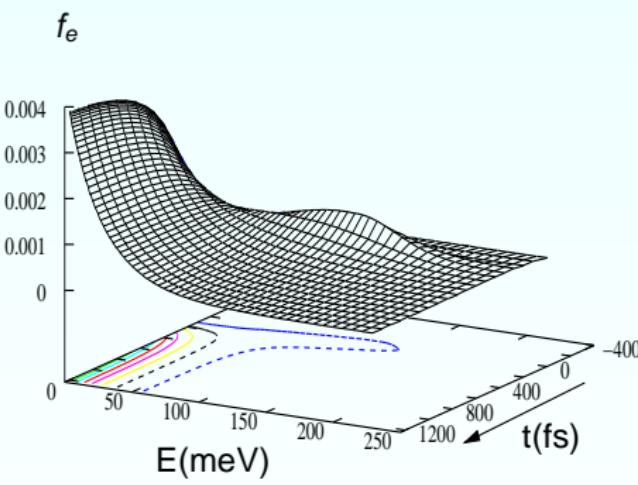


1-time

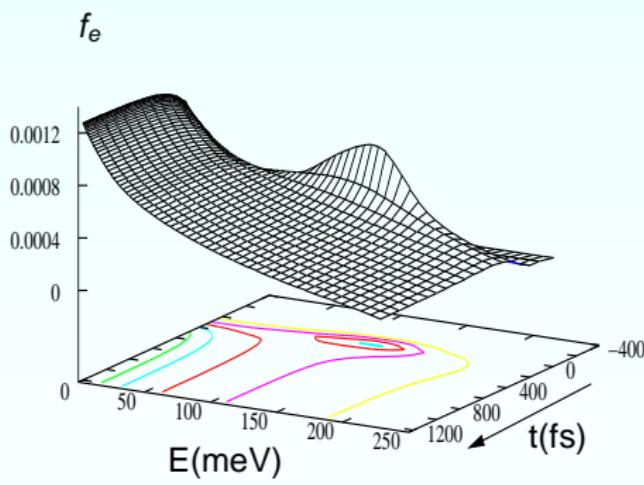
Strong dephasing

Quantum well results: electron population

CdTe $\alpha = 0.31$ T = 300K



2-time



1-time

Steady state reached
Not the same!

Kubo-Martin-Schwinger condition

- Exact relation in thermal equilibrium

KMS condition

$$f_\alpha = \int \frac{d(\hbar\omega)}{2\pi} F(\omega) \hat{G}_\alpha(\omega)$$

Kubo-Martin-Schwinger condition

- Exact relation in thermal equilibrium

KMS condition

$$f_\alpha = \int \frac{d(\hbar\omega)}{2\pi} F(\omega) \hat{G}_\alpha(\omega)$$

- Non-interacting system

$$\rightarrow \hat{G}_\alpha(\omega) = 2\pi \delta(\hbar\omega - \epsilon_\alpha)$$

$$\rightarrow f_\alpha = F(\epsilon_\alpha)$$

Kubo-Martin-Schwinger condition

- Exact relation in thermal equilibrium

KMS condition

$$f_\alpha = \int \frac{d(\hbar\omega)}{2\pi} F(\omega) \hat{G}_\alpha(\omega)$$

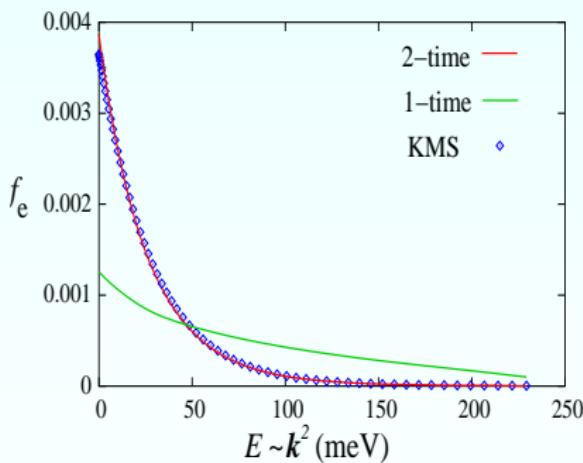
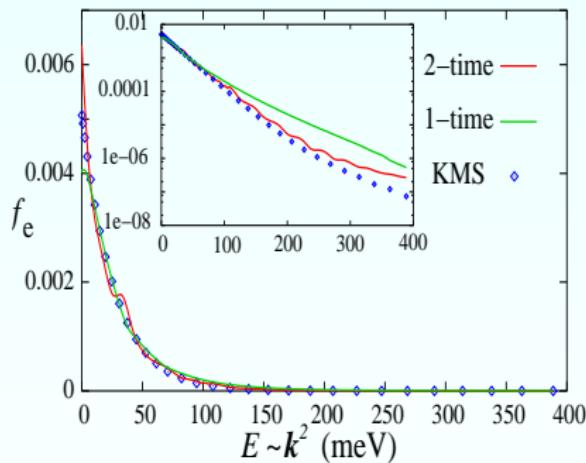
- Non-interacting system

$$\begin{aligned}\rightarrow \quad & \hat{G}_\alpha(\omega) = 2\pi \delta(\hbar\omega - \epsilon_\alpha) \\ \rightarrow \quad & f_\alpha = F(\epsilon_\alpha)\end{aligned}$$

- Interacting system

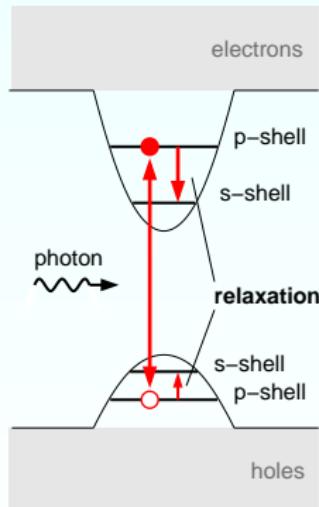
→ Generalization of Fermi-Dirac distribution

Kubo-Martin-Schwinger test in quantum wells

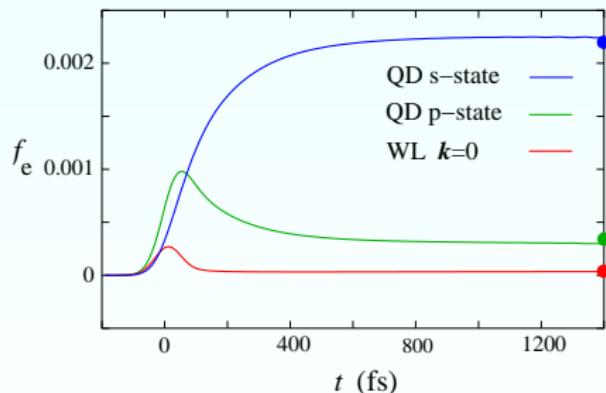
CdTe, $\alpha = 0.31$ GaAs, $\alpha = 0.06$ P. Gartner, J. Seebek, F. Jahnke, Phys. Rev. **B 73**, 115307 (2006)

Kubo-Martin-Schwinger test in quantum dots

- CdTe $\alpha = 0.31$ $\Delta E = 2.4 \hbar \omega_{\text{LO}}$ p-level excitation



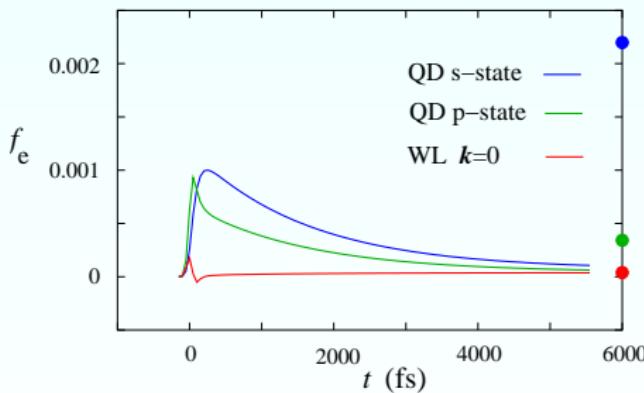
2-time calculation



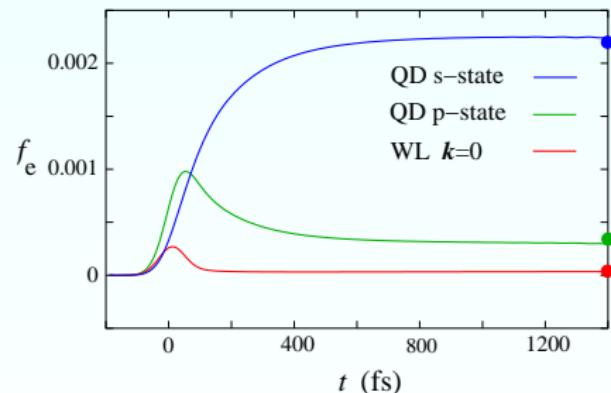
Kubo-Martin-Schwinger test in quantum dots

- CdTe $\alpha = 0.31$ $\Delta E = 2.4 \hbar \omega_{\text{LO}}$ p-level excitation

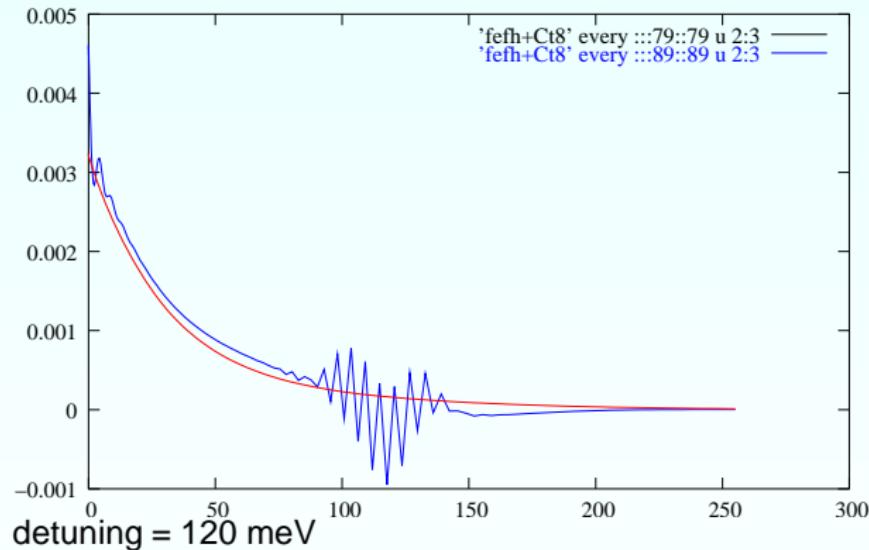
1-time calculation



2-time calculation



Numerics: instabilities



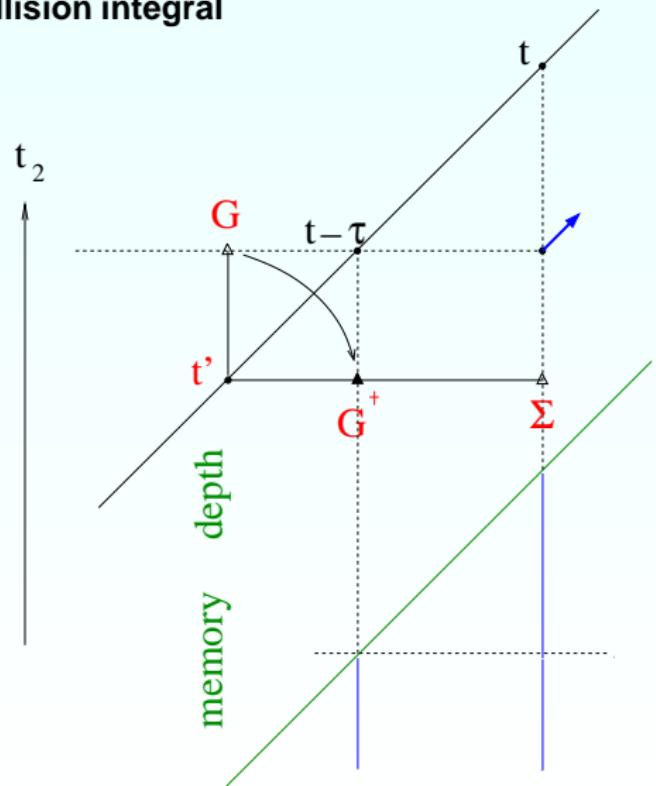
t = 550fs

t = 650fs

abrupt cut of the collision integrals at memory **depth = 500 fs**

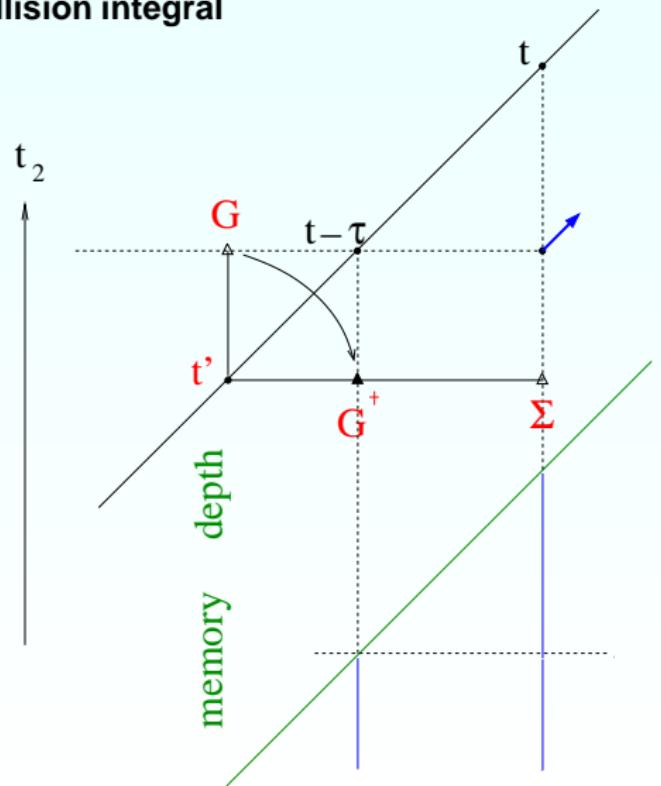
Numerics: instabilities

Collision integral



Numerics: instabilities

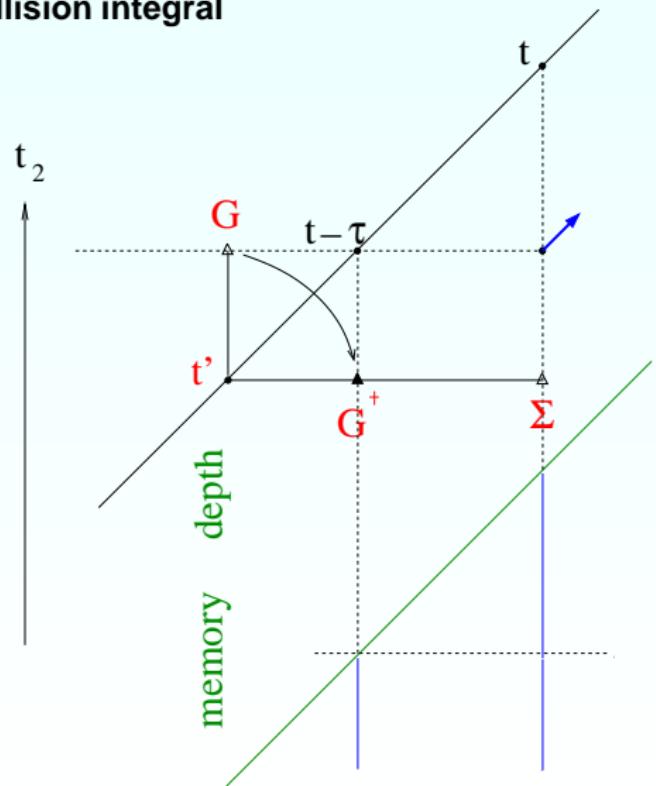
Collision integral



- integral abruptly cut at memory depth

Numerics: instabilities

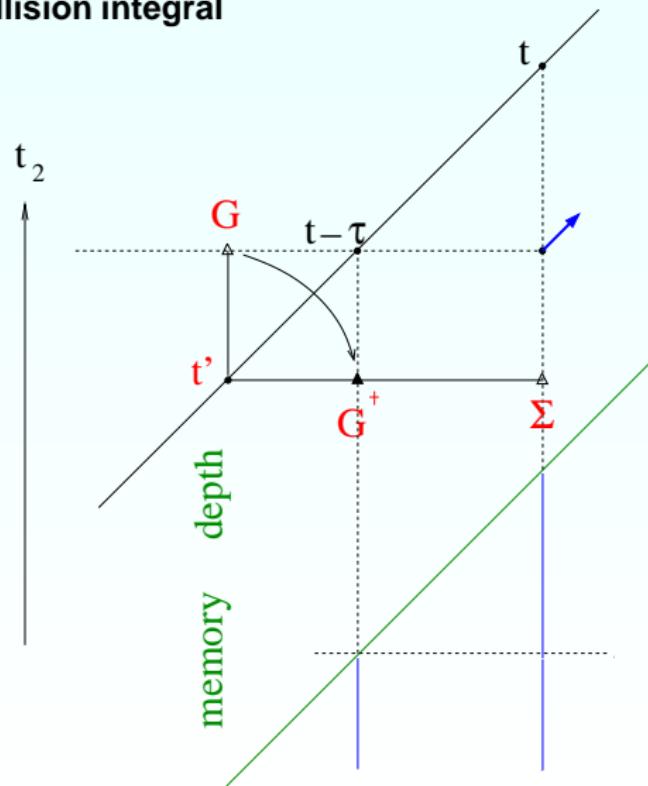
Collision integral



- integral abruptly cut at memory depth
- beyond the memory depth extend with equilibrium Σ , G

Numerics: instabilities

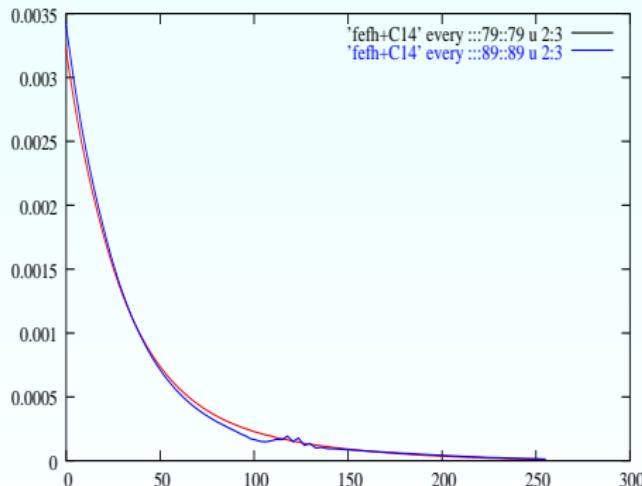
Collision integral



- integral abruptly cut at memory depth
- beyond the memory depth extend with **equilibrium Σ , G**
- smooth interpolation to **equilibrium Σ , G**

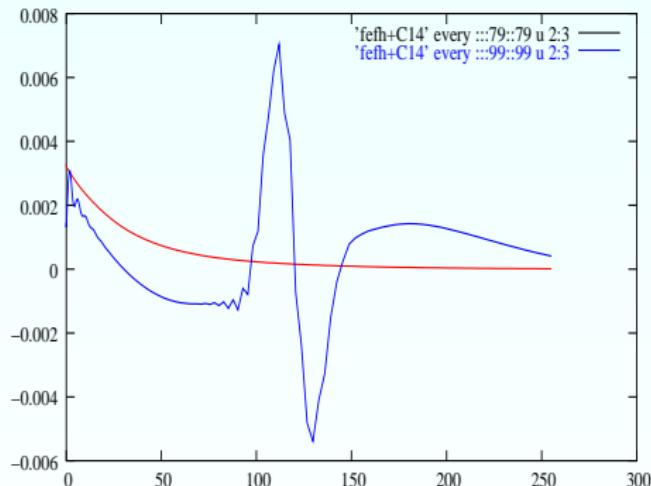
Numerics: instabilities

Collision integrals extended with equilibrium GFs



$t = 550\text{fs}$

$t = 650\text{fs}$



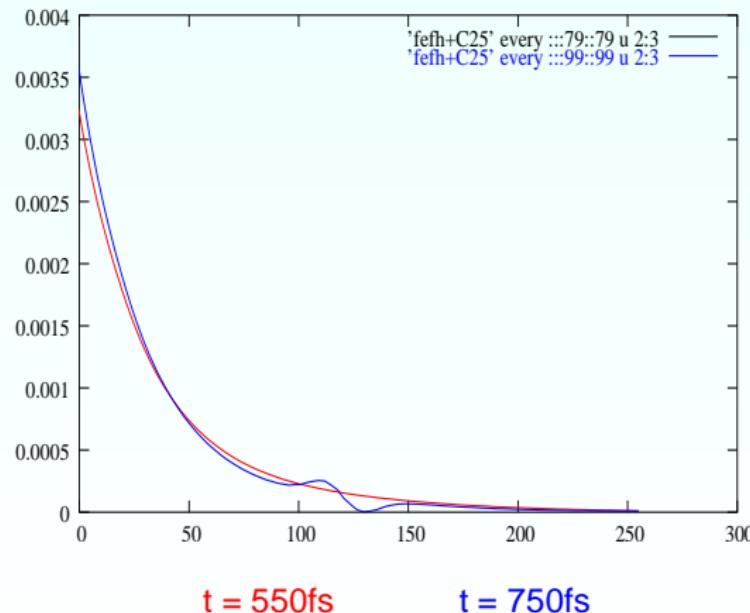
$t = 550\text{fs}$

$t = 750\text{fs}$

Numerics: instabilities

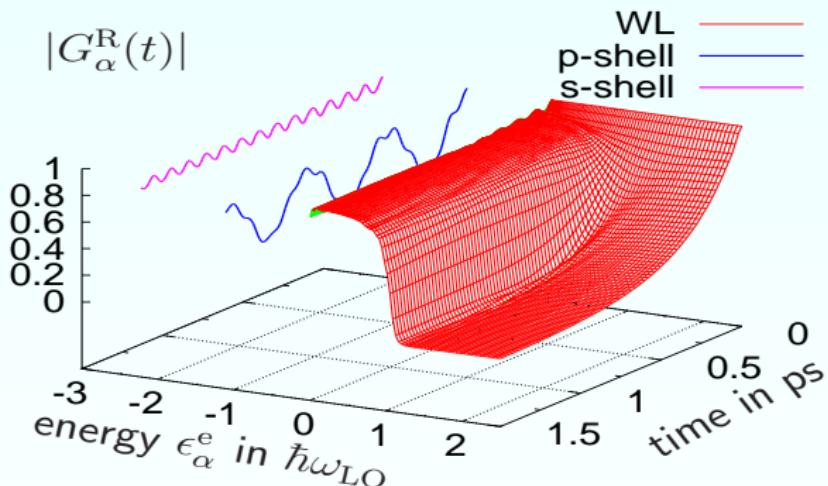
Collision integrals extended with equilibrium GFs

- smooth change using an interpolating (Fermi-like) function



Low temperatures

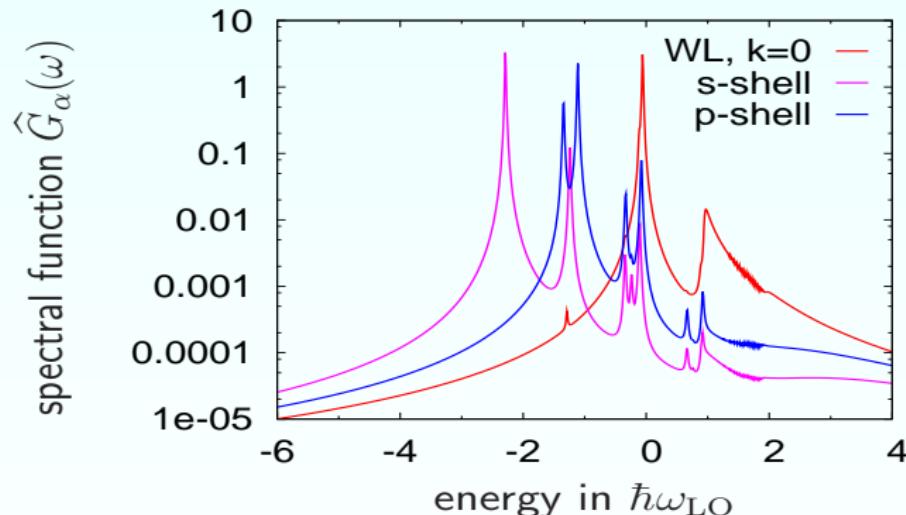
The polaron



Polaronic GF: GaAs at $T=10K$

Low temperatures

The polaron



Spectral function: GaAs at $T=10\text{K}$

Low temperatures

Quantum kinetics 1-time

$$\frac{d}{dt} f_\alpha(t) = 2\text{Re} \int_{-\infty}^t dt' \sum_{\beta q} |M_{\alpha,\beta}(q)|^2 G_\beta^\text{R}(t-t') [G_\alpha^\text{R}(t-t')]^* \\ \times \left\{ -f_\alpha(\textcolor{red}{t'}) [1-f_\beta(\textcolor{red}{t'})] D_q^>(t-t') \right. \\ \left. + [1-f_\alpha(\textcolor{red}{t'})] f_\beta(\textcolor{red}{t'}) D_q^<(t-t') \right\}$$

Low temperatures

Quantum kinetics 1-time

$$\frac{d}{dt} f_\alpha(t) = 2\text{Re} \int_{-\infty}^t dt' \sum_{\beta q} |M_{\alpha,\beta}(q)|^2 G_\beta^R(t-t') [G_\alpha^R(t-t')]^* \\ \times \left\{ -f_\alpha(\textcolor{red}{t'}) [1-f_\beta(\textcolor{red}{t'})] D_q^>(t-t') \right. \\ \left. + [1-f_\alpha(\textcolor{red}{t'})] f_\beta(\textcolor{red}{t'}) D_q^<(t-t') \right\}$$

$$G_\alpha^R(t) = \frac{1}{i\hbar} \Theta(t) \left[\sum_j e^{-\frac{i}{\hbar}(\epsilon_\alpha - \Delta_{\alpha,j})t} + G_\alpha^R(t) \right]$$
$$G_\alpha^R(t) \rightarrow 0 \quad \text{for} \quad t \rightarrow \infty$$

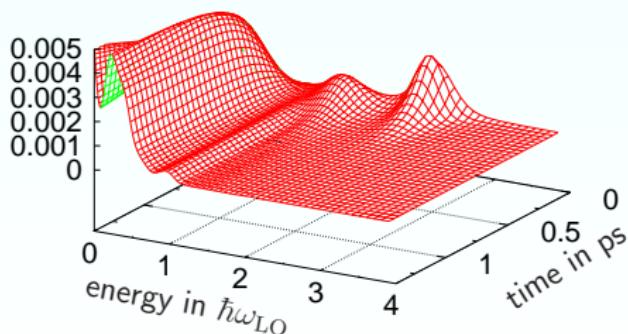
Low temperatures

WL electron population

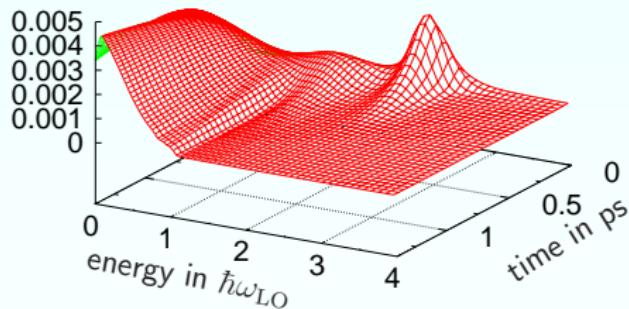
2-time



population



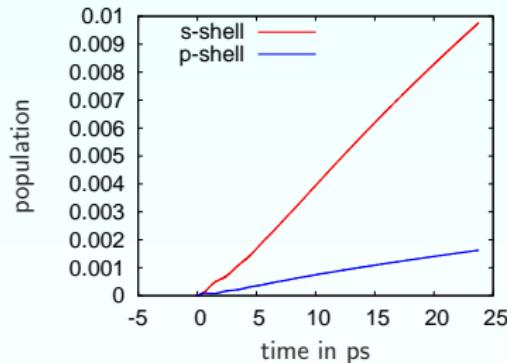
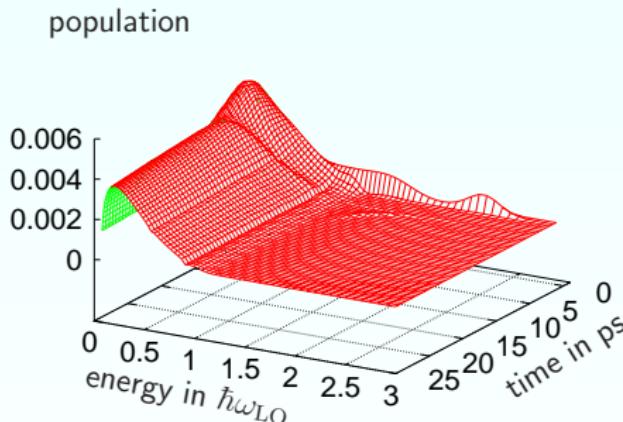
population



1-time

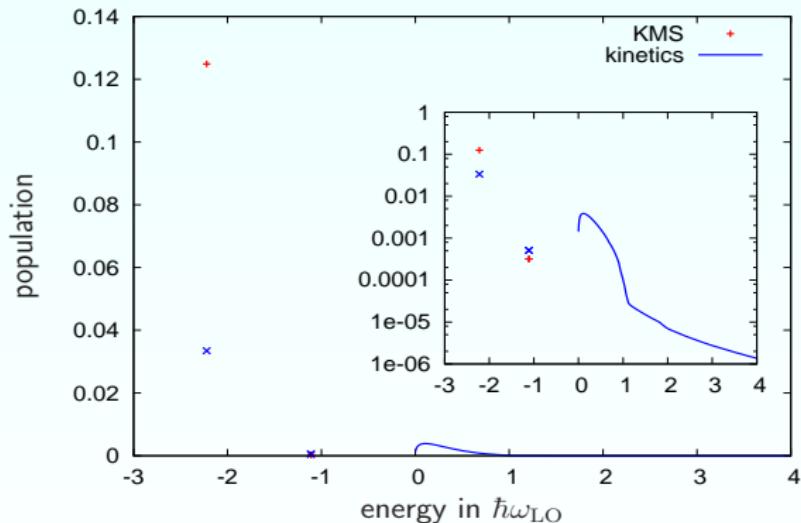
Low temperatures

Electron population (long time)



Low temperatures

KMS test of the steady state



no thermalization (asymptotic bottleneck)

Summary and conclusions

- Carrier-LO-phonon interaction role - twofold:
 - equilibrium: polaron
 - kinetics: polaron-phonon scattering
- Relaxation properties (room temp.):
 - Steady state reached both in 2-time and in 1-time kinetics
 - Thermalization:
 - 2-time kinetics: Yes!
 - 1-time kinetics, only low α
- Problems with low temperatures:
 - 2-time - only the early kinetics
 - 1-time - no thermalization (asymptotic bottleneck ?)