Max Planck Institute for Solid State Research

Density-Matrix Theory for high-Tc superconductors in non-equilibrium: Higgs mode and pairing glue

Dirk Manske

co-workers and papers:

(1) A. Knorr (TU Berlin), DM, PRB 77, 180509 (R) (2008)
(2) A. Schnyder (MPI Stuttgart), A. Avella (Uni Salerno), DM, PRB 84, 214513 (2011)
(3) Exp.: M. Rübhausen + team (Uni Hamburg), DM, PRL 102, 177004 (2009)
(4) A. Schnyder, A. Akbari (MPI Stuttgart), I. Eremin (Uni Bochum), DM, EPL 101, 17002 (2013)
(5) G. Uhrig + team, DM, arXiv:1309.7318, PRB 2014

YITP@Kyoto, June 24th, 2014

Phase diagram (hole-doped)

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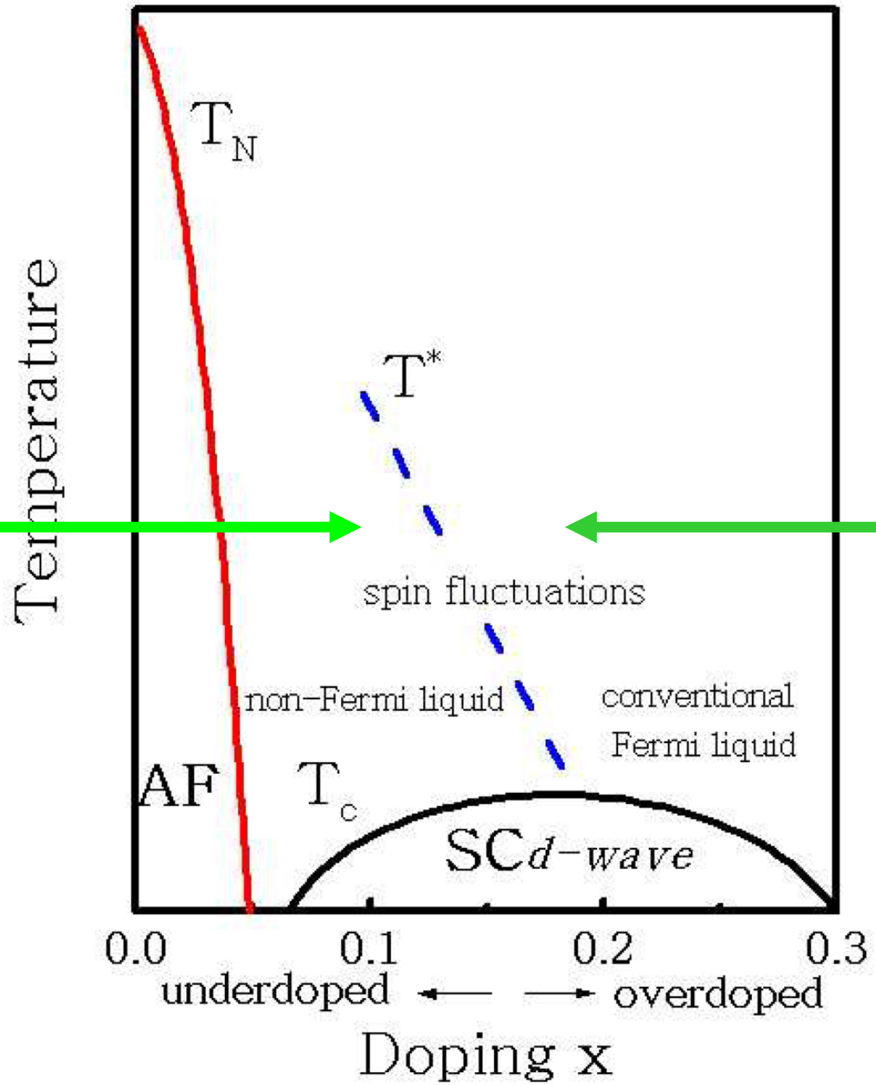
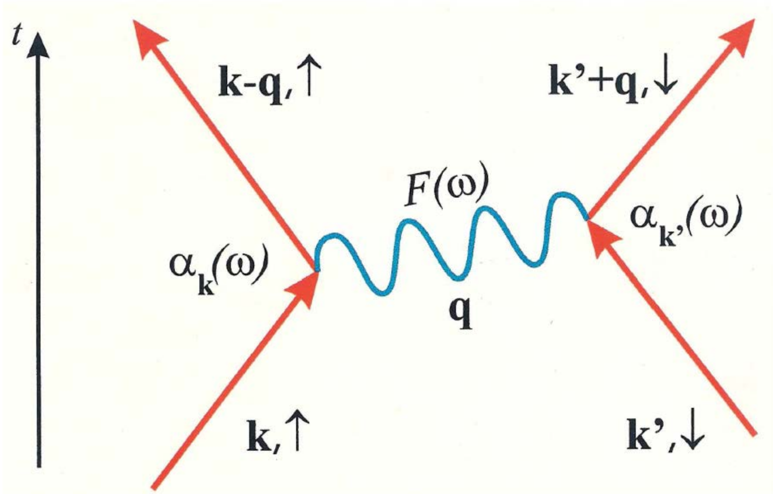
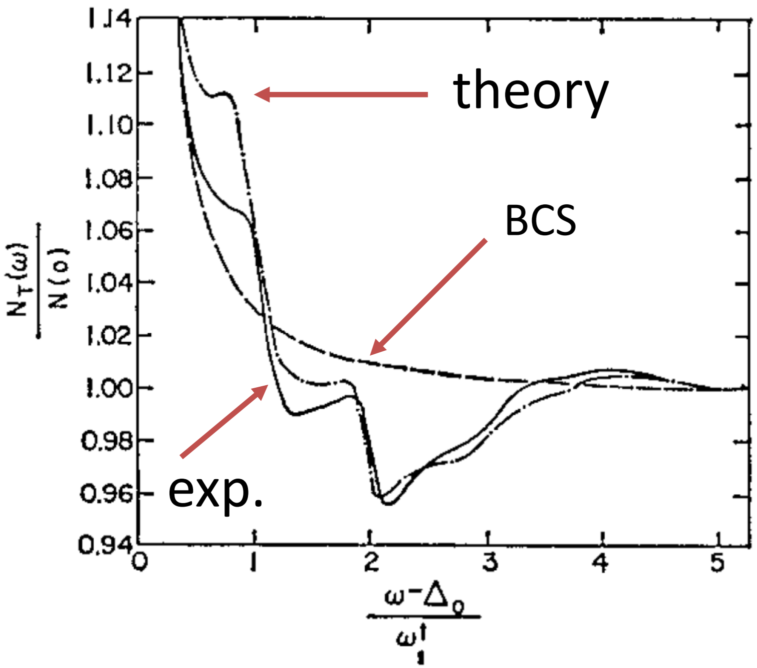
Theory I



Theory II

Pairing due to phonons





pairing interaction is determined by $V_{eff} = \alpha^2_{k,k'} F(\omega)$
Eliashberg equations yield $\Delta(\omega)$ and tunneling density of states

$$\frac{N_T(\omega)}{N(0)} = \mathrm{Re}\left[\frac{\omega}{\sqrt{\omega^2 - \Delta^2(\omega)}}\right]$$

D.J. Scalapino, J.R. Schrieffer, J.W. Wilkins PR **148**, 148 (1966)

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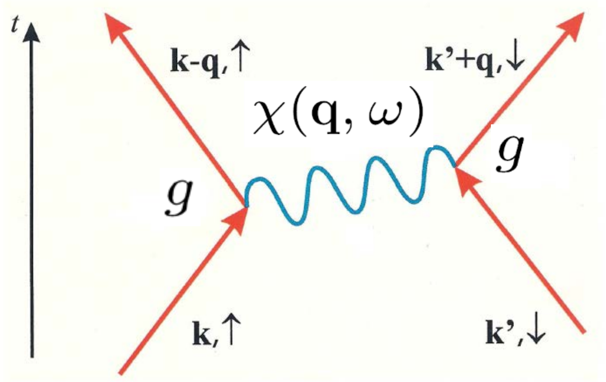
Coupling of holes to spin excitations



□ Cooper-pairing is controlled by spin excitations:

Ornstein-Zernicke form for the spin susceptibility ($\mathbf{Q} = (\pi, \pi)$), parameters from NMR (Millis, Monien, Pines (PRB 1989))

$$\chi(\mathbf{q},\omega) = \frac{\chi_{\mathbf{Q}}}{1 + \xi^2(\mathbf{q}-\mathbf{Q})^2 - i\frac{\omega}{\omega_{sf}}}$$

leads with $g = U_{eff} = U$

$$V_{eff}(\mathbf{q},\omega) = g^2\,\chi(\mathbf{q},\omega)$$

$\Longrightarrow$ high-T_c and d-wave is possible

Microscopic approach: e.g. FLEX (Scalapino, Bickers, Manske), Spin-Fermion (Chubukov. …) , …

FLEX (3rd generation): method and applications

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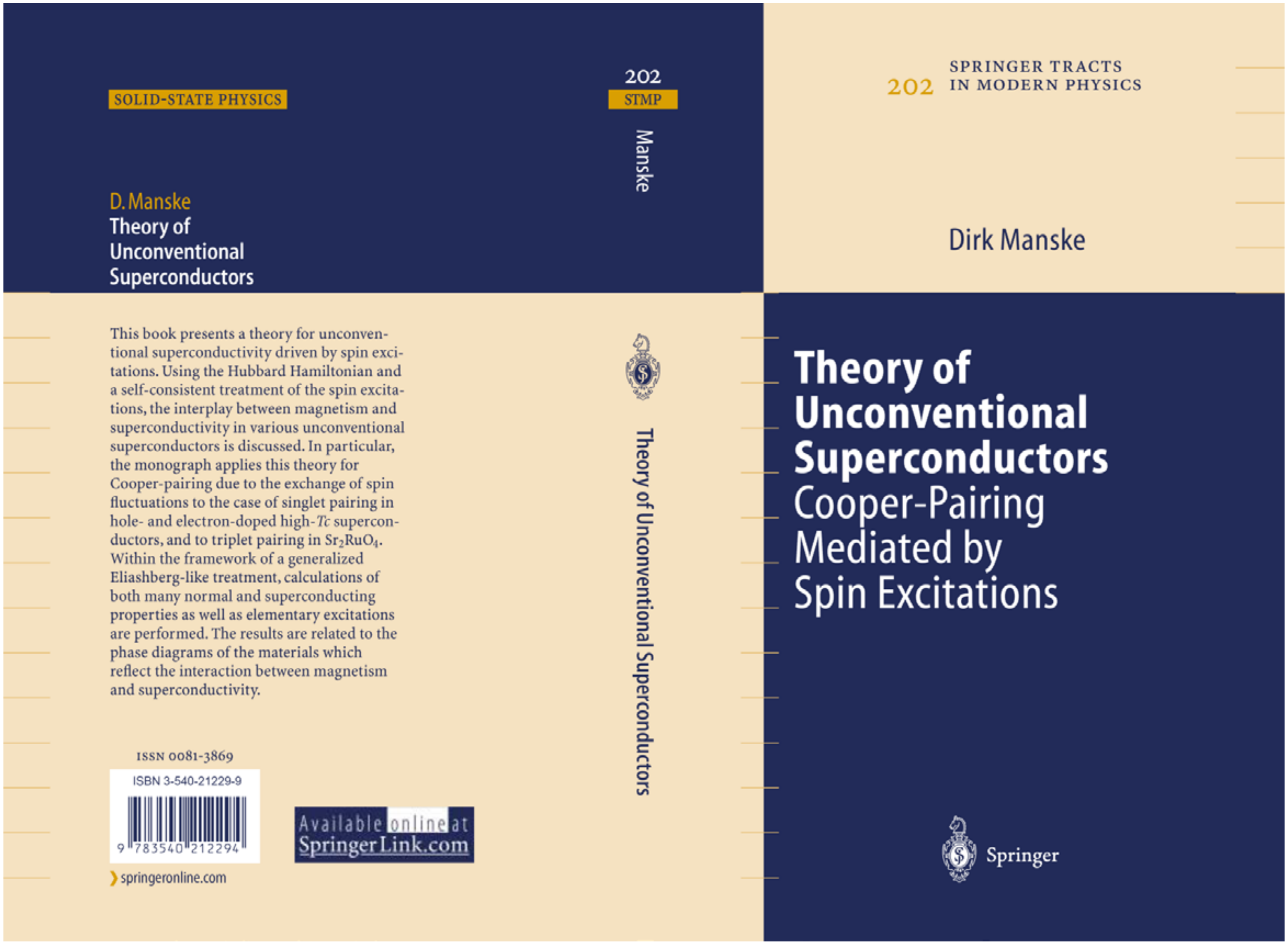

published 2004

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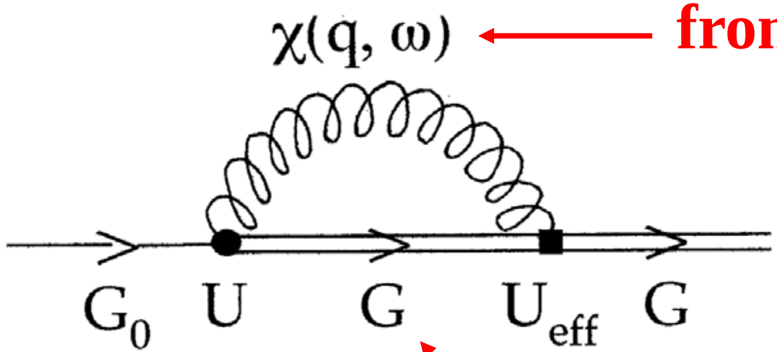
Idea: analysis of the elementary excitations

$$\omega(\mathbf{k}) = \epsilon_{\mathbf{k}} + \mathrm{Re}\ \Sigma(\mathbf{k},\omega)$$

$$\Sigma(\mathbf{k},\omega) =$$



from INS, RIXS

from ARPES

structure in Re $\Sigma(\mathbf{k},\omega)$?

- ☐ characteristic for interaction of quasiparticles $\longleftrightarrow$ spin fluctuations?
- ☐ anisotropy in momentum space?
- ☐ feedback on $\chi(\mathbf{q},\omega)$?
- ☐ doping dependence?

Fingerprints of the glue?

nature physics

LETTERS

PUBLISHED ONLINE: 18 JANUARY 2009 | DOI: 10.1038/NPHYS1180

Strength of the spin-fluctuation-mediated pairing interaction in a high-temperature superconductor

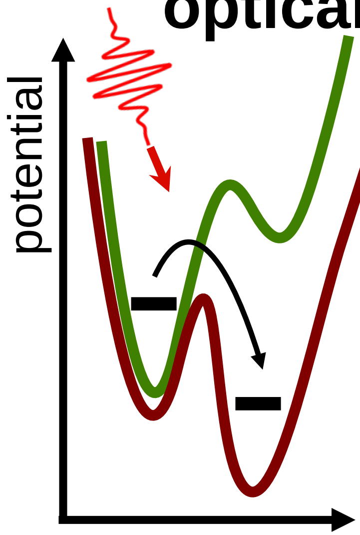
T. Dahm[1], V. Hinkov[2], S. V. Borisenko[3], A. A. Kordyuk[3], V. B. Zabolotnyy[3], J. Fink[3,4], B. Büchner[3], D. J. Scalapino[5], W. Hanke[6] and B. Keimer[2]*

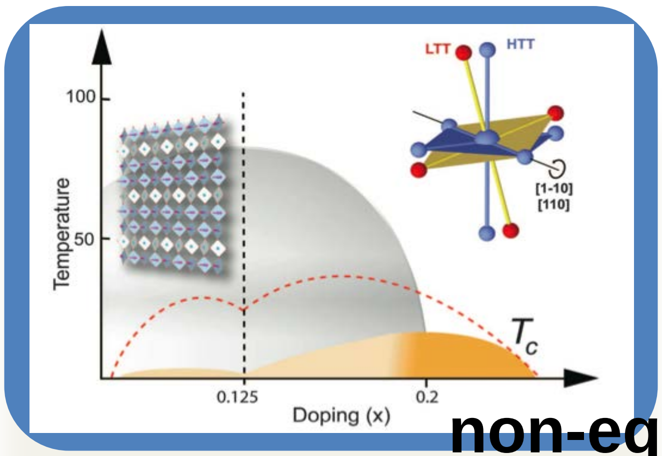
- ❑ simultaneous explanation of the resonance peak and kinks is possible

→ extract U ≈ 2eV (high Tc is possible)

3 types of non-equilibrium experiments

optical control new transient ground state





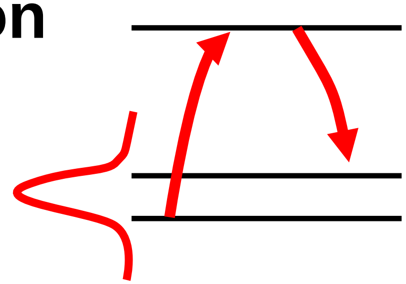
D. Fausti et al.,
Science **331**, 189 (2011)

non-equilibrium spectroscopy

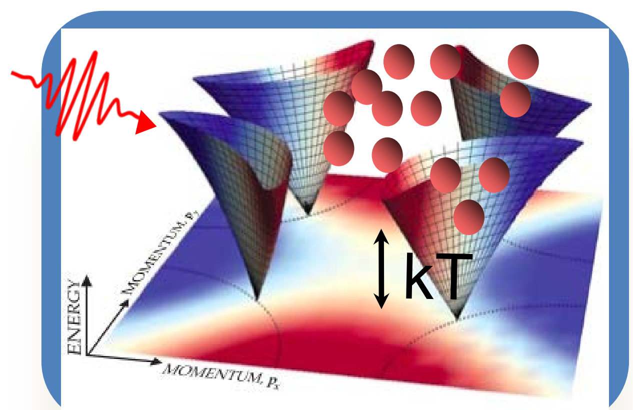
recovery of the ground state

coherent excitation

coherent oscillation



bandwidth



Content

- Motivation: how does the superconducting condensate response? Role of phonons?

- Theory: Equations of motion for coherent dynamics, quantum kinetic equations in the nonadiabatic regime (DMT)

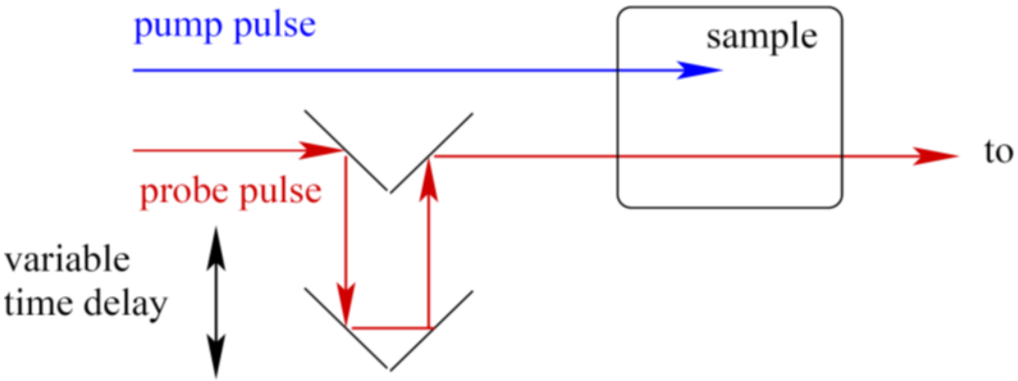
- Results: order parameter (Higgs) oscillations

  role of electron-phonon coupling

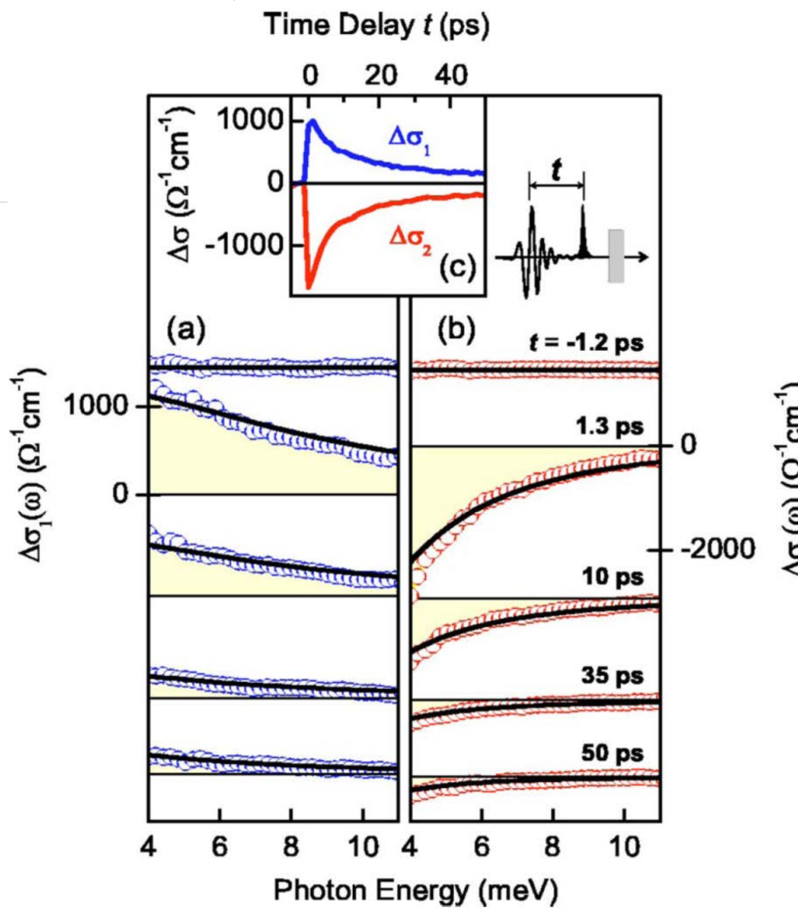
  coherent phonons vs. phonon bath

  multi-band effects

Motivation I: pump-probe spectroscopy



Bi2212



R.A. Kaindl *et al.*, PRB 72, 060510(R) (2005)

Two kinds of information can be extracted:

- **Time domain: conductivity change $\Delta\sigma$, depending on time delay Δt**
- **Energy domain: change in the conductivity spectra**

Motivation II: time-resolved ARPES (1)

PRL **99,** 197001 (2007) PHYSICAL REVIEW LETTERS week ending 9 NOVEMBER 2007

Ultrafast Electron Relaxation in Superconducting $Bi_2Sr_2CaCu_2O_{8+\delta}$ by Time-Resolved Photoelectron Spectroscopy

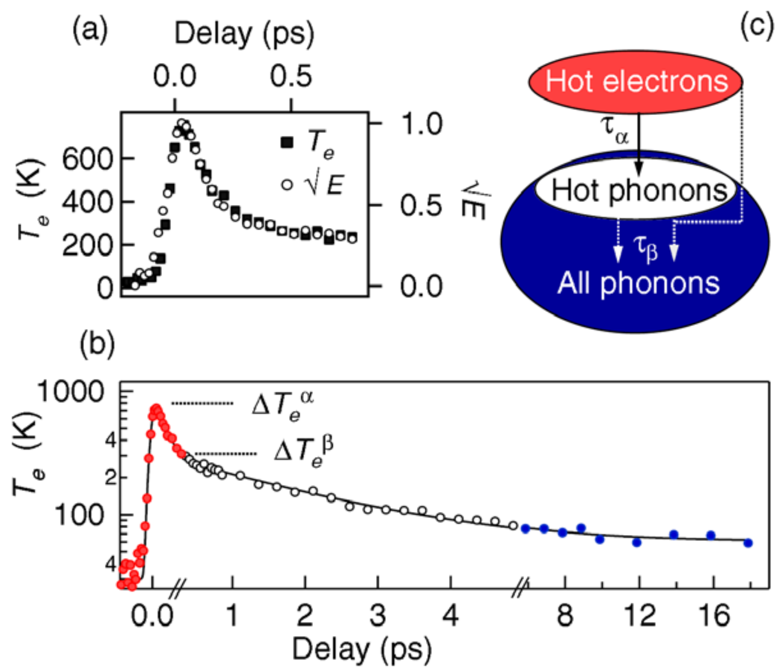
L. Perfetti,[1] P. A. Loukakos,[1] M. Lisowski,[1] U. Bovensiepen,[1] H. Eisaki,[2] and M. Wolf[1]

[1]*Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany*

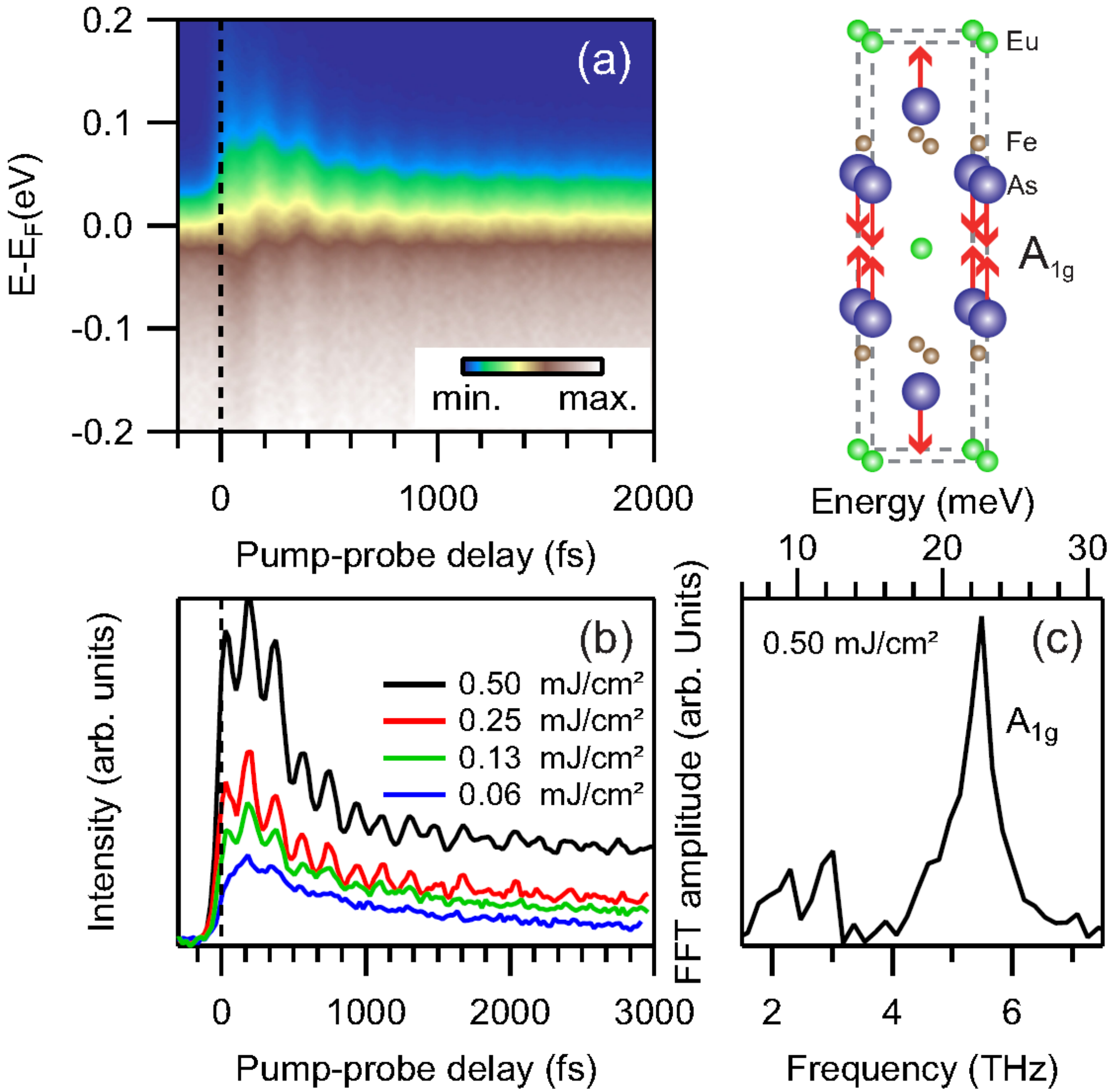
[2]*AIST Tsukuba Central 2, 1-1-1 Umenzono, Tsukuba, Ibaraki 305-8568, Japan*

(Received 18 April 2007; published 9 November 2007)

- **Hot electrons dissipate on 2 distinct time scales: 110fs and 2ps**
- **Only 10-20 % of the total lattice modes dominate the coupling strength**
- **(averaged) electron-phonon coupling λ < 0.25**



Motivation III: time-resolved ARPES (2)



- **Observation of coherent phonons in $EuFe_2As_2$**

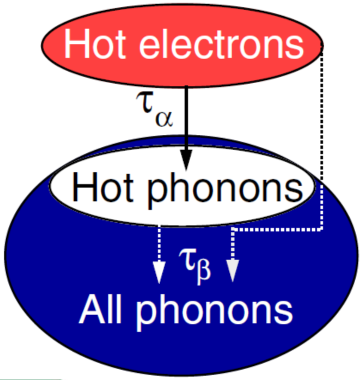
PRL 108, 097002 (2012)

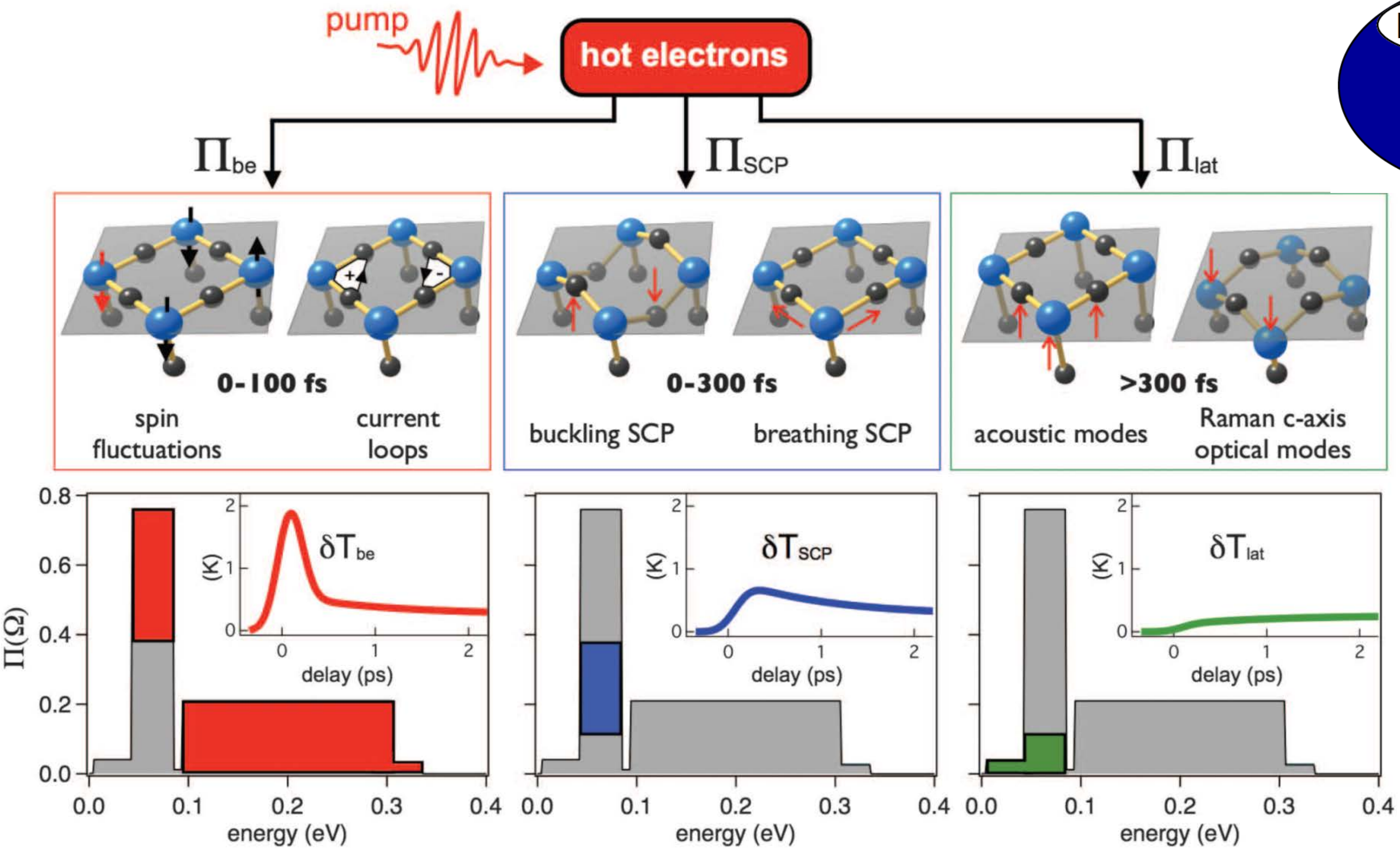
J. Fink and co-workers

Motivation IV: glue of high-Tc cuprates?

Science AAAS

Disentangling the Electronic and Phononic Glue in a High-T_c Superconductor
S. Dal Conte *et al.*
Science **335**, 1600 (2012);
DOI: 10.1126/science.1216765





Often used: effective theories

Two different models for the description of time-resolved experiments:

- „effective models“: μ^*, T^* model [PRB **67**, 214506 (2003)]:
  describe excited quasiparticle distribution as equilibrium distribution with new temperatature T^* / chemical potential μ^*

- rate equations [PRL **95**, 147002 (2005)]:
  equations of motion for quasiparticle (*n*) and phonon (*N*) distributions:

$$\frac{dn}{dt} = I_0 + \eta N - Rn^2,$$

$$\frac{dN}{dt} = J_0 - \eta \frac{N}{2} + \frac{Rn^2}{2} - \gamma (N - N_0)$$

with phenomenological parameters for pair-breaking, recombination, and phonon decay

Microscopic approach:

$$H = \sum_{\mathbf{k}s} \epsilon_{\mathbf{k}} c^+_{\mathbf{k}s} c_{\mathbf{k}s} + \sum_{\mathbf{k}} \left(\Delta_{\mathbf{k}} c^+_{\mathbf{k}\uparrow} c^+_{-\mathbf{k}\downarrow} + \mathbf{c.c} \right)$$

$$- \frac{e\hbar}{m} \sum_{\mathbf{kq}s} (\mathbf{k} \cdot \mathbf{A_q}) c^+_{\mathbf{k}+\frac{\mathbf{q}}{2}s} c_{\mathbf{k}-\frac{\mathbf{q}}{2}s} + \frac{e^2}{2m} \sum_{\mathbf{kq}s} (\mathbf{A_{q-k}} \cdot \mathbf{A_q}) c^+_{\mathbf{k}s} c_{\mathbf{k}s}$$

$$+ \sum_{\mathbf{q}j} \hbar\omega_{\mathbf{q}j} \left(b^+_{\mathbf{q}j} b_{\mathbf{q}j} + \frac{1}{2} \right) + \sum_{\mathbf{p}j\mathbf{k}s} \left(g_{\mathbf{pk}js} (b^+_{-\mathbf{p}j} + b_{\mathbf{p}j}) c^+_{\mathbf{k}+\mathbf{p},s} c_{\mathbf{k}s} + \mathbf{c.c.} \right)$$

with $$\Delta_{\mathbf{k}} = \sum_{\mathbf{k}'} V_{\mathbf{kk}'} \langle c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow} \rangle$$

we consider:
(a) tetragonal lattice
(b) tight-binding band structure, e.g. from Kordyuk *et al*. ('03)
(c) *s*- or *d*-wave order parameter

DMT: Calculation of coherent dynamics

Superconducting state: Bogoliubov transformation

$$\alpha^\dagger_{\boldsymbol{k}} = u_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k}\uparrow} + v^*_{\boldsymbol{k}} c_{-\boldsymbol{k}\downarrow} \qquad \beta^\dagger_{\boldsymbol{k}} = u_{\boldsymbol{k}} c^\dagger_{-\boldsymbol{k}\downarrow} - v^*_{\boldsymbol{k}} c_{\boldsymbol{k}\uparrow}$$

$$\Delta_{\boldsymbol{k}} = \sum_{\boldsymbol{k}} W_{\boldsymbol{k},\boldsymbol{k}'} \left[u_{\boldsymbol{k}'} v_{\boldsymbol{k}'} \left(1 - \left\langle \alpha^\dagger_{\boldsymbol{k}'} \alpha_{\boldsymbol{k}'} \right\rangle - \left\langle \beta^\dagger_{\boldsymbol{k}'} \beta_{\boldsymbol{k}'} \right\rangle \right) + u^2_{\boldsymbol{k}'} \left\langle \beta_{\boldsymbol{k}'} \alpha_{\boldsymbol{k}'} \right\rangle - v^2_{\boldsymbol{k}'} \left\langle \alpha^\dagger_{\boldsymbol{k}'} \beta^\dagger_{\boldsymbol{k}'} \right\rangle \right]$$

All quantities of interest can be expressed in terms of these four dynamical variables

$$\left\langle \alpha^\dagger_{\boldsymbol{k}} \alpha_{\boldsymbol{k}'} \right\rangle (t), \quad \left\langle \beta^\dagger_{\boldsymbol{k}} \beta_{\boldsymbol{k}'} \right\rangle (t), \quad \left\langle \alpha^\dagger_{\boldsymbol{k}} \beta^\dagger_{\boldsymbol{k}'} \right\rangle (t), \quad \left\langle \alpha_{\boldsymbol{k}} \beta_{\boldsymbol{k}'} \right\rangle (t)$$

For example, current density:

$$\boldsymbol{j}(\boldsymbol{q},\omega) \simeq \frac{e\hbar}{mV} \sum_{\boldsymbol{k}} \boldsymbol{k} \left[\left\langle \alpha^\dagger_{\boldsymbol{k}} \alpha_{\boldsymbol{k}+\boldsymbol{q}} \right\rangle - \left\langle \beta^\dagger_{\boldsymbol{k}+\boldsymbol{q}} \beta_{\boldsymbol{k}} \right\rangle + \boldsymbol{k}\cdot\boldsymbol{q} \frac{\hbar^2 |\Delta_1|}{2m\,(E^2_{\boldsymbol{k}})} \left(\left\langle \alpha^\dagger_{\boldsymbol{k}} \beta^\dagger_{\boldsymbol{k}+\boldsymbol{q}} \right\rangle + \left\langle \alpha_{\boldsymbol{k}+\boldsymbol{q}} \beta_{\boldsymbol{k}} \right\rangle \right) \right]$$

Density-matrix theory:

$$\frac{d}{dt} \left(c^\dagger_{\boldsymbol{k}_1} c_{\boldsymbol{k}_2} \right) = \frac{i}{\hbar} \left[H, c^\dagger_{\boldsymbol{k}_1} c_{\boldsymbol{k}_2} \right] + \frac{\partial}{\partial t} \left(c^\dagger_{\boldsymbol{k}_1} c_{\boldsymbol{k}_2} \right)$$

$\Longrightarrow$ yields equations of motions for the above four expectation values

Results

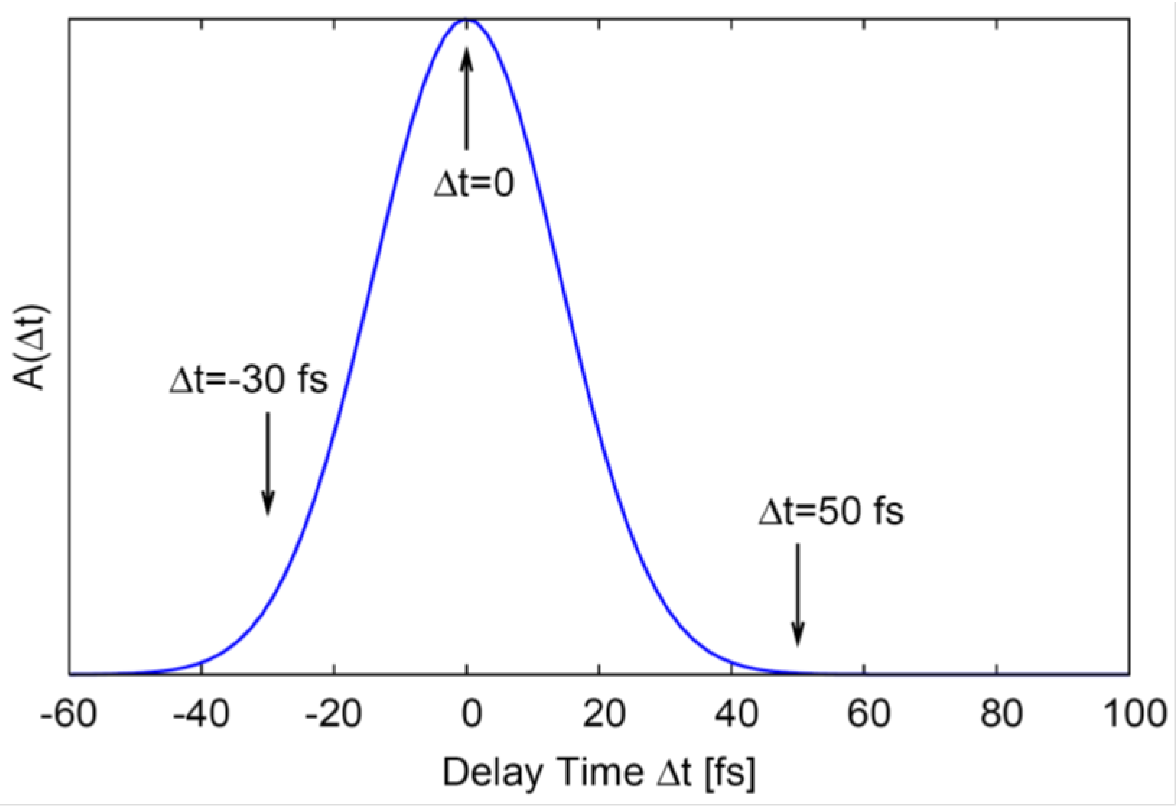
Case I: single band
no phonons

Calculating the superconductor's response

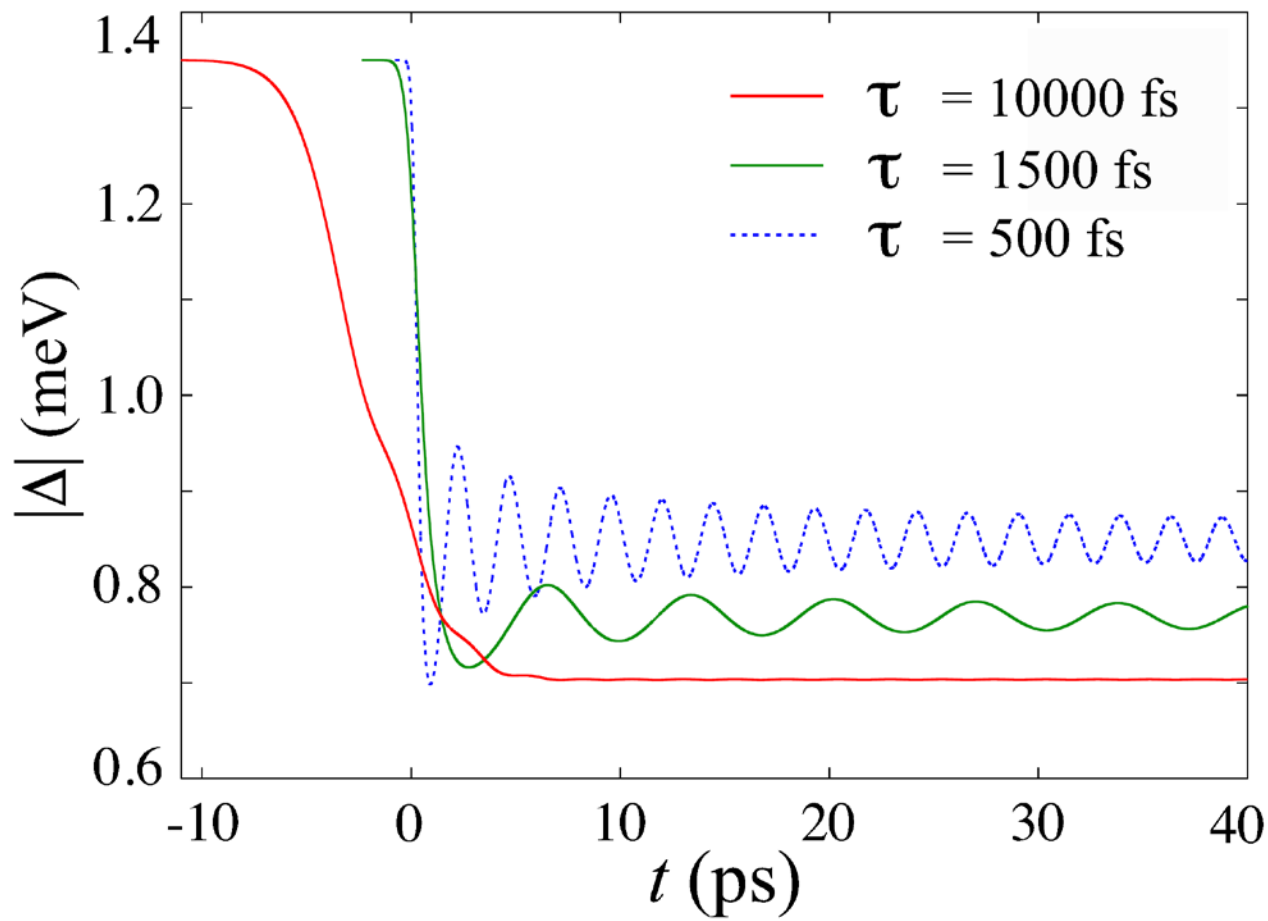
→ **arriving at a closed set of differential equations**
(case I : no phonons)

- **Gaussian pump and probe pulses**

- **Pulse duration will become important!**



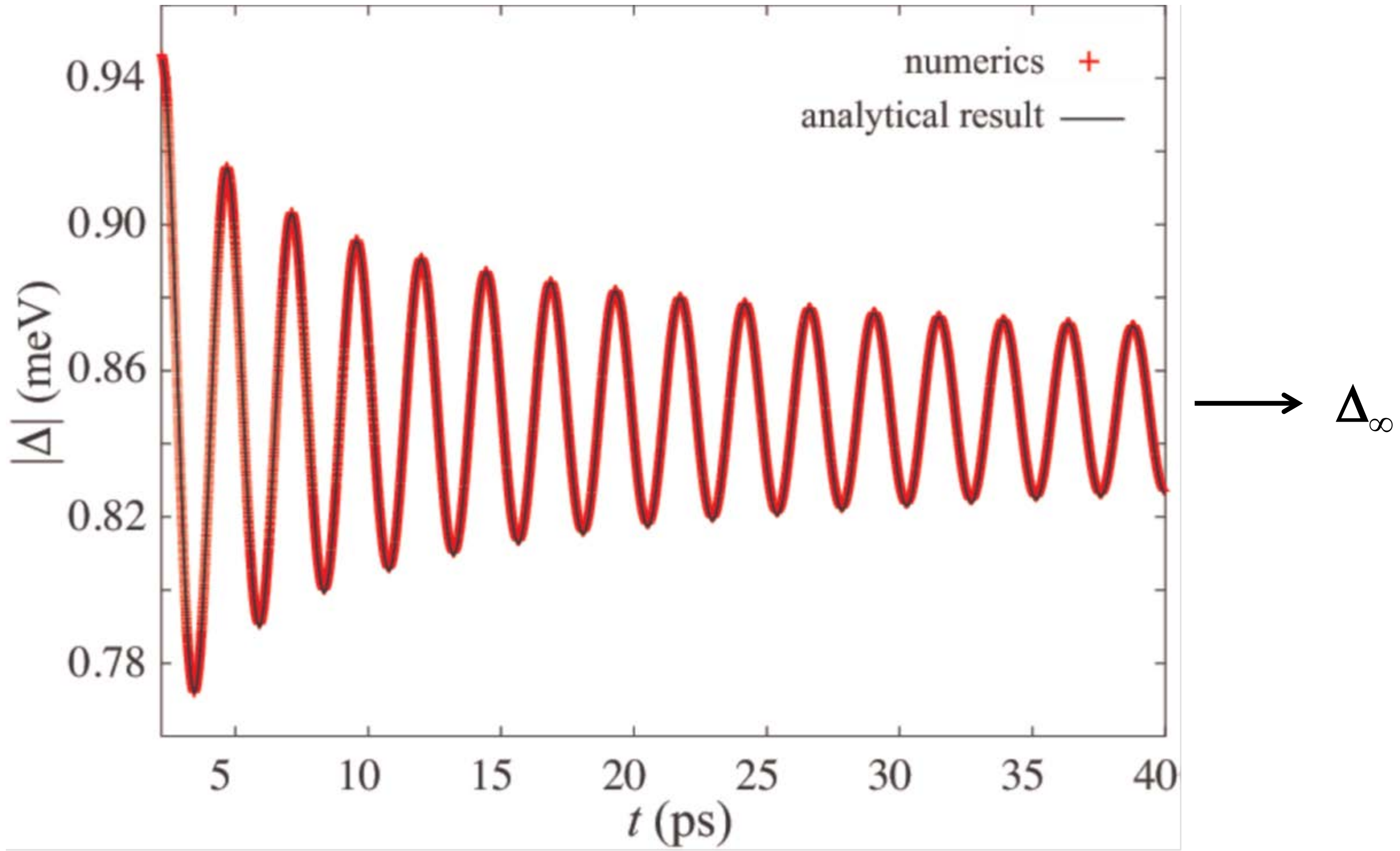
Order parameter oscillations: 2 regimes



lead:
$2\Delta_0$ = 2.7mev

Non-adiabatic regime: **gap continues to oscillate (Higgs) even when the pump pulse has been switched off long ago** $(\Delta(t{=}\infty) = \Delta_\infty)$

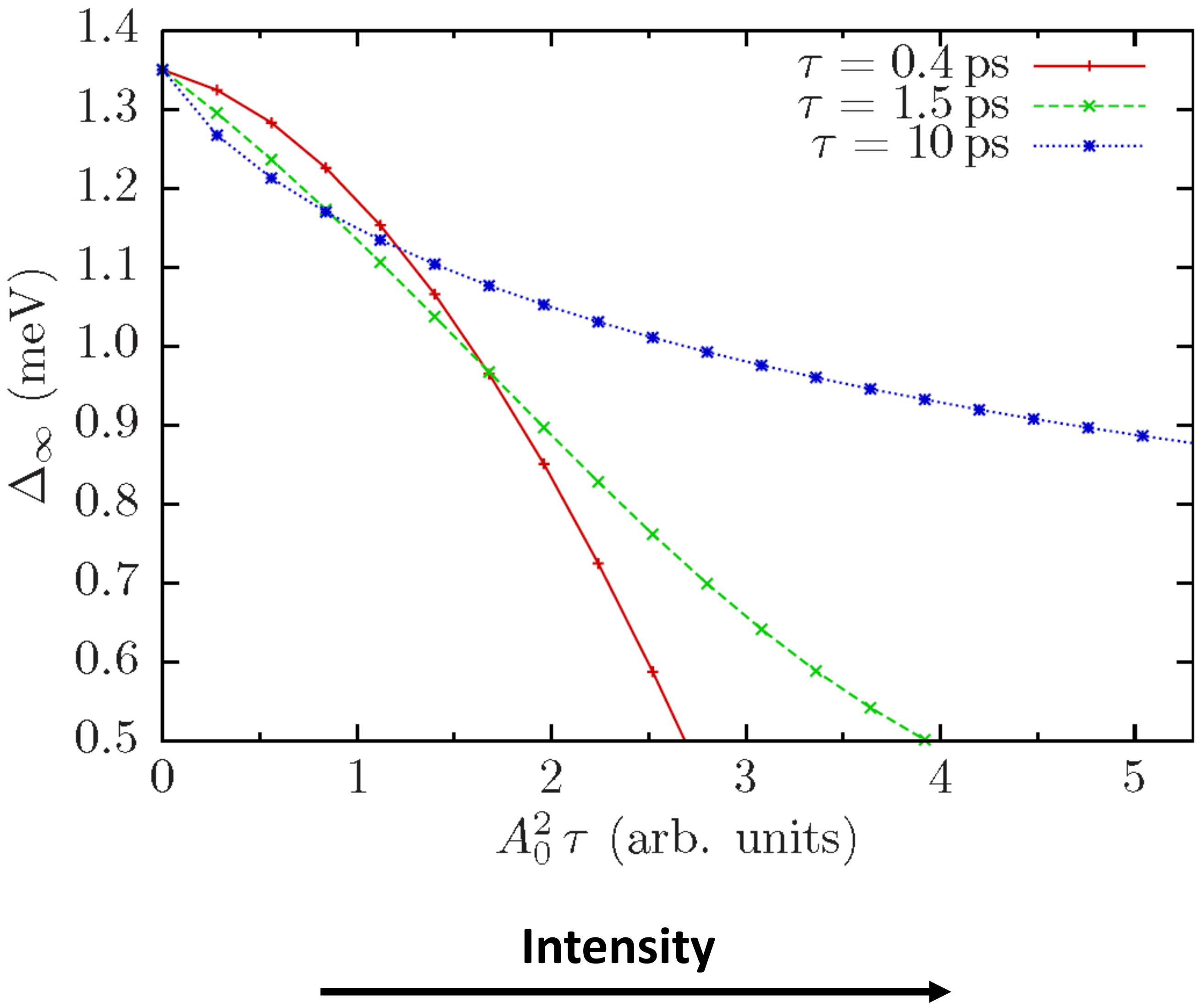
Analytic solution possible



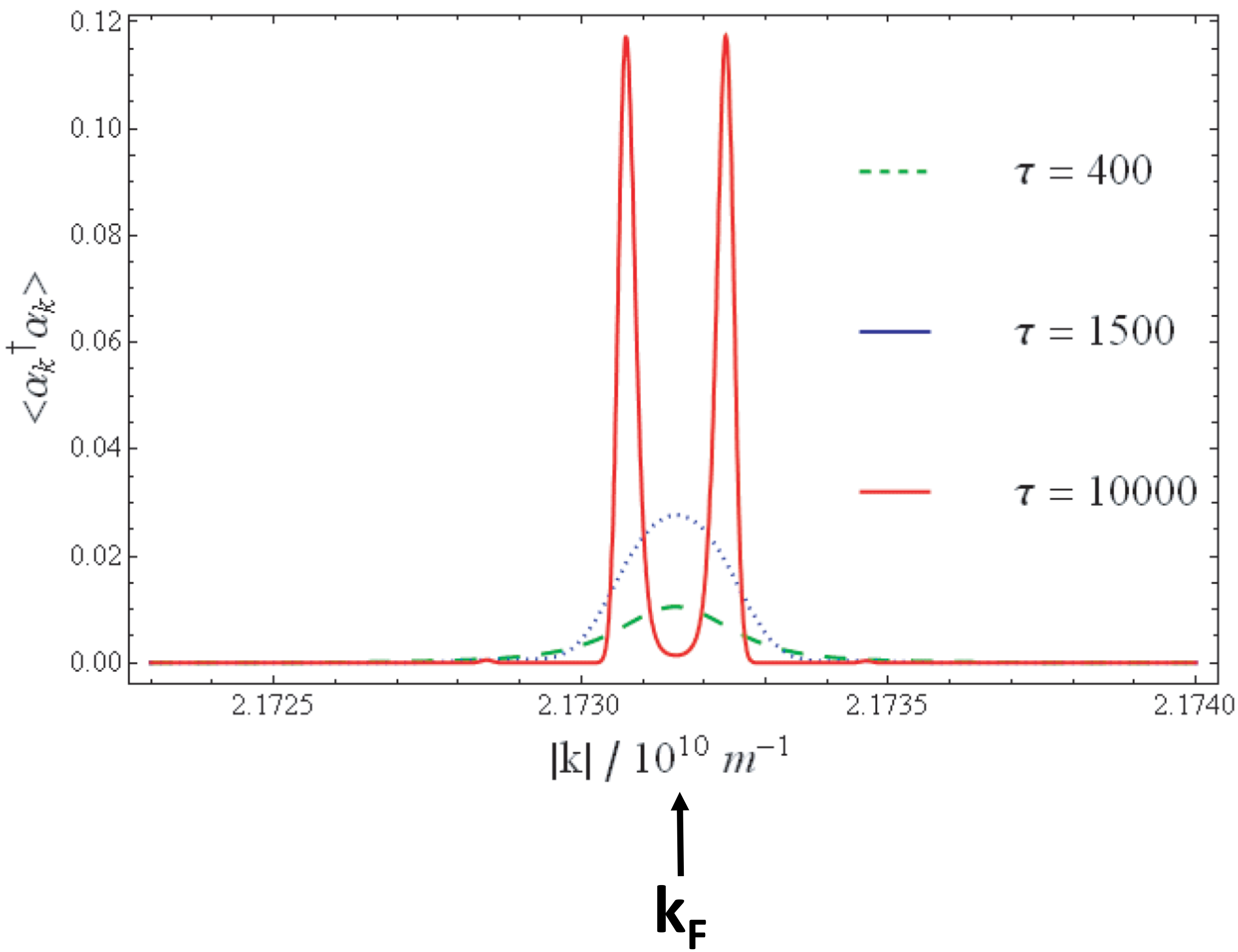
$$|\Delta| = |\Delta_\infty| + \Gamma \frac{\cos(\frac{2|\Delta_\infty|}{\hbar}t + \Phi)}{\sqrt{t}}$$

Yuzbashyan, Tsyplyatyev, Altshuler, PRL 2006

Intensity dependence

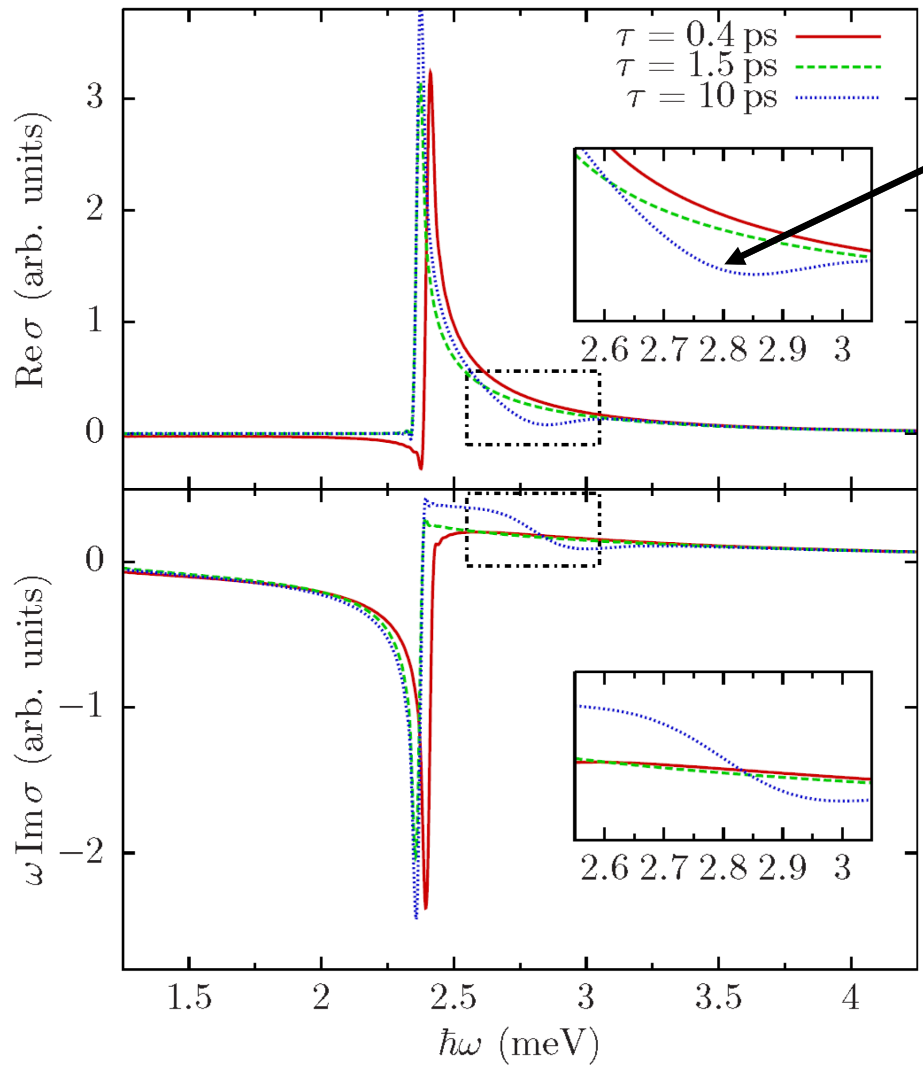


Quasiparticle occupations: no oscillations



- **Peak position(s) related to pump energy**

Probe spectra: no oscillations (well known)



Pauli blocking

- **Gap oscilllations cannot be perceived by means of a simple probe specrum**

See also:
Papenkort, Axt, and Kuhn, PRB '07

Case II: single band, coherent phonons $\langle b \rangle \neq 0$

Role of	τ_p ...	pulse duration
	τ_{ph} ...	phonon period
and	τ_Δ ...	dynamical time scale $\sim h / (2\|\Delta\|)$?

Density-Matrix Formalism

No bath approximation $\longrightarrow$ Cluster expansion:

coupling of phonon-assisted quantities such as

$$\langle \alpha_{\mathbf{k}+\mathbf{q}} \beta_{\mathbf{k}} b_{\mathbf{q}j} \rangle (t) \quad \text{and} \quad \langle \alpha^{+}_{\mathbf{k}_1+\mathbf{q}} \alpha_{\mathbf{k}_2} (b^{+}_{-\mathbf{q}j} + b_{\mathbf{q}j}) \rangle$$

→ solve numerically 6 Boltzmann-like equations

Phonon equations for $B_{\boldsymbol{q}} = \langle b_{\boldsymbol{q}} \rangle$ **and** $B^{*}_{-\boldsymbol{q}} = \langle b^{\dagger}_{-\boldsymbol{q}} \rangle$

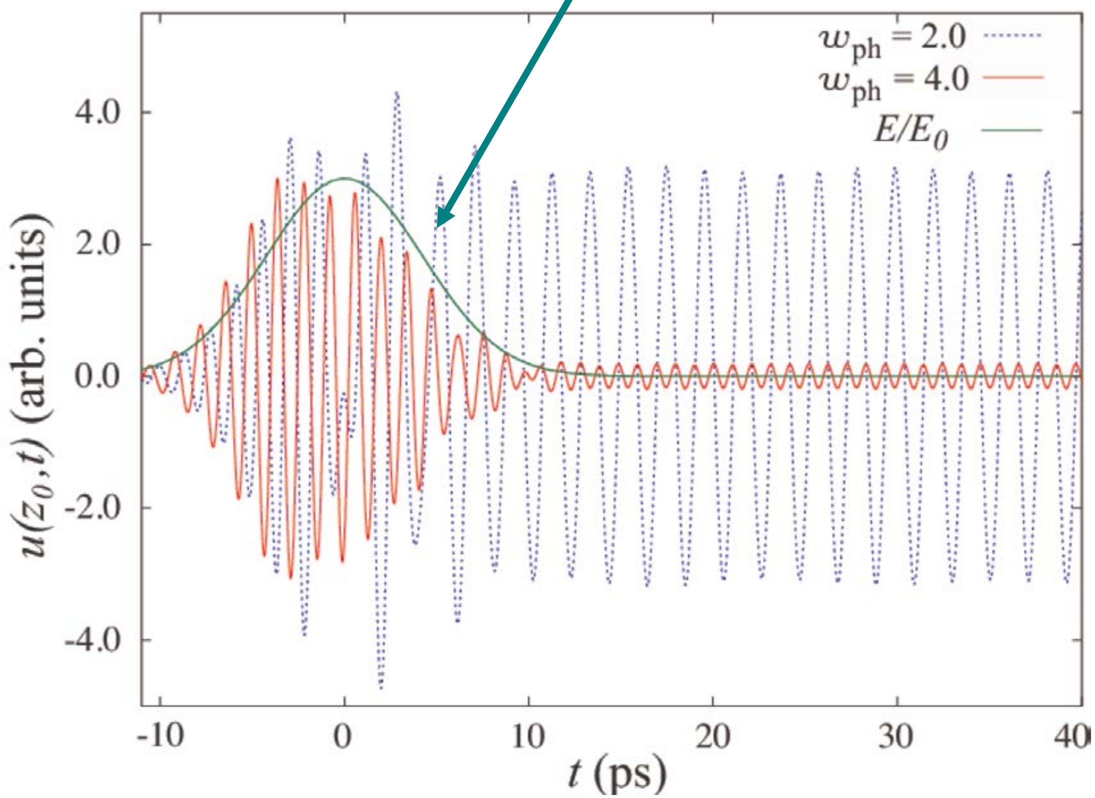
$$\boxed{\frac{d}{dt} B_{\boldsymbol{p}} = -i\omega_{\boldsymbol{p}} B_{\boldsymbol{p}} - \frac{i}{\hbar} g_{\boldsymbol{p}} \mathcal{F}(t)}$$

$$\mathcal{F}(t) = \sum_{\boldsymbol{k}} \Big[M^{+}_{\boldsymbol{k},\boldsymbol{p}} \Big(\langle \alpha_{\boldsymbol{k}+\boldsymbol{p}} \beta_{\boldsymbol{k}} \rangle - \langle \alpha^{\dagger}_{\boldsymbol{k}} \beta^{\dagger}_{\boldsymbol{k}+\boldsymbol{p}} \rangle \Big) + L^{-}_{\boldsymbol{k},\boldsymbol{p}} \Big(\langle \alpha^{\dagger}_{\boldsymbol{k}} \alpha_{\boldsymbol{k}+\boldsymbol{p}} \rangle + \langle \beta^{\dagger}_{\boldsymbol{k}+\boldsymbol{p}} \beta_{\boldsymbol{k}} \rangle \Big) \Big]$$

$$M^{+}_{\boldsymbol{k},\boldsymbol{p}} = v_{\boldsymbol{k}} u_{\boldsymbol{k}+\boldsymbol{p}} + u_{\boldsymbol{k}} v_{\boldsymbol{k}+\boldsymbol{p}}$$

Phonon amplitude: Adiabatic regime $\tau_p > \tau_\Delta , \tau_{ph}$

pulse

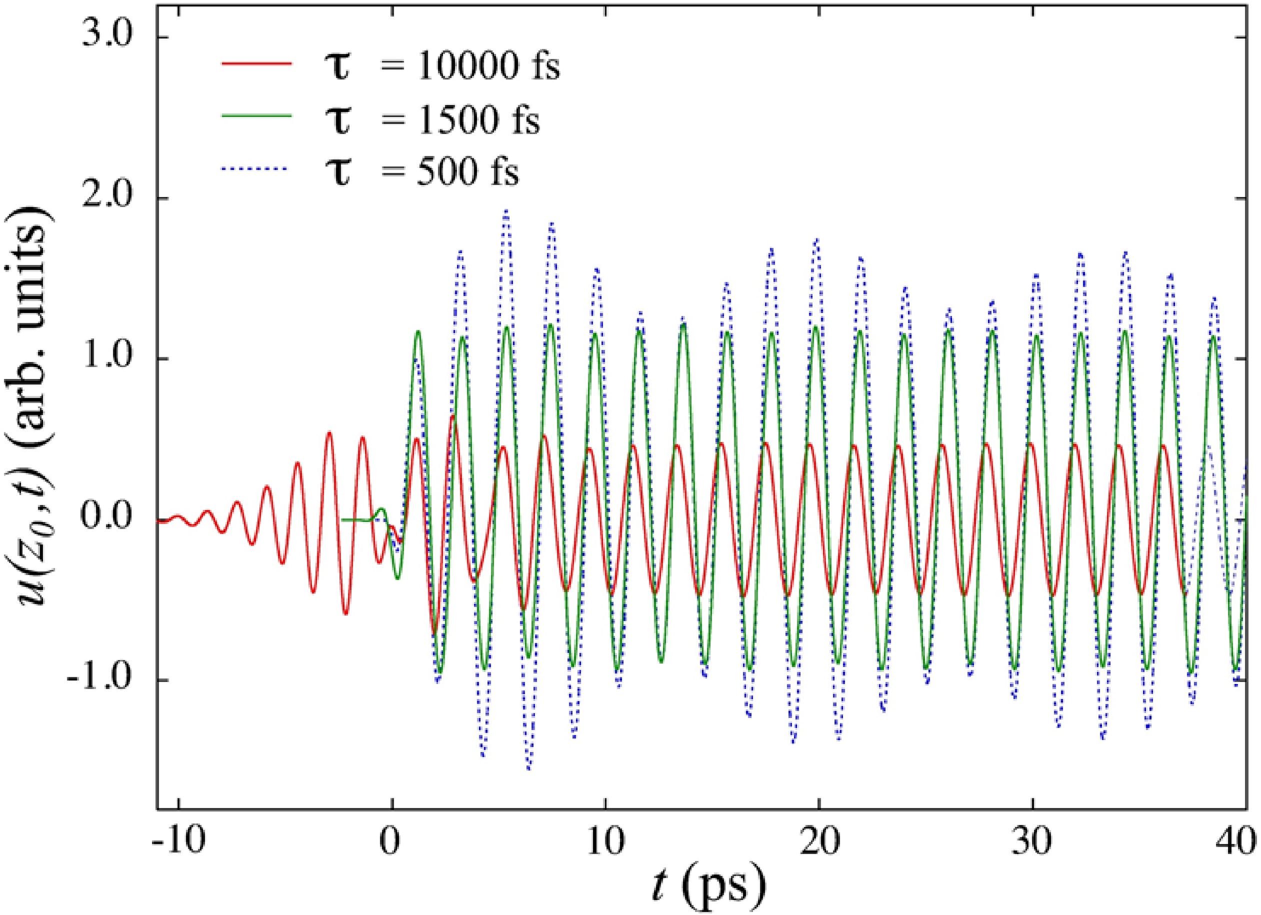


τ_p = 20000fs
Δ = 1.35

- only transient effect, <u>no</u> coupling to Higgs oscillations

- Creation of coherent phonons possible for $\tau_{ph} < \tau_\Delta << \tau_p$
- Inclusion of incoherent phonons would lead to damping

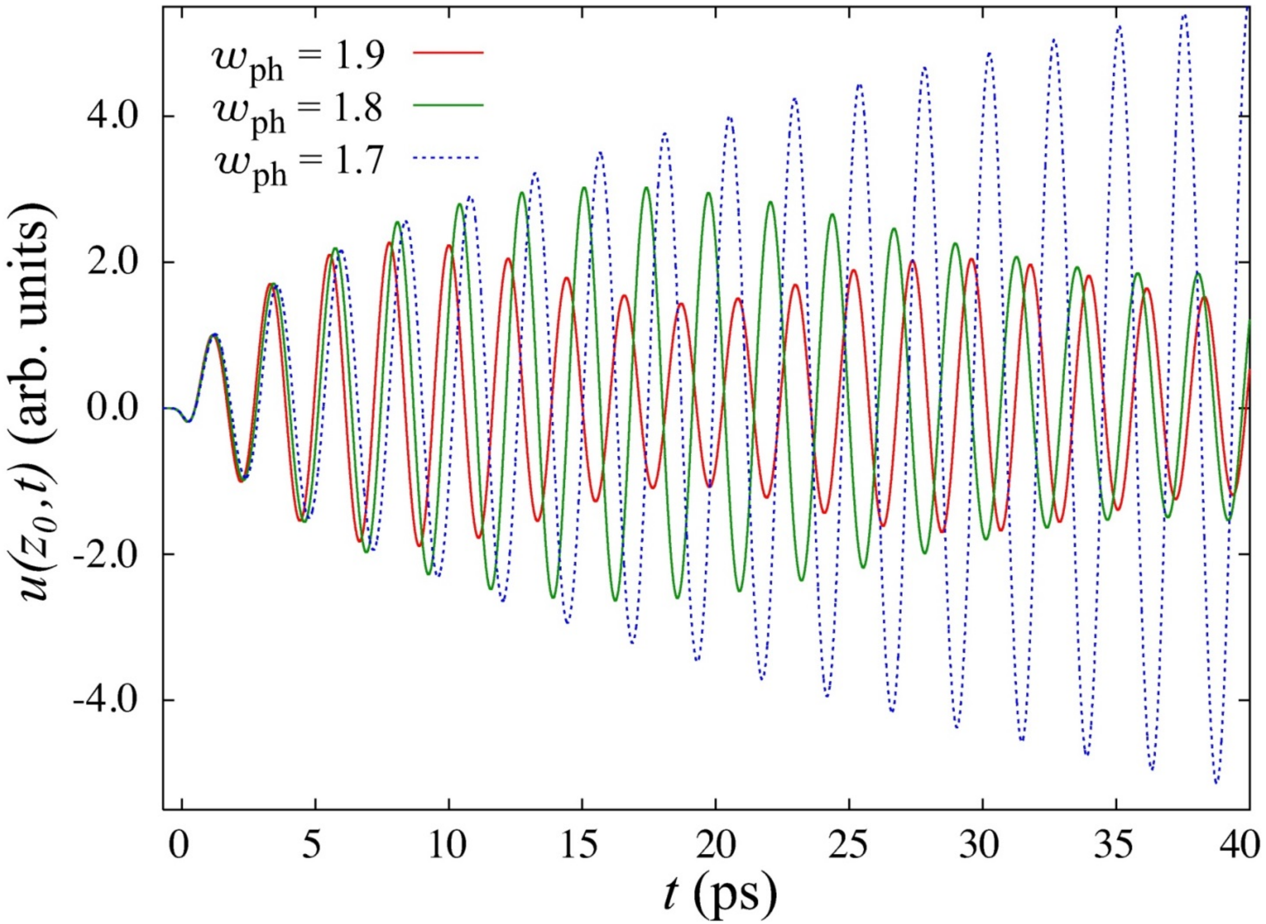
Crossover to non-adiabatic regime



ω_{ph} = 2.0
Δ = 1.35

- **Occurence of Quantum beats:** $|2\Delta_\infty/\hbar - \omega_{\rm ph}| \ll \omega_{\rm ph}$

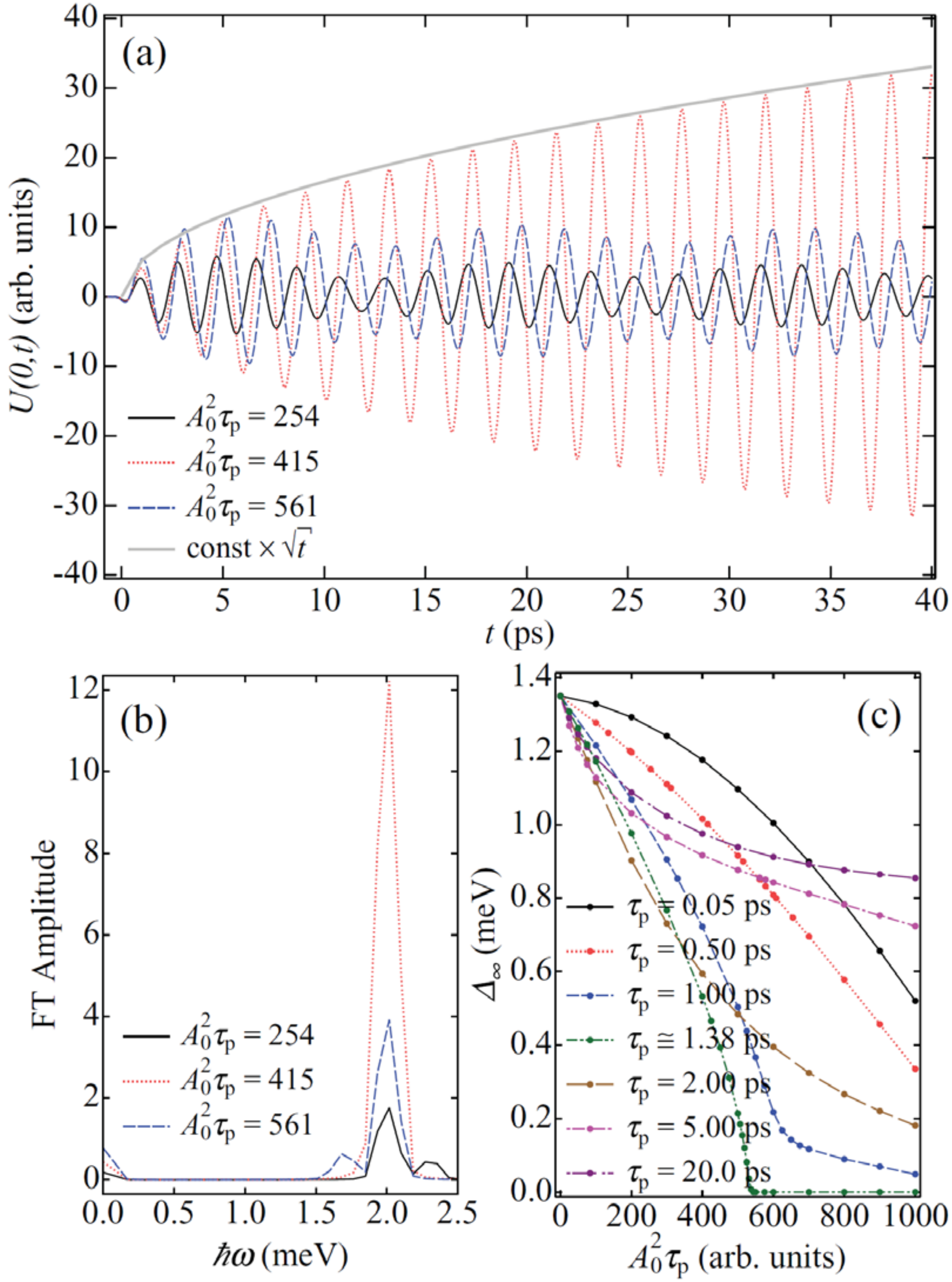
Non-adiabatic regime $\tau_p < \tau_\Delta$



τ_p = 500fs
Δ= 1.35

Δ_∞ = 0.85

- **Coherent phonons are resonantly enhanced**



- **off-resonant:**

$2\Delta_\infty$ = 1.7 and 2.3meV

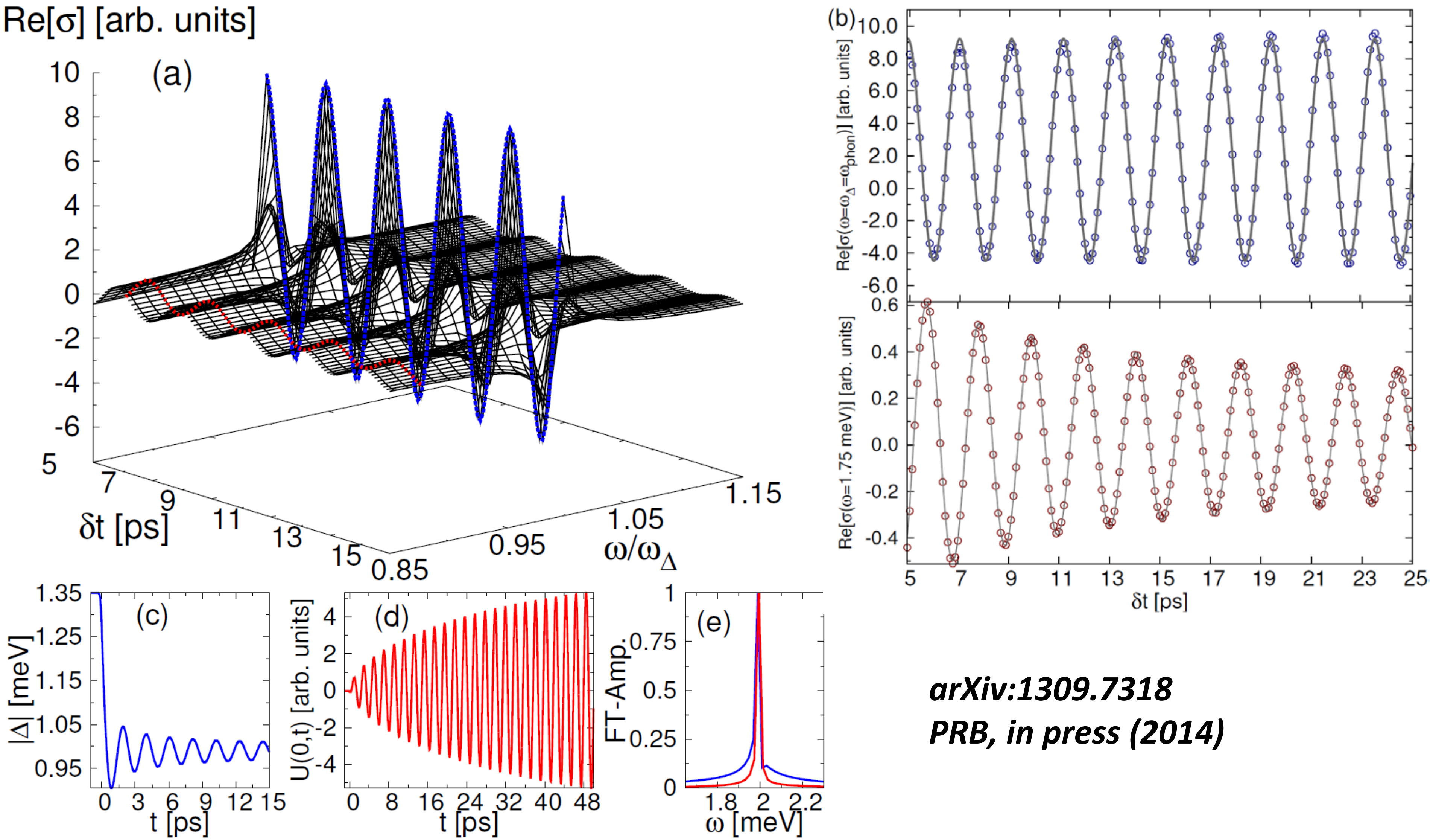
- **resonant:**

$2\Delta_\infty$ = 2.0meV = ω_{ph}

- **tune the order parameter oscillations exactly to resonance by adjusting the integrated pump intensity**

PRB 84, 214513 (2011)

Order parameter oscillations: theory



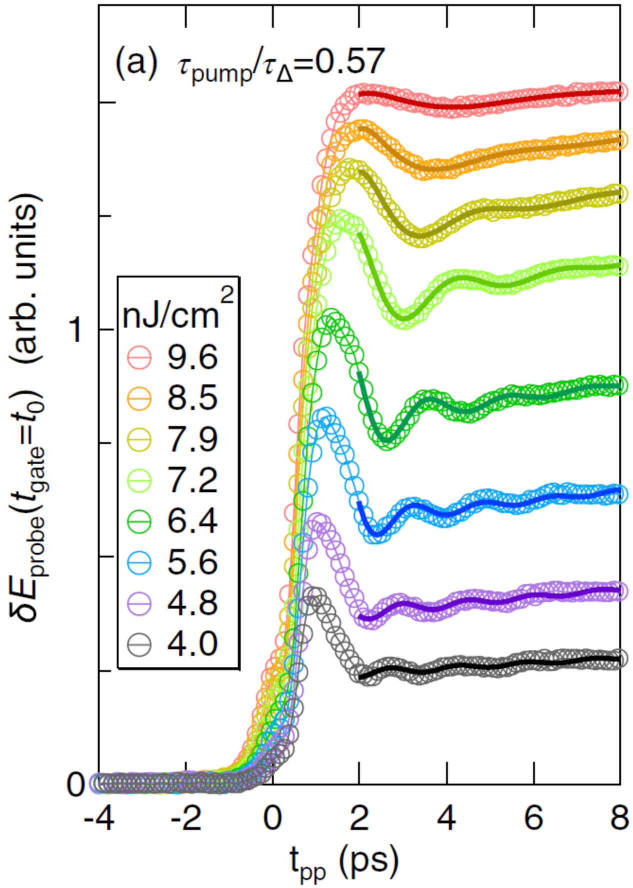
arXiv:1309.7318

PRB, in press (2014)

Order parameter oscillations: Experiment (1)

PRL **111**, 057002 (2013) PHYSICAL REVIEW LETTERS week ending 2 AUGUST 2013

Higgs Amplitude Mode in the BCS Superconductors $Nb_{1-x}Ti_xN$ Induced by Terahertz Pulse Excitation



- s-wave superconductor, non-adiabatic regime
- oscillation frequency in excellent accordance with asymptotic gap value
- collective Higgs mode detected

Ryo Shimano and co-workers, University of Tokyo

Order parameter oscillations: Experiment (2)

arXiv.org > cond-mat > arXiv:1112.0737

Search or A

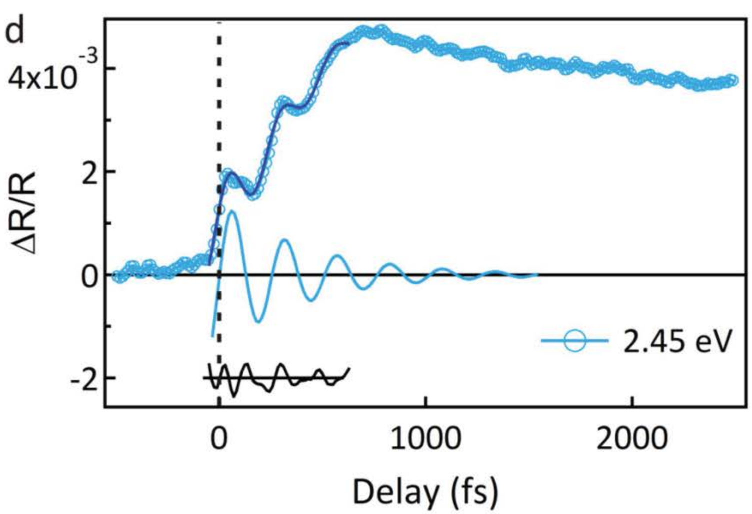
Condensed Matter > Superconductivity

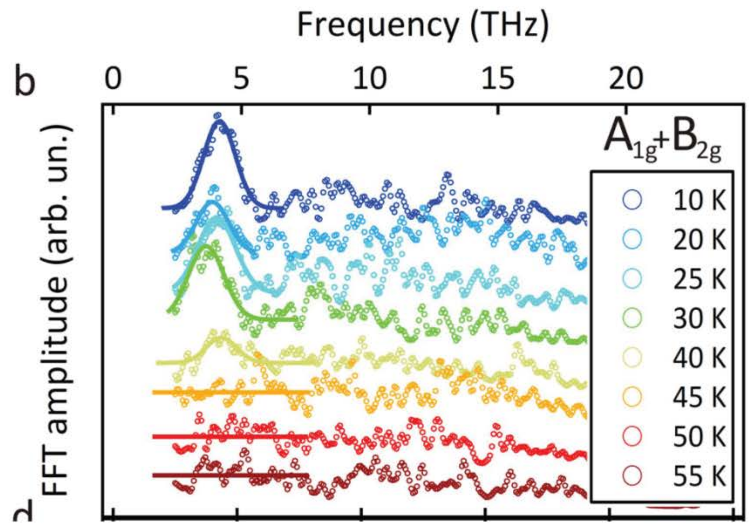
PNAS 2013

Direct observation of real-time oscillations of the Cooper-pairs condensate in a high-Tc superconductor

B. Mansart, J. Lorenzana, M. Scarongella, M. Chergui, F. Carbone

- Pump-probe optical spectroscopy of LSCO (Tc = 40 K); 1.55 eV laser
- Oscillations observed with period of same order as $\tau_\Delta \sim h/(2\,|\Delta|)$





Case III: single band, phonons in equilibrium $\langle b \rangle = 0$ (bath approximation)

Motivation: time-resolved Raman scattering

Density-Matrix Formalism (bath approximation)

apply Markovian approximation (energy conservation), then:

$$\partial_t \langle \alpha^+_{\mathbf{k}} \alpha_{\mathbf{k}} \rangle = -\frac{ie}{m} \mathbf{k} \cdot \mathbf{A}_{\mathbf{q}} M_{\mathbf{kq}} \left(\langle \alpha_{\mathbf{k}} \beta_{\mathbf{k}} \rangle - \langle \alpha^+_{\mathbf{k}} \beta^+_{\mathbf{k}} \rangle \right)$$

$$+ \sum_{\mathbf{qj}} \frac{\pi |g_{\mathbf{q}j}|^2}{\hbar^2} \Big(\Gamma^{(1)}_{\mathbf{kq}j} \langle \alpha^+_{\mathbf{k}} \alpha_{\mathbf{k}} \rangle (1 - \langle \alpha^+_{\mathbf{k+q}} \alpha_{\mathbf{k+q}} \rangle)$$

$$- \Gamma^{(2)}_{\mathbf{kq}j} \langle \alpha^+_{\mathbf{k+q}} \alpha_{\mathbf{k+q}} \rangle (1 - \langle \alpha^+_{\mathbf{k}} \alpha_{\mathbf{k}} \rangle) - \Gamma^{(3)}_{\mathbf{kq}j} \langle \beta^+_{\mathbf{k+q}} \beta_{\mathbf{k+q}} \rangle \langle \alpha^+_{\mathbf{k}} \alpha_{\mathbf{k}} \rangle \Big)$$

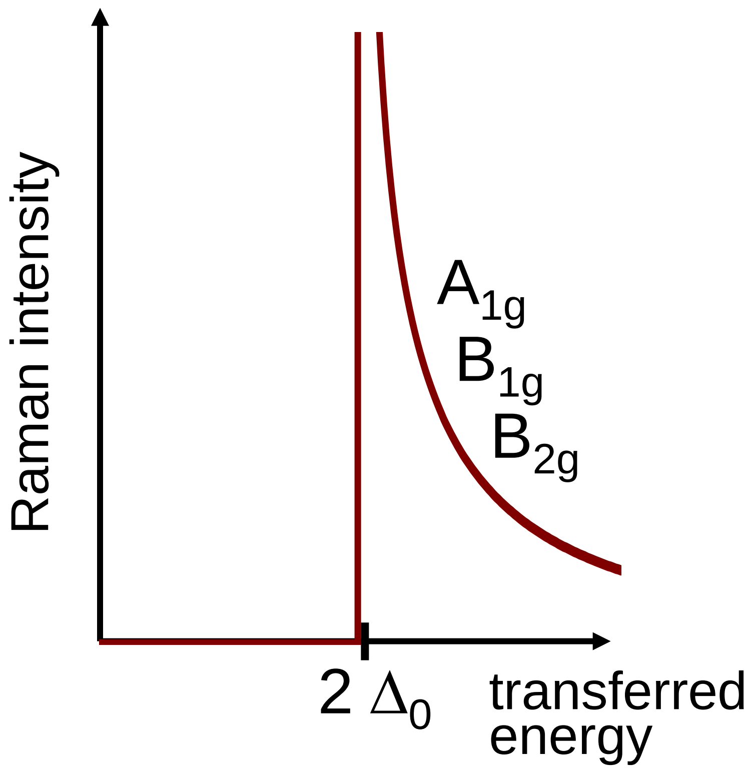
with $M_{\mathbf{kq}} = u_{\mathbf{k}_+\mathbf{q}} v_{\mathbf{k}} - v_{\mathbf{k+q}} u_{\mathbf{k}}$ $\qquad L_{\mathbf{kq}} = u_{\mathbf{k+q}} u_{\mathbf{k}} + v_{\mathbf{k+q}} v_{\mathbf{k}}$

$$\Gamma^{(1)}_{\mathbf{kq}j} = (1 + n_{\mathbf{q}j}) u_{\mathbf{k+q}} u_{\mathbf{k}} L_{\mathbf{kq}} \delta(\omega_{\mathbf{k+q}} - \omega_{\mathbf{k}} + \omega_{\mathbf{q}j})$$

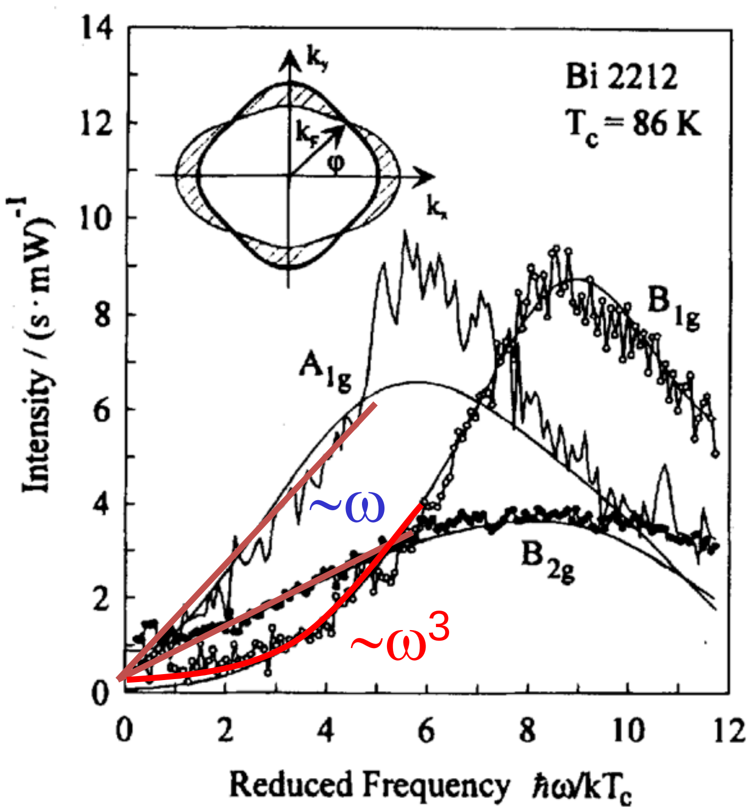
$$\Gamma^{(2)}_{\mathbf{kq}j} = n_{\mathbf{q}j} u_{\mathbf{k+q}} u_{\mathbf{k}} L_{\mathbf{kq}} \delta(\omega_{\mathbf{k+q}} - \omega_{\mathbf{k}} - \omega_{\mathbf{q}j})$$

$$\Gamma^{(3)}_{\mathbf{kq}j} = u_{\mathbf{k+q}} v_{\mathbf{k}} M_{\mathbf{kq}} \delta(\omega_{\mathbf{k+q}} - \omega_{\mathbf{k}} + \omega_{\mathbf{q}j})$$

Reminder: 'Conventional' Raman scattering



same spectra for
A_{1g}, B_{1g} and B_{2g}



polarization dependence

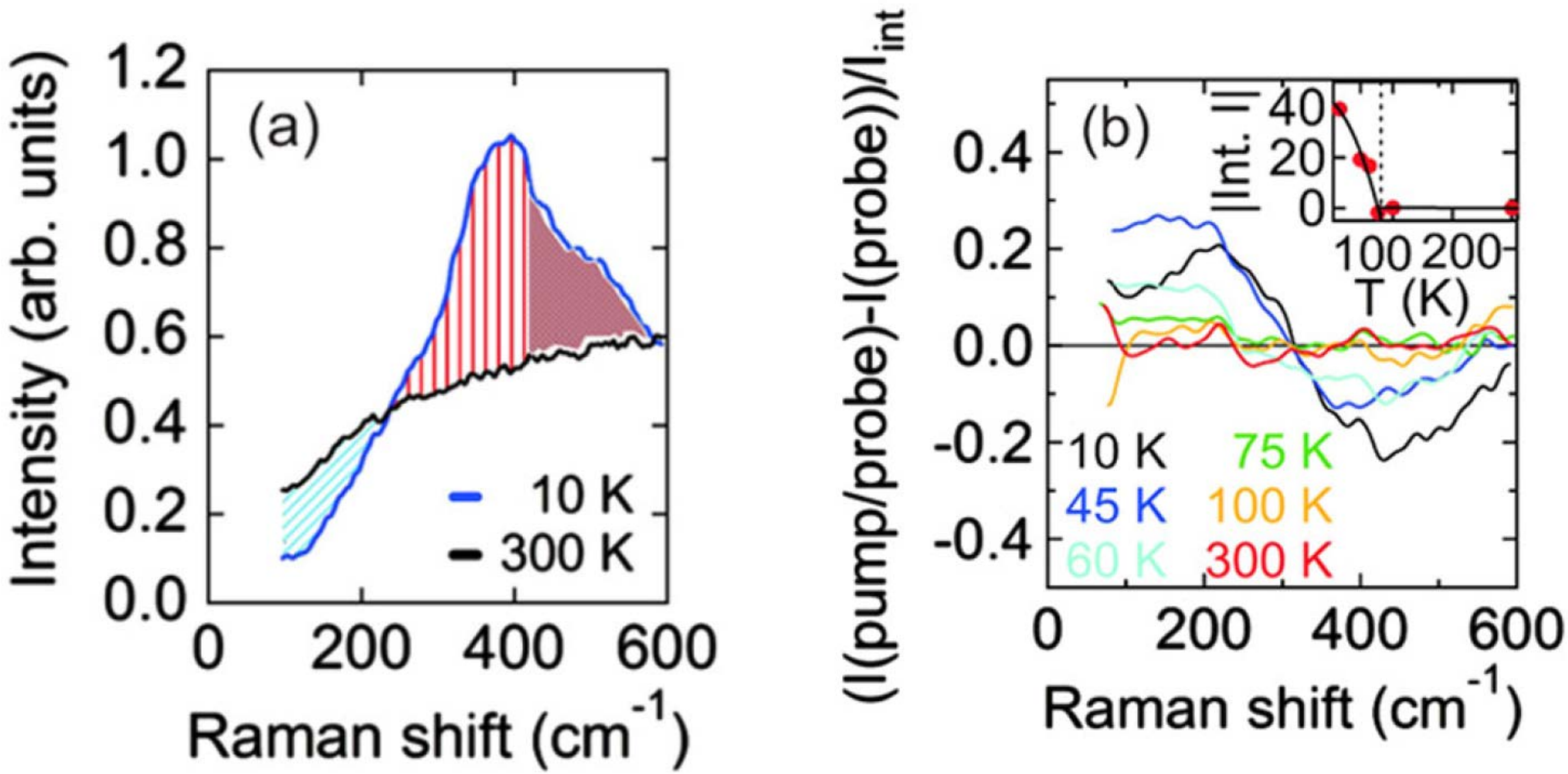
R. Hackl, D. Einzel *et al*. (1995)

$$B_{1g} \propto (\cos k_x - \cos k_y)$$

D. Manske *et al*. (PRB (RC)1997)

Exp.: Time-resolved Raman scattering (I)

Bi2212, B_{1g}-polarization

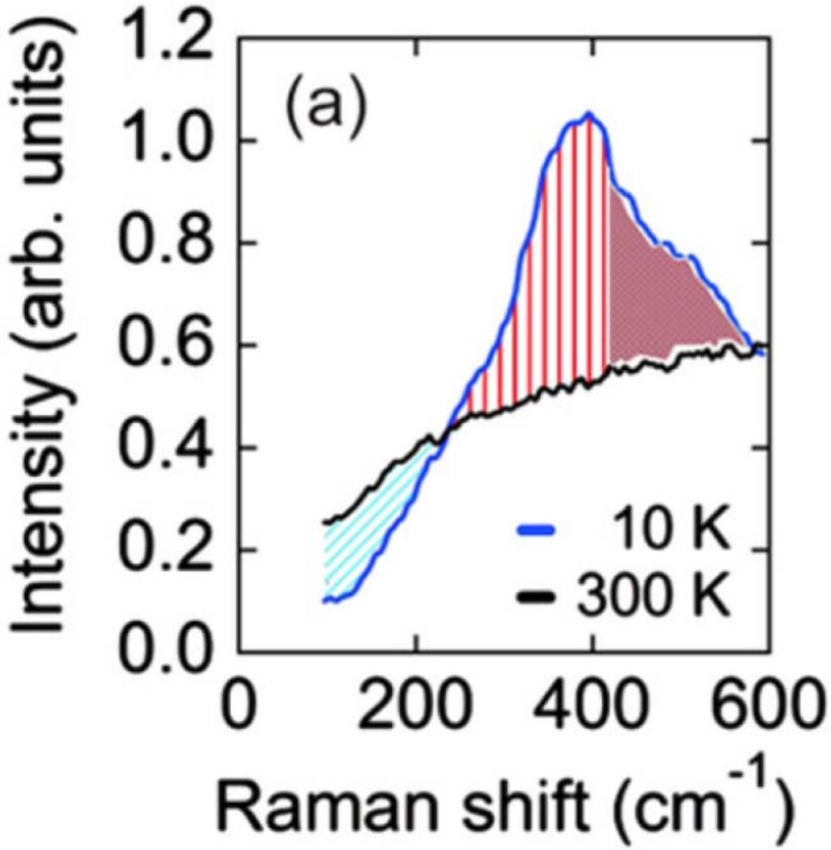


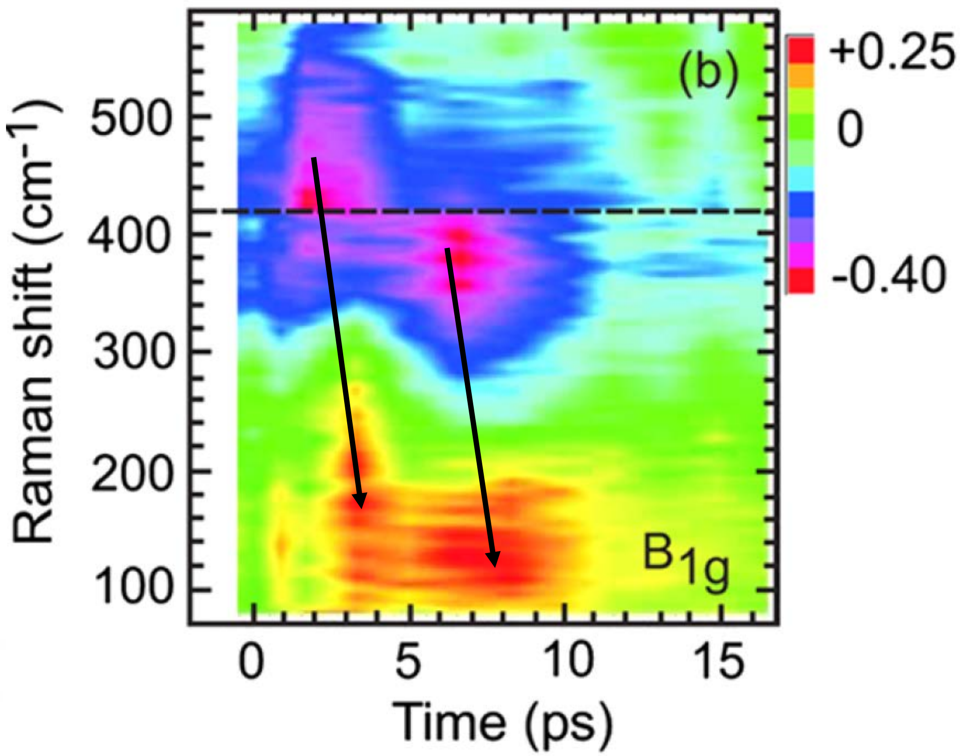
Phys. Rev. Lett. 102, 177004 (2009)

Δt = 3ps

Exp.: Time-resolved Raman scattering (II)

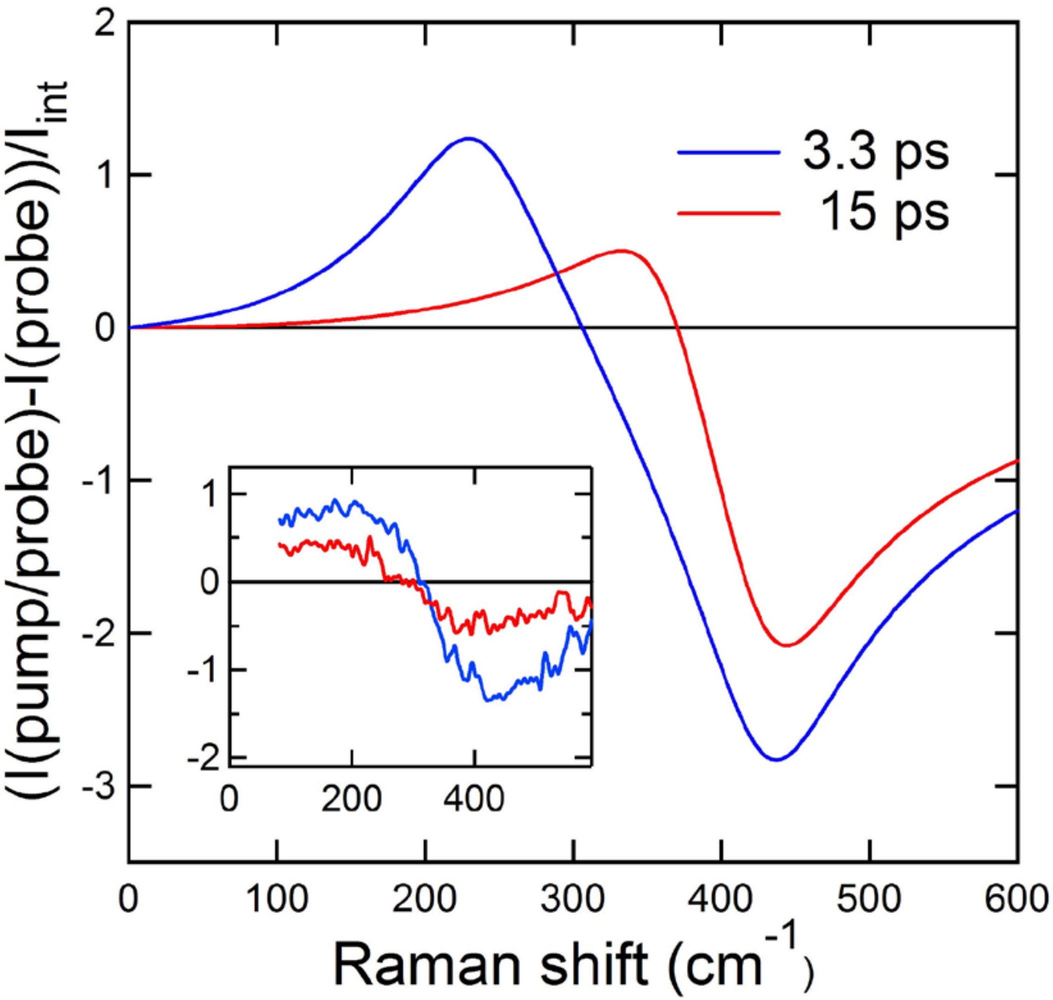
Bi2212, B_{1g}-polarization





Phys. Rev. Lett. 102, 177004 (2009)

Comparison with experiment



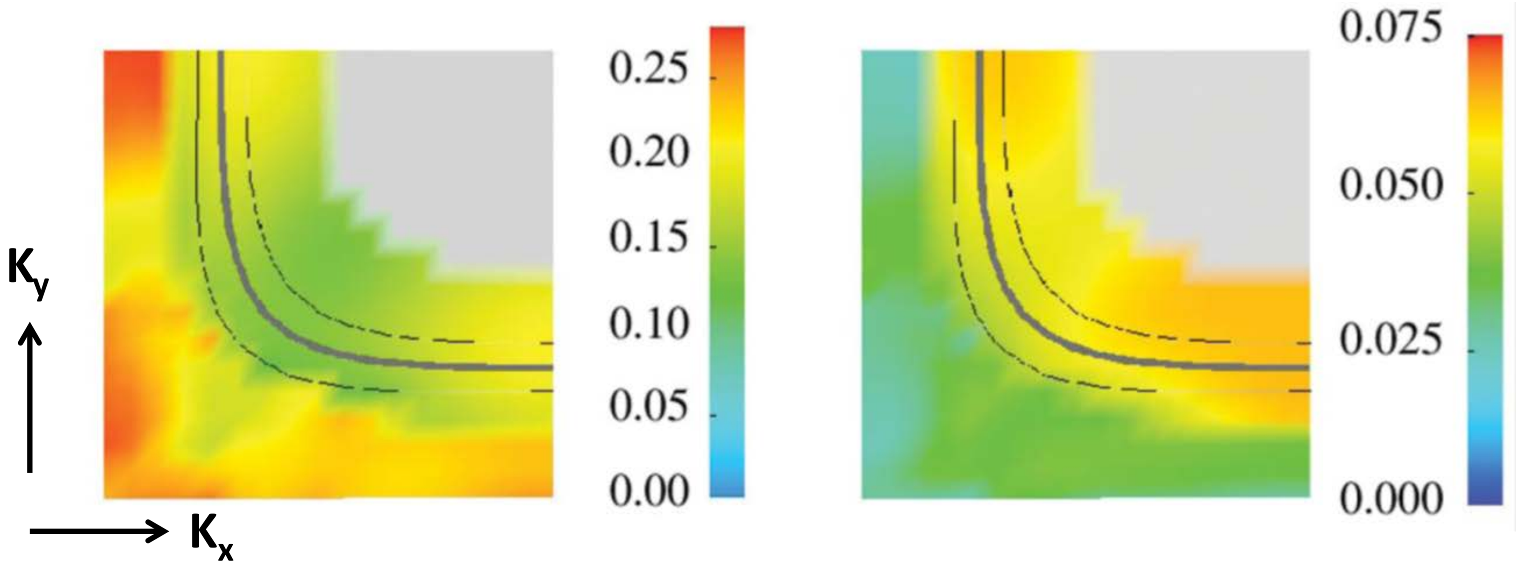
Phys. Rev. Lett. 102, 177004 (2009)

- **signatures of phonons**

Compare with YBCO, bonding band

- **LDA calculation of the electron-phonon coupling strength**

$$\lambda_\nu(\mathbf{k},\omega) = \frac{2}{\omega}\sum_{\mathbf{q},j,\mu} |g_j(\mathbf{k}\nu,\mathbf{k}+\mathbf{q}\mu)|^2 \cdot \delta(\omega-\omega_{\mathbf{q}j})\delta(\epsilon_{\mathbf{k}+\mathbf{q}\mu})$$

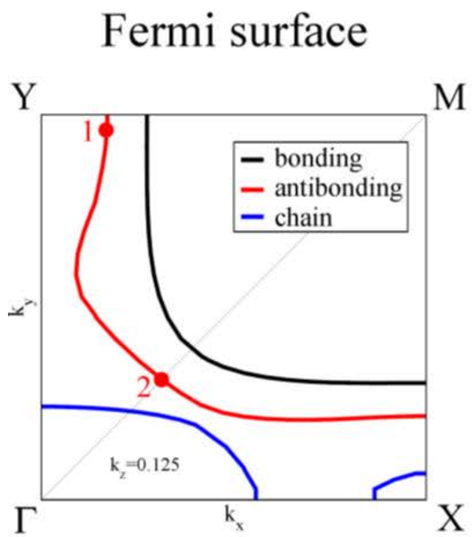


widely used assumptions:

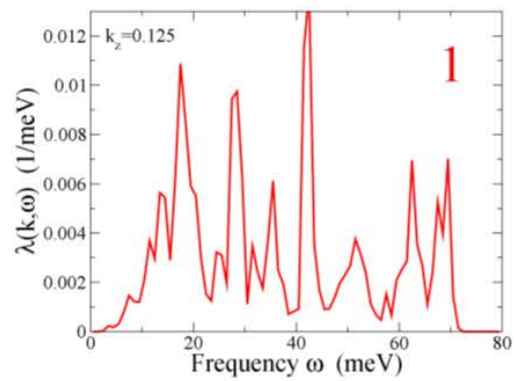
- **buckling mode $\propto$ $\cos^2(q_x/2) + \cos^2(q_y/2)$**
- **breathing mode $\propto$ $\sin^2(q_x/2) + \sin^2(q_y/2)$**

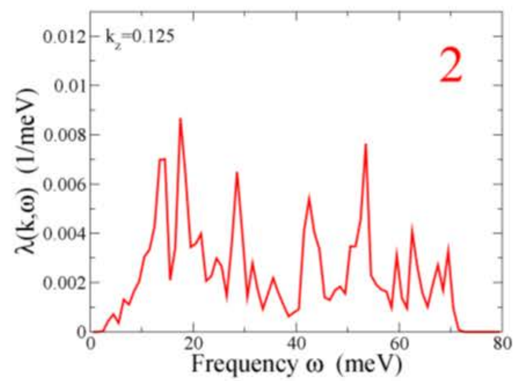
R. Heid, K.-P- Bohnen, R. Zeyher, and D. Manske, Phys. Rev. Lett. 100, 137001 (2009)

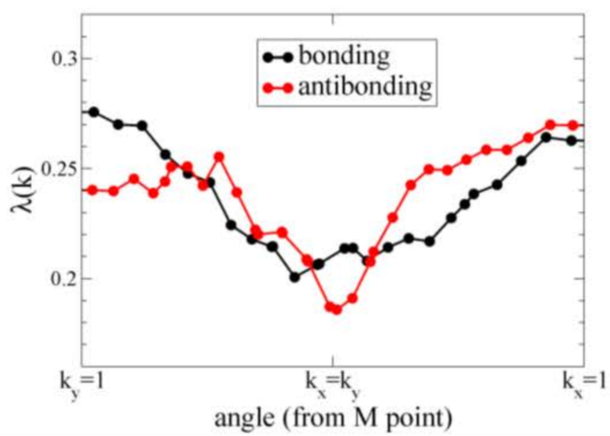
Momentum- and frequency-resolved coupling



$$\lambda_\nu(\mathbf{k},\omega) = \frac{2}{\omega}\sum_{\mathbf{q}j}\sum_{\nu'}|g^{\mathbf{q}j}_{\mathbf{k}\nu,\mathbf{k}+\mathbf{q}\nu'}|^2\delta(\epsilon_{\mathbf{k}+\mathbf{q}\nu'})\delta(\omega-\omega_{\mathbf{q}j})$$







$$\lambda_\nu(\mathbf{k}) = \int d\omega\,\lambda_\nu(\mathbf{k},\omega)$$

- weak anisotropy
- many phonon modes contribute

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Case IV: 2 bands, no phonons

Density-Matrix Formalism

$$
\begin{aligned}
i\hbar\frac{d}{dt}\langle\alpha^{\dagger}_{\gamma'\mathbf{k}'}\alpha_{\gamma\mathbf{k}}\rangle \;=\;& (\eta_{1\gamma\mathbf{k}}-\eta_{1\gamma'\mathbf{k}'})\langle\alpha^{\dagger}_{\gamma'\mathbf{k}'}\alpha_{\gamma\mathbf{k}}\rangle-\eta_{2\gamma\mathbf{k}}\langle\beta^{\dagger}_{\gamma\mathbf{k}}\alpha^{\dagger}_{\gamma'\mathbf{k}'}\rangle+\eta^{*}_{2\gamma'\mathbf{k}'}\langle\alpha_{\gamma\mathbf{k}}\beta_{\gamma'\mathbf{k}'}\rangle \\
&+\sum_{\gamma_0,\mathbf{q}'=\pm\mathbf{q}_0}-\frac{2e\hbar}{m}\mathbf{k}\cdot\mathbf{A}_{\mathbf{q}'}\Big(M^{+}_{\gamma\gamma_0\mathbf{k},\mathbf{k}\;\mathbf{q}'}\langle\alpha^{\dagger}_{\gamma'\mathbf{k}'}\alpha_{\gamma_0\mathbf{k}-\mathbf{q}'}\rangle+L^{-}_{\gamma\gamma_0\mathbf{k},\mathbf{k}\;\mathbf{q}'}\langle\beta^{\dagger}_{\gamma'\mathbf{k}\;\mathbf{q}'}\alpha^{\dagger}_{\gamma_0\mathbf{k}'}\rangle\Big) \\
&-M^{+}_{\gamma_0\gamma'\mathbf{k}'-\mathbf{q}',\mathbf{k}'}\langle\alpha^{\dagger}_{\gamma_0\mathbf{k}'+\mathbf{q}'}\alpha_{\gamma\mathbf{k}}\rangle-L^{-*}_{\gamma'\gamma_0\mathbf{k}',\mathbf{k}'+\mathbf{q}'}\langle\alpha_{\gamma\mathbf{k}}\beta_{\gamma_0\mathbf{k}'+\mathbf{q}'}\rangle\Big) \\
&+\sum_{\gamma_0,\mathbf{q}'=\pm\mathbf{q}_0;\;\mathbf{q}_i=0,\pm2\mathbf{q}_0}\frac{e^2}{2m}(\mathbf{A}_{\mathbf{q}'-\mathbf{q}_i}\cdot\mathbf{A}_{\mathbf{q}'})\times\Big(M^{-}_{\gamma\gamma_0\mathbf{k},\mathbf{k}\;\mathbf{q}'}\langle\alpha^{\dagger}_{\gamma'\mathbf{k}'}\alpha_{\gamma_0\mathbf{k}-\mathbf{q}'}\rangle+L^{+}_{\gamma\gamma_0\mathbf{k}\;\mathbf{q}',\mathbf{k}}\langle\beta^{\dagger}_{\gamma'\mathbf{k}\;\mathbf{q}'}\alpha^{\dagger}_{\gamma_0\mathbf{k}'}\rangle \\
&-M^{-}_{\gamma_0\gamma'\mathbf{k}'+\mathbf{q}',\mathbf{k}'}\langle\alpha^{\dagger}_{\gamma_0\mathbf{k}'+\mathbf{q}'}\alpha_{\gamma\mathbf{k}}\rangle-L^{+*}_{\gamma'\gamma_0\mathbf{k}',\mathbf{k}'+\mathbf{q}'}\langle\alpha_{\gamma\mathbf{k}}\beta_{\gamma_0\mathbf{k}'+\mathbf{q}'}\rangle\Big)
\end{aligned}
$$

$$
\eta_{1\gamma\mathbf{k}} \;=\; \frac{\hat{\varepsilon}_{\gamma\mathbf{k}}\hat{\varepsilon}^{\star}_{\gamma\mathbf{k}}+Re[\Delta^{*}_{\gamma\mathbf{k}}\Delta^{\star}_{\gamma\mathbf{k}}]}{E^{\star}_{\gamma\mathbf{k}}}
\qquad
\eta_{2\gamma\mathbf{k}} \;=\; \Delta^{\star}_{\gamma\mathbf{k}}\left[\frac{\hat{\varepsilon}_{\gamma\mathbf{k}}Re\left[\frac{\Delta_{\gamma\mathbf{k}}}{\Delta^{\star}_{\gamma\mathbf{k}}}\right]-\hat{\varepsilon}^{\star}_{\gamma\mathbf{k}}}{E^{\star}_{\gamma\mathbf{k}}}+iIm\left[\frac{\Delta_{\gamma\mathbf{k}}}{\Delta^{\star}_{\gamma\mathbf{k}}}\right]\right]
$$

→ solve numerically 8 Boltzmann-like equations (still no phonons)

Multiband effects

$$\Delta_{\gamma\mathbf{k}} = \sum_{\gamma'\mathbf{k}'} g^{\gamma\gamma'}_{\mathbf{k}\mathbf{k}'} \langle c_{\gamma' -\mathbf{k}'\downarrow} c_{\gamma'\mathbf{k}'\uparrow} \rangle$$

$$= \sum_{\gamma'\mathbf{k}'} g^{\gamma\gamma'}_{\mathbf{k}\mathbf{k}'} \Big[u_{\gamma'\mathbf{k}'} v_{\gamma'\mathbf{k}'} \big(\langle \alpha^{\dagger}_{\gamma'\mathbf{k}'} \alpha_{\gamma'\mathbf{k}'} \rangle + \langle \beta^{\dagger}_{\gamma'\mathbf{k}'} \beta_{\gamma'\mathbf{k}'} \rangle - 1 \big)$$

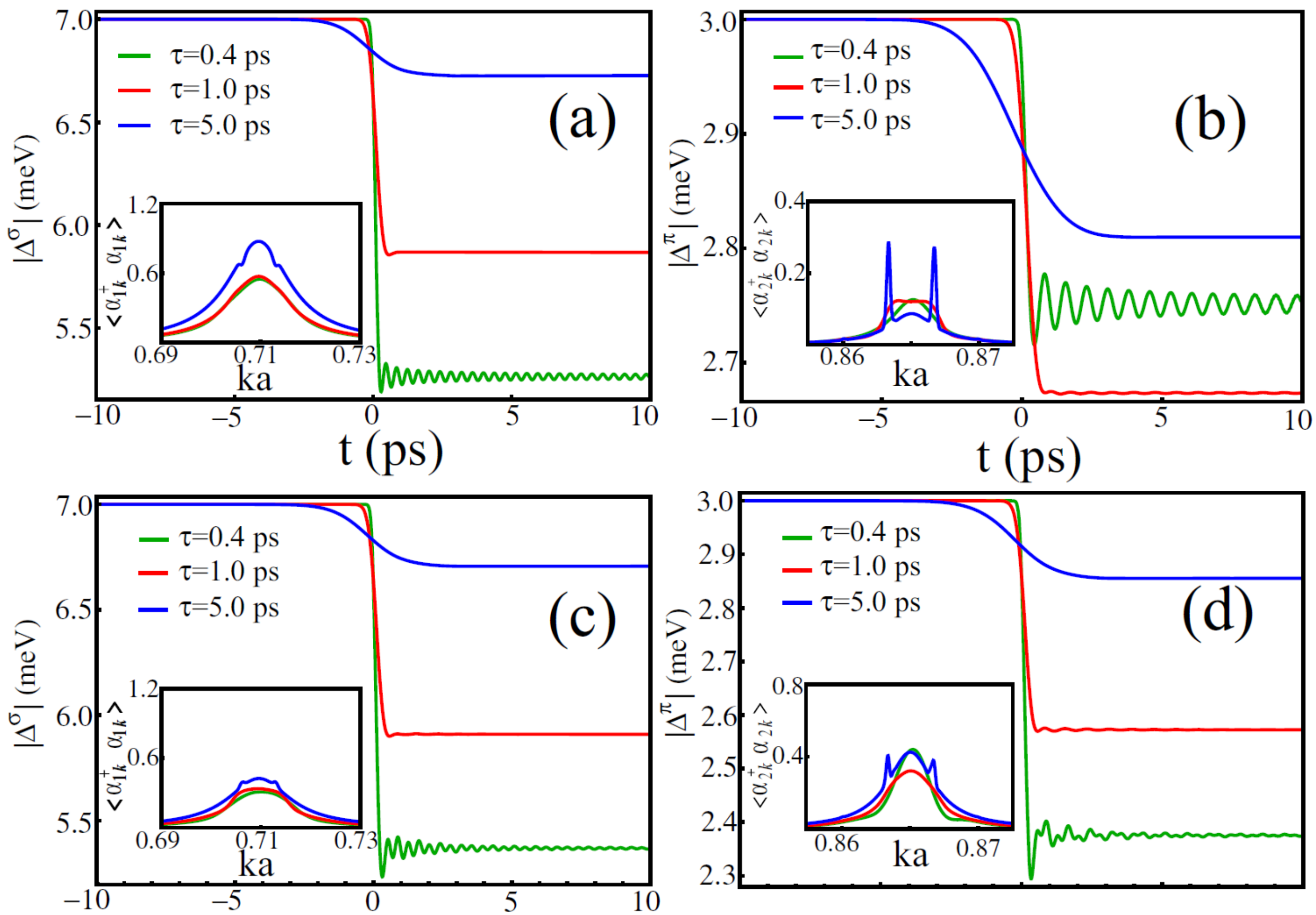
$$+ \quad u^2_{\gamma'\mathbf{k}'} \langle \beta_{\gamma'\mathbf{k}'} \alpha_{\gamma'\mathbf{k}'} \rangle + v^2_{\gamma'\mathbf{k}'} \langle \beta^{\dagger}_{\gamma'\mathbf{k}'} \alpha^{\dagger}_{\gamma'\mathbf{k}'} \rangle \Big]$$

Calculation for pnictides: $g^{11} = 0 = g^{22}$ and $g^{12} < 0$

$$|\Delta^l(t)| = |\Delta^l_\infty| + \sum_{l,l'} (a_{ll} + a_{ll'}) \frac{\cos(\omega_1 t + \phi_l)\cos(\omega_2 t + \phi_l)}{\sqrt{|\Delta^l_\infty| t}}$$

$$+ \quad (a_{ll} - a_{ll'}) \frac{\sin(\omega_1 t + \phi_l)\sin(\omega_2 t + \phi_l)}{\sqrt{|\Delta^l_\infty| t}}$$

Order parameter oscillations (1): MgB_2

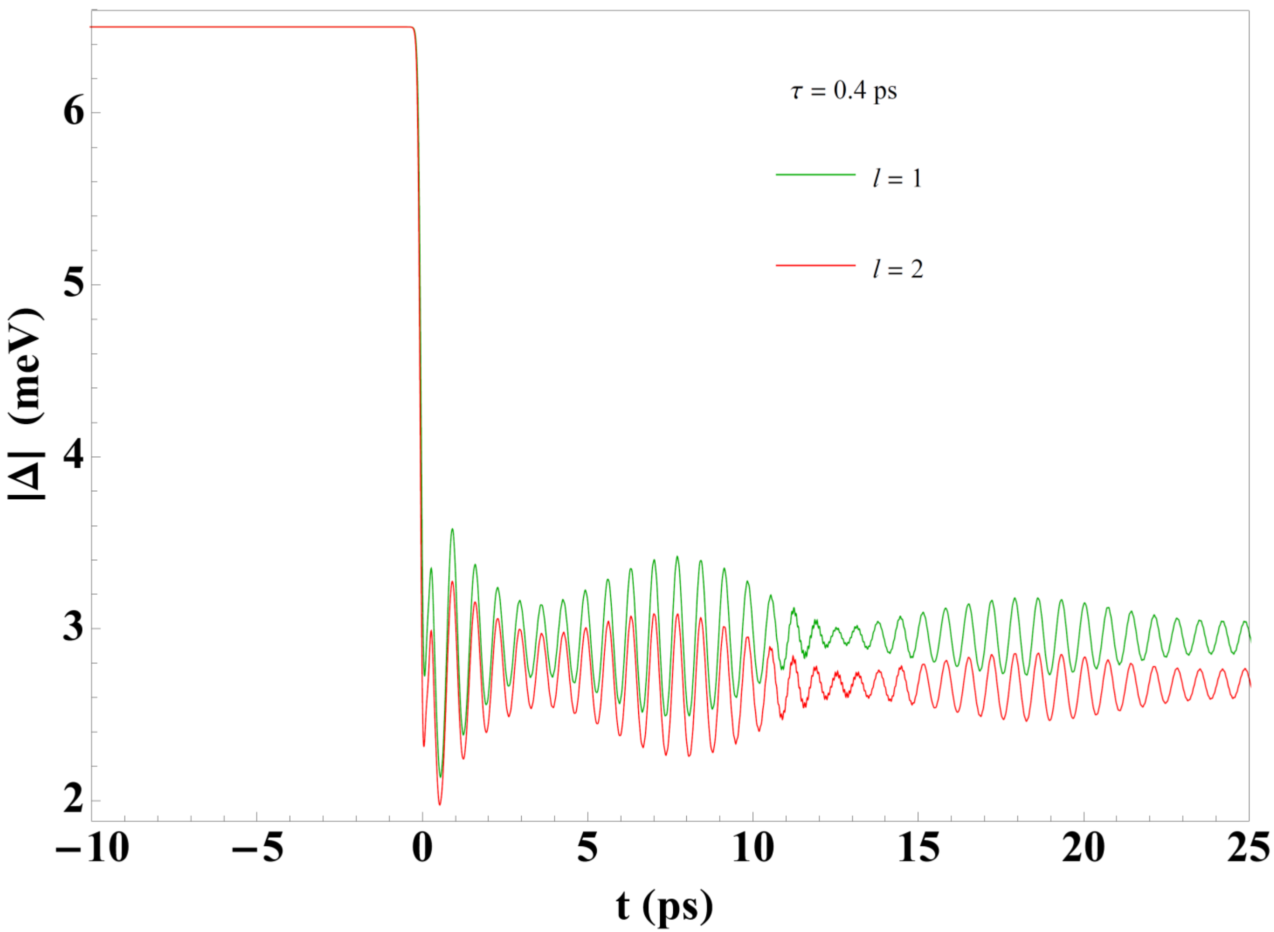


- **Characteristic changes due to inter-band scattering:**

2 coupled harmonic oscillators

A. Akbari *et al.*, EPL <u>101</u>. 17002 (2013)

Order parameter oscillations (2): pnictides ?



- **Quantum beats are possible**

Summary

Micoscopic theory for ultrafast dynamics in superconductors employing Density Matrix Theory:
What happens after the pump pulse?

- **case 1: no phonons, single band**

$\rightarrow$ OP oscillations in the non-adiabatic regime if $\tau_p < \tau_\Delta$

- **case 2: coherent phonons, single band**

$\rightarrow$ Quantum Beats and resonance effects if $|2\Delta_\infty/\hbar - \omega_{\mathrm{ph}}| \ll \omega_{\mathrm{ph}}$

- **case 3: incoherent (bath) phonons, single band**

$\rightarrow$ Comparison with time-resolved Raman scattering

- **case 4: no phonons, two bands**

$\rightarrow$ 2 damped oscillators, quantum beats

Outlook

● **consideration of non-centrosymmetric superconductors**
(E. Bauer and M. Sigrist (Eds.), 'Non-centrosymmetric superconductors', Lecture Notes in Physics 847, Springer 2012)

→ **Interdependence of singlet- and triplet-pairing**

● **light-induced superconductivity (A. Cavalleri, MPI)**

→ **Pumping pre-formed pairs (within Density-Matrix Theory)**

● **consideration of strong electron-electron interaction**
(together with T. Tohyama (Tokyo), 1D extended Hubbard model)

END OF TALK

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Thank you!

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