Theory of ultrafast dynamics in superconductors

PRB 92, 224517 (2015)
PRB 93, 144506 (2016)
arXiv:1611.04307
arXiv:1607.02314

Collaborators:
A. F. Kemper, B. Moritz, J. K. Freericks, T. P. Devereaux,
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E. Pomarico, I. Gierz, A. Cavalleri

Michael Sentef

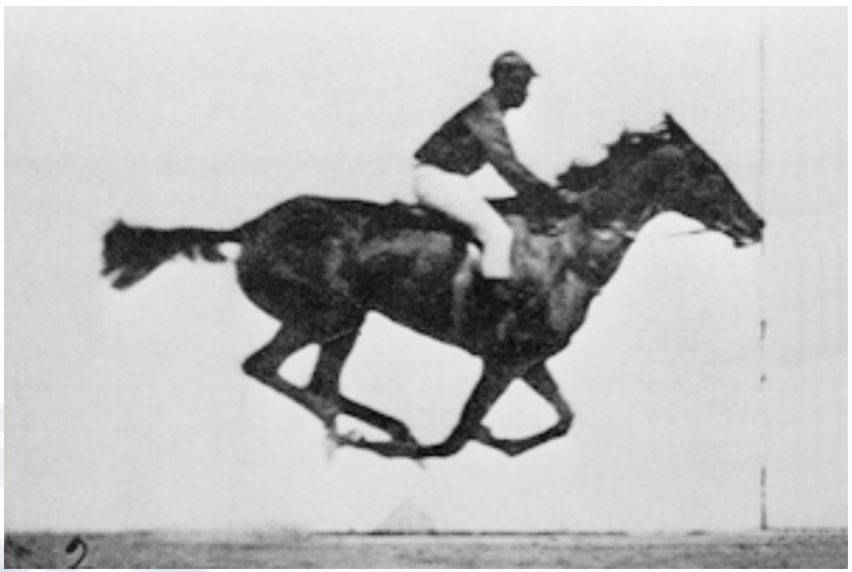
SFB 1242 Kickoff Meeting

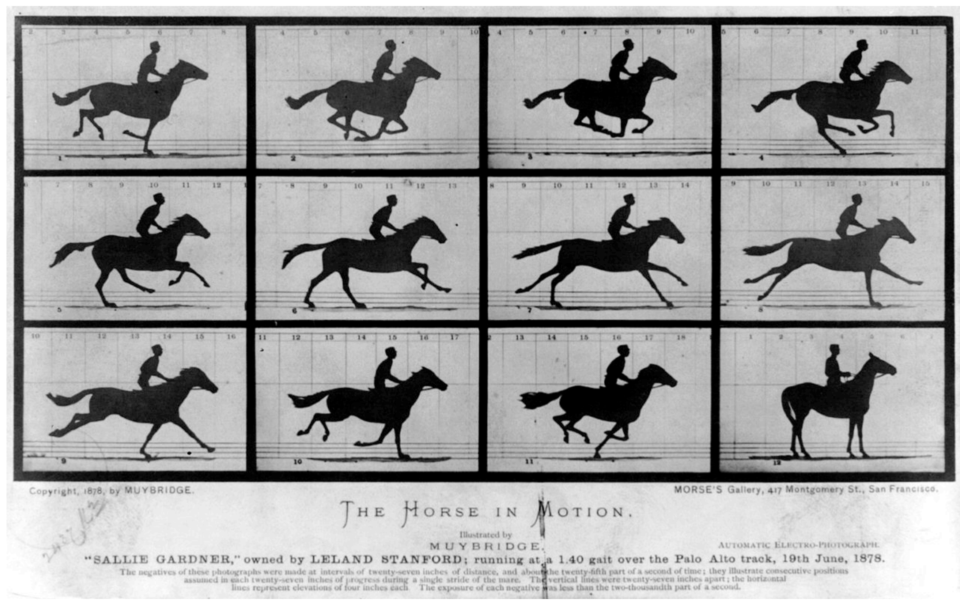
Bad Honnef, November 23, 2016

Max Planck Institute for the Structure and Dynamics of Matter

Pump-probe spectroscopy (1887)

- stroboscopic investigations of dynamic phenomena



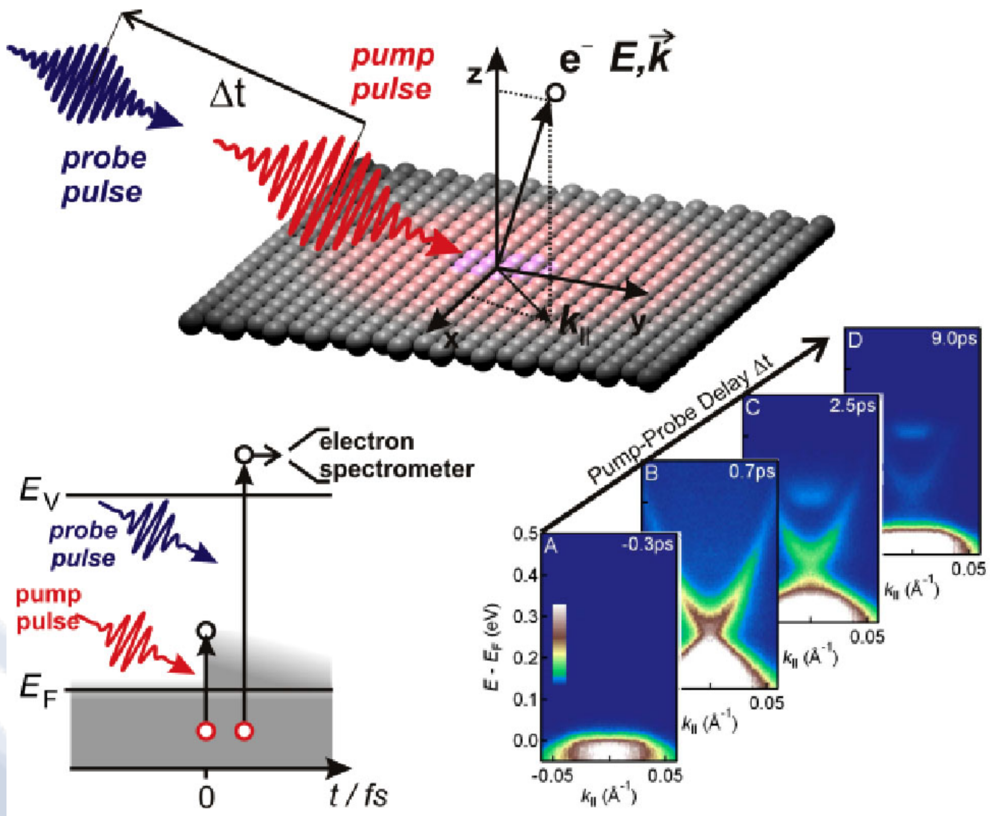


Muybridge 1887

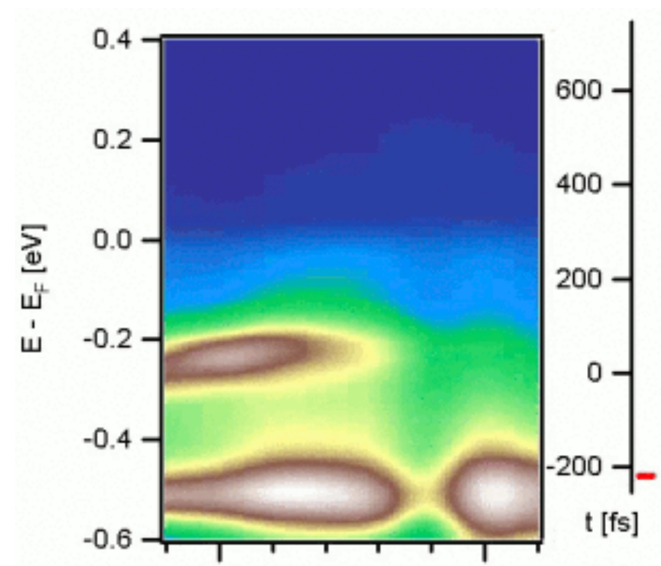
Pump-probe spectroscopy (today)

mpsd

- stroboscopic investigations of dynamic phenomena



TbTe3 CDW metal



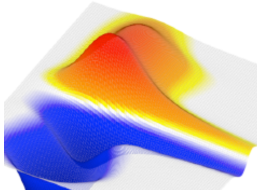
J. Sobota et al., PRL 108, 117403 (2012)
F. Schmitt et al., Science 321, 1649 (2008)
Image courtesy: J. Sobota / F. Schmitt

Ultrafast Materials Science

Understanding the nature of quasiparticles

- Relaxation dynamics

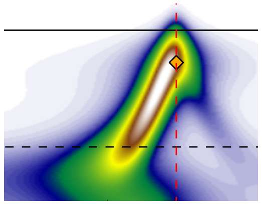
PRL 111, 077401 (2013)
PRX 3, 041033 (2013)
PRB 87, 235139 (2013)
PRB 90, 075126 (2014)
arXiv:1505.07055, Nature Comm.
arXiv:1607.02314

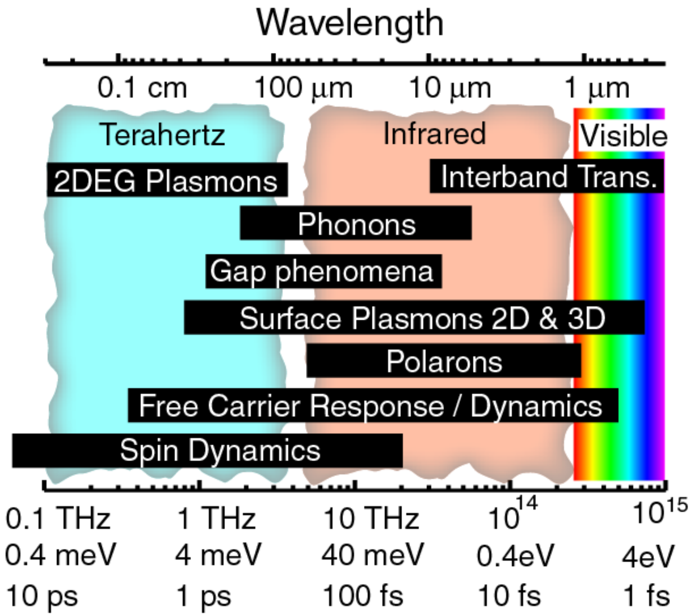


Understanding ordered phases

- Collective oscillations
- Competing order parameters

PRB 92, 224517 (2015)
PRB 93, 144506 (2016)
arXiv:1611.04307





Creating new states of matter

- Photo-induced phase transitions
- Floquet topological states

Nature Commun. 6, 7047 (2015)
arXiv:1604.03399, Nature Comm.

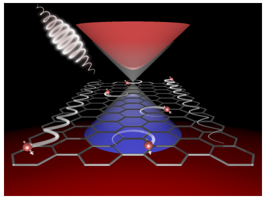


Image courtesy:
D. Basov

Outline

mpsd

- Part I: Driven superconductors
  - Higgs amplitude mode oscillations for optical pumping (1.5 eV laser)

    PRB 92, 224517 (2015)
  - light-enhanced superconductivity via hopping control

    PRB 93, 144506 (2016)
- Part II: Laser-controlled competing orders

  arXiv:1611.04307
- Part III: Light-enhanced electron-phonon coupling

  arXiv:1607.02314

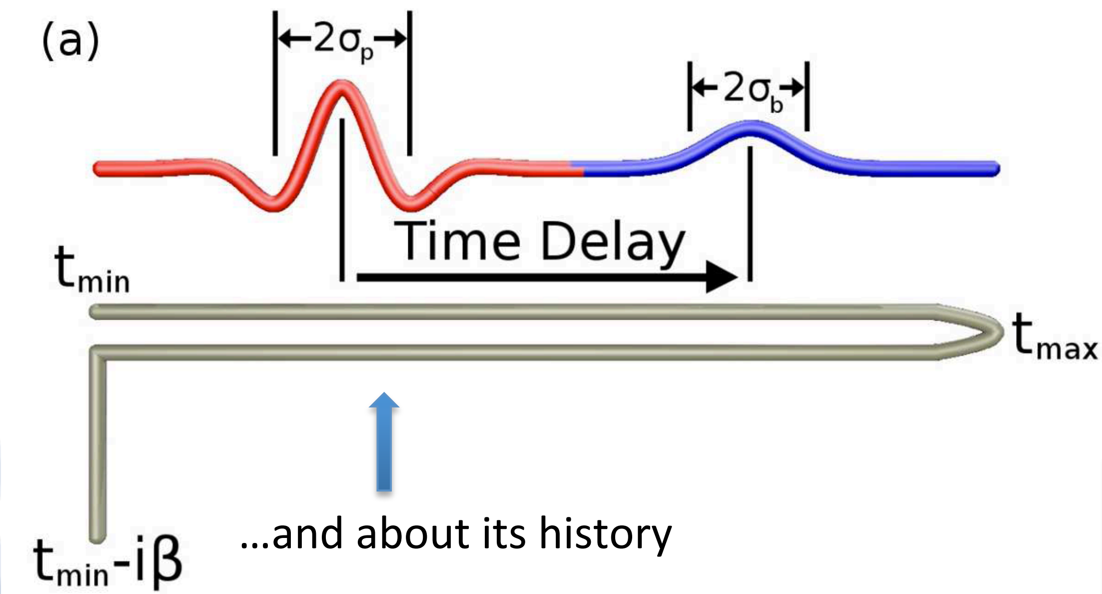
Non-Equilibrium Keldysh Formalism

Beyond BCS

$$G(t,t') = G^0(t,t') + \oint dt_1\, dt_2\, G^0(t,t_1)\,\underline{\Sigma(t_1,t_2)}\,G(t_2,t')$$

$$G_{\mathbf{k}}(\omega) = G^0_{\mathbf{k}}(\omega) + G^0_{\mathbf{k}}(\omega)\,\Sigma(\omega)\,G_{\mathbf{k}}(\omega)$$

self-energy Σ:
electron-electron scattering
electron-phonon scattering
...



System knows about its thermal initial state...

Include the effects of driving field through time-dependent electronic dispersion

$$\varepsilon(k) \rightarrow \varepsilon(k,t)$$

Model and Method

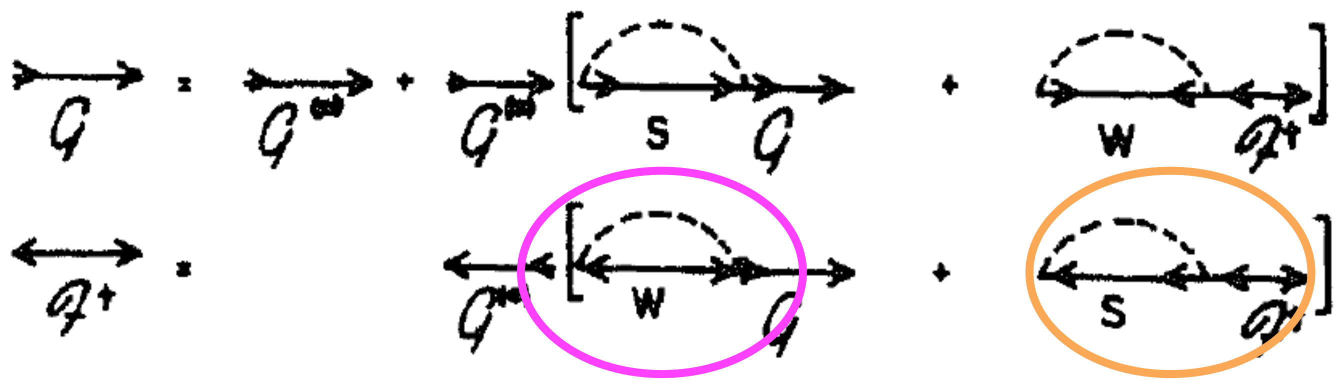
$$\mathcal{H} = \sum_{\boldsymbol{k}\sigma} \epsilon(\boldsymbol{k},t) c^\dagger_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma} + \sum_{\boldsymbol{q},\gamma} \Omega_\gamma b^\dagger_{\boldsymbol{q},\gamma} b_{\boldsymbol{q},\gamma} - \sum_{\boldsymbol{q},\gamma,\sigma} g_\gamma c^\dagger_{\boldsymbol{k}+\boldsymbol{q}\sigma} c_{\boldsymbol{k}\sigma} \left(b_{\boldsymbol{q},\gamma} + b^\dagger_{-\boldsymbol{q},\gamma} \right)$$

- electrons (2D square latt.) + spectrum of phonons + el-ph coupling (Holstein)
- Migdal-Eliashberg (1st Born) + phonon heat bath approximation

superconductor:

normal

anomalous

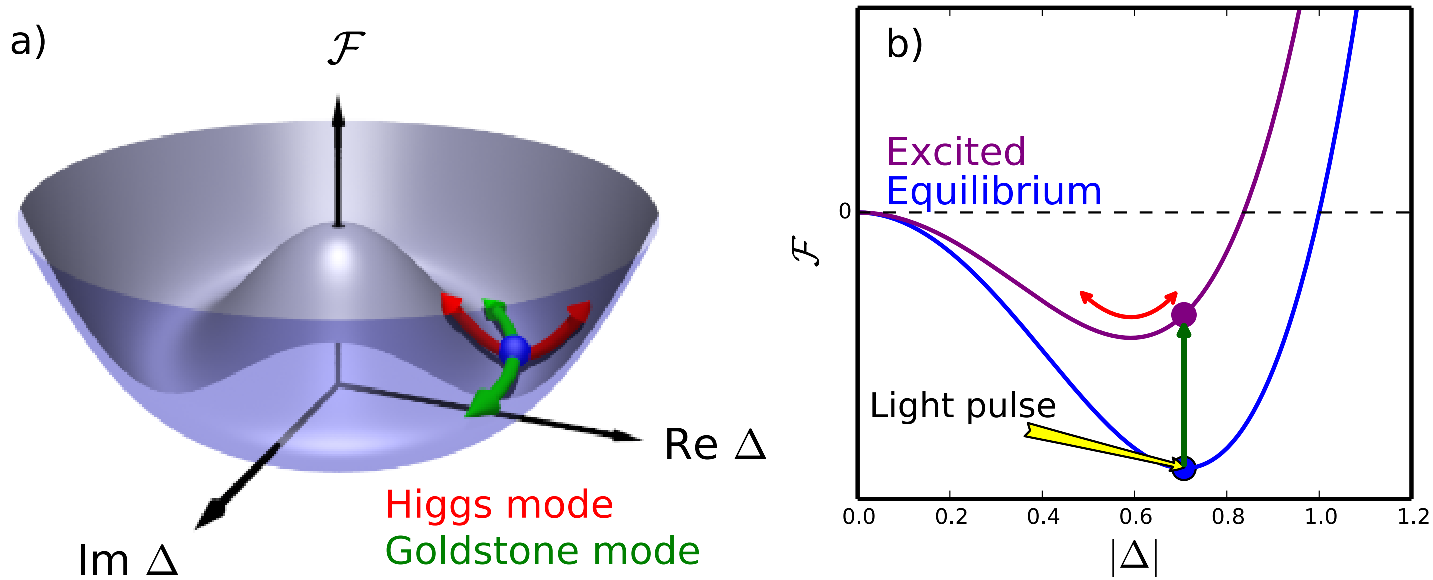


order parameter Δ, condensate dynamics

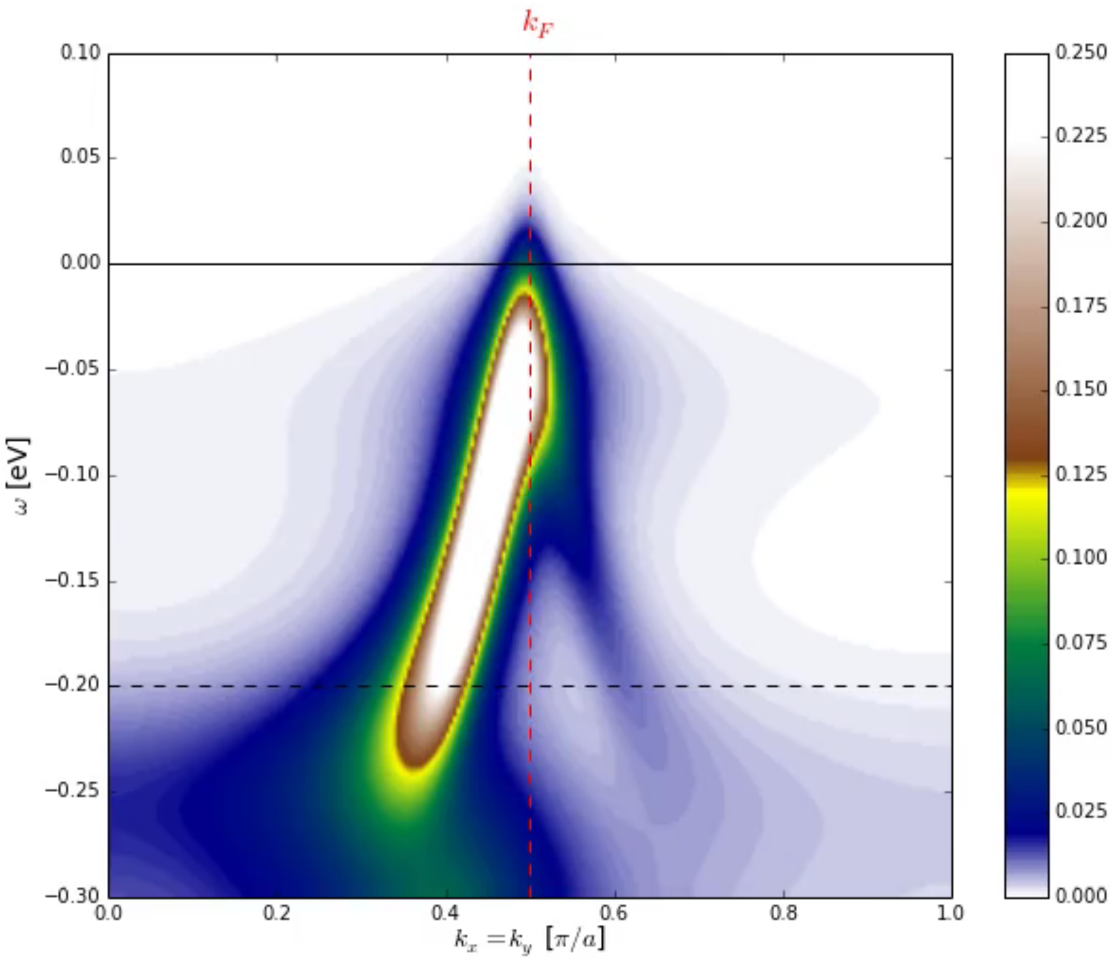
el-ph single-particle scattering

also see:
Murakami, Werner et al., PRB 93, 094509 (2016)

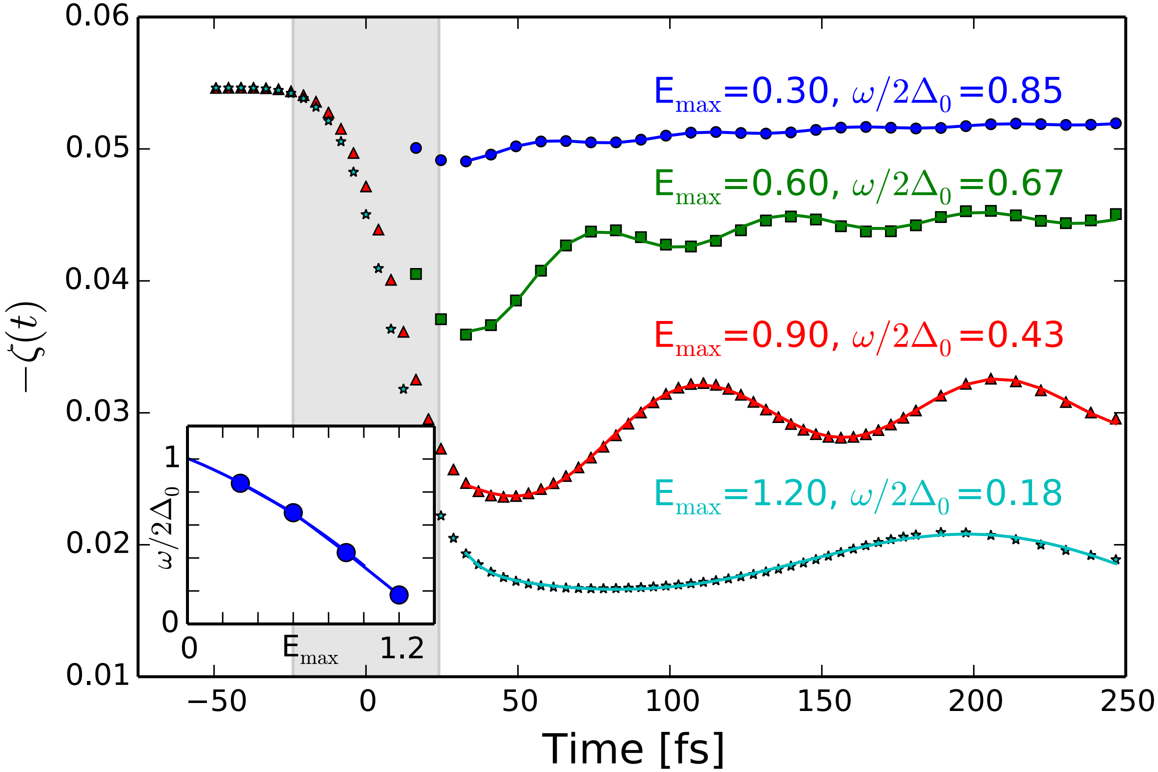
Higgs amplitude mode



Oscillations in photocurrent



Amplitude mode oscillations



PRB 92, 224517 (2015)

- Amplitude ("Higgs") mode oscillations predicted in time-resolved ARPES
- Reduced order parameter sets oscillation frequency
- Dissipation: Exciting Higgs even far away from gap resonance

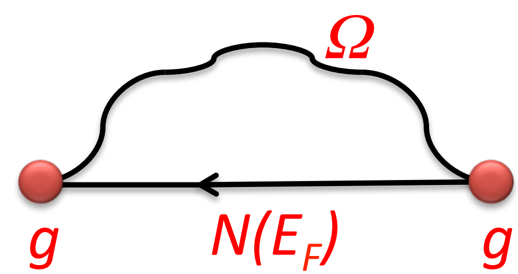
Optics: Matsunaga et al., Phys. Rev. Lett. 111, 057002 (2013), Science 2014 [10.1126/science.1254697]
Theory: Volkov & Kogan 1974, Barankov PRL 2004, Yuzbashyan PRL 2006, Tsuji PRL 2013, Murakami PRB 2016, Schnyder et al, PRB 2011, Krull et al., PRB 2014

How to enhance boson-mediated SC?

- BCS theory – plain vanilla SC (weak coupling)

$$\Delta \approx 2\hbar\Omega_c \exp(-1/V_0 N(E_F))$$

  - effective attraction $V_0 \sim g^2/(\hbar\ \Omega)$
  - e-boson coupling g
  - boson frequency Ω
  - electronic DOS $N(E_F)$

$\Sigma =$ 

Migdal-Eliashberg theory
boson-mediated pairing

How to enhance boson-mediated SC?

- nonlinear phononics Q^2Q: resonant excitation of vibrational modes – effects?

1. tune model parameters
   - e-boson coupling g
   - boson frequency Ω

   } $\alpha^2 F$ – Eliashberg function

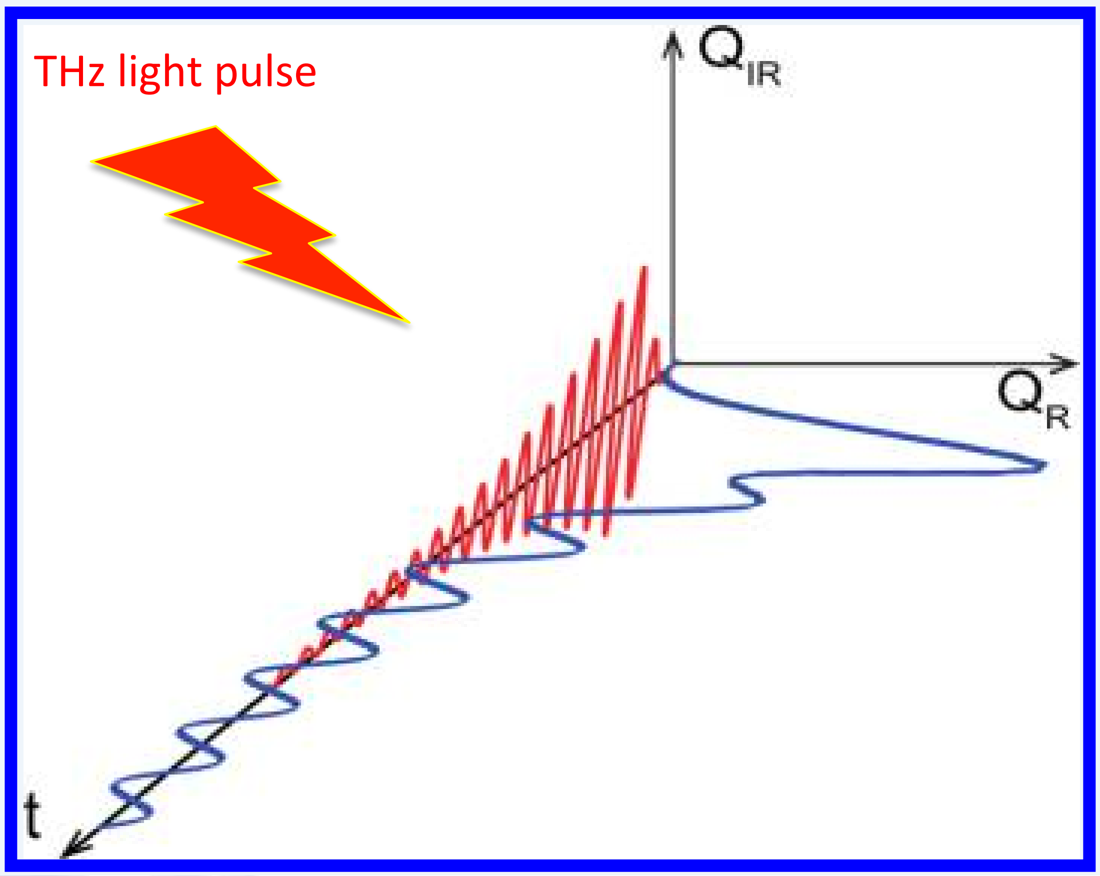
   - electronic DOS $N(E_F)$

   Gedankenexperiment (what if?)

2. dynamical effect
   - effective Hamiltonian (e.g., Floquet)

also see: Knap et al., arXiv:1511.07874,
Patel & Eberlein PRB 93, 195139 (2016), Komnik & Thorwart arXiv:1607.03858

Classical lattice dynamics



$$\ddot{Q}_{IR} + \Omega_{IR}^2 Q_{IR} = \frac{e^* E_0}{\sqrt{M_{IR}}} \sin(\Omega_{IR} t) F(t)$$

$$\ddot{Q}_{RS} + \Omega_{RS}^2 Q_{RS} = A Q_{IR}^2$$

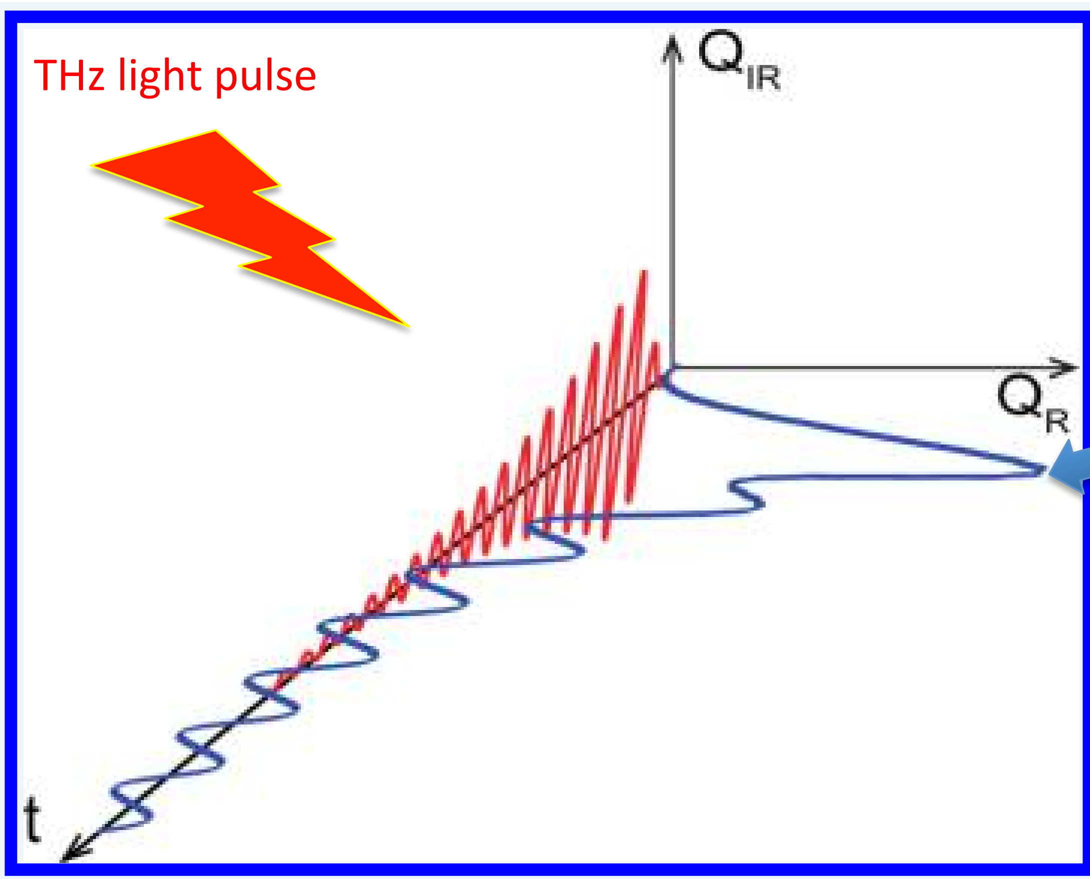
Rectification of a second (Raman) phonon via coherent driving of a first (IR) phonon

„Nonlinear phononics"

M. Först et al., Nature Physics 7, 854 (2011)

A. Subedi, A. Cavalleri, A. Georges, PRB 89, 220301R (2014)

Classical lattice dynamics



Displaced Raman mode assumed to lead to temporal change of electronic hopping

Gedankenexperiment (what if?)

Include the effects of driving field through time-dependent electronic dispersion

$$\varepsilon(k) \rightarrow \varepsilon(k,t)$$

„Nonlinear phononics"

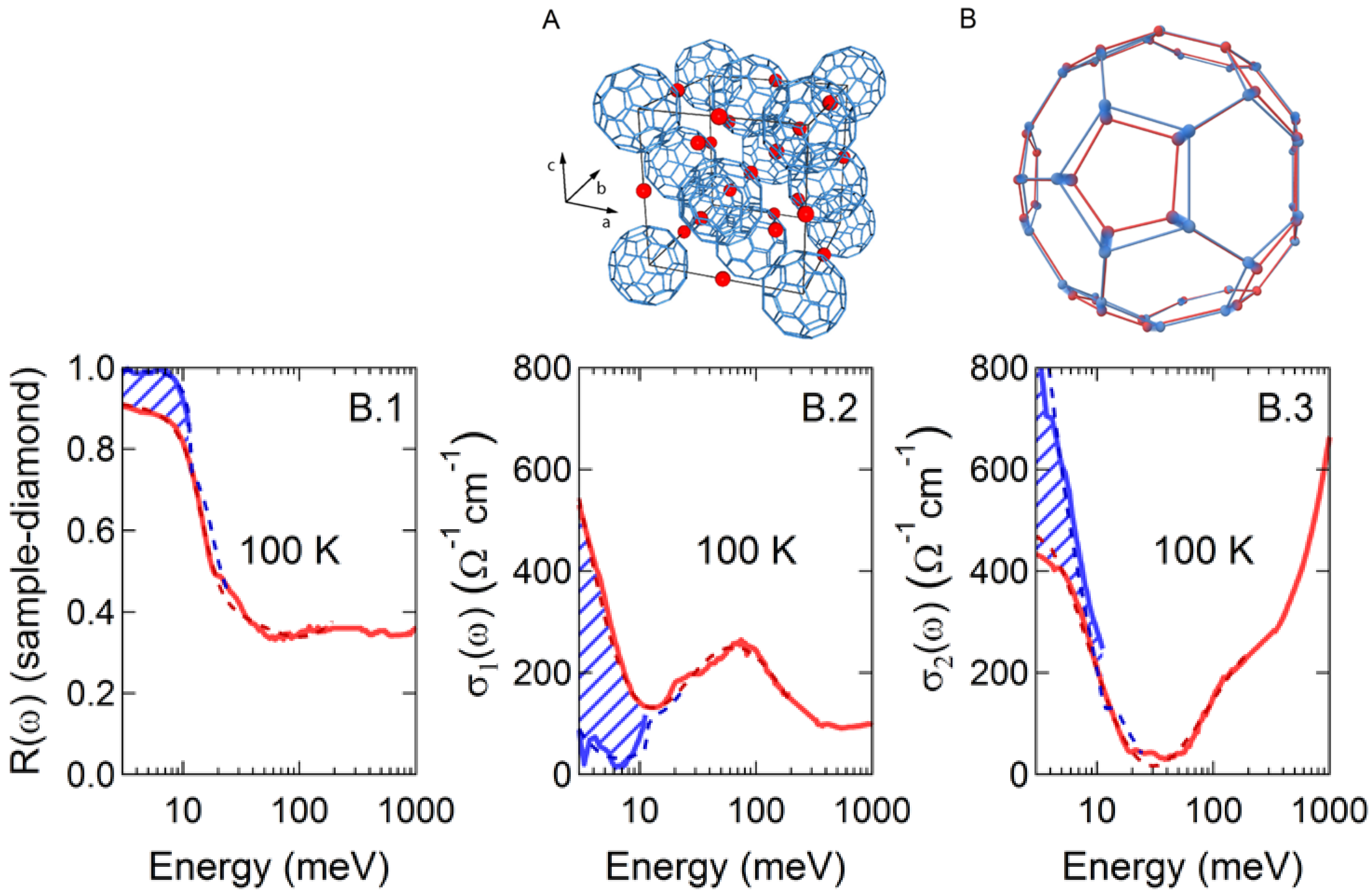
M. Först et al., Nature Physics 7, 854 (2011)

A. Subedi, A. Cavalleri, A. Georges, PRB 89, 220301R (2014)

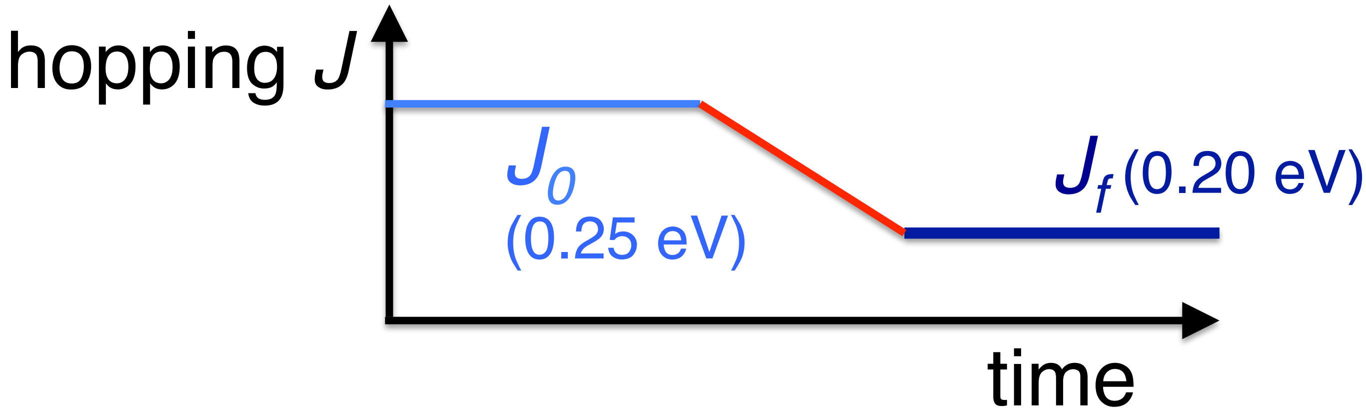
Experimental motivation

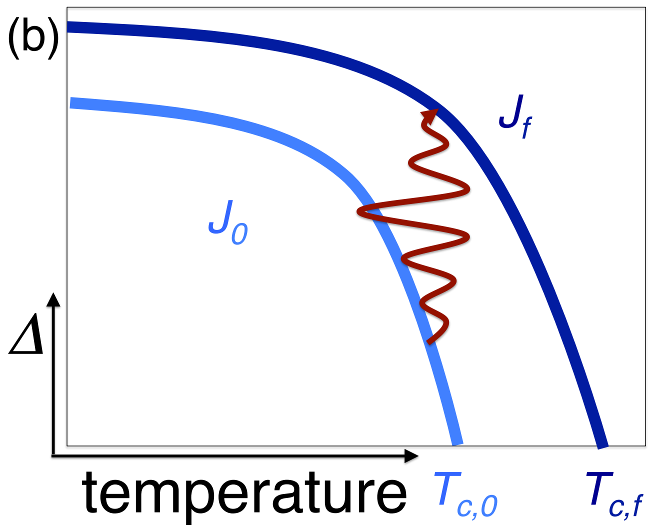
„Possible light-induced superconductivity in K3C60 at high temperature“

M. Mitrano et al., Nature 530, 461 (2016)



Simplest model: hopping ramp

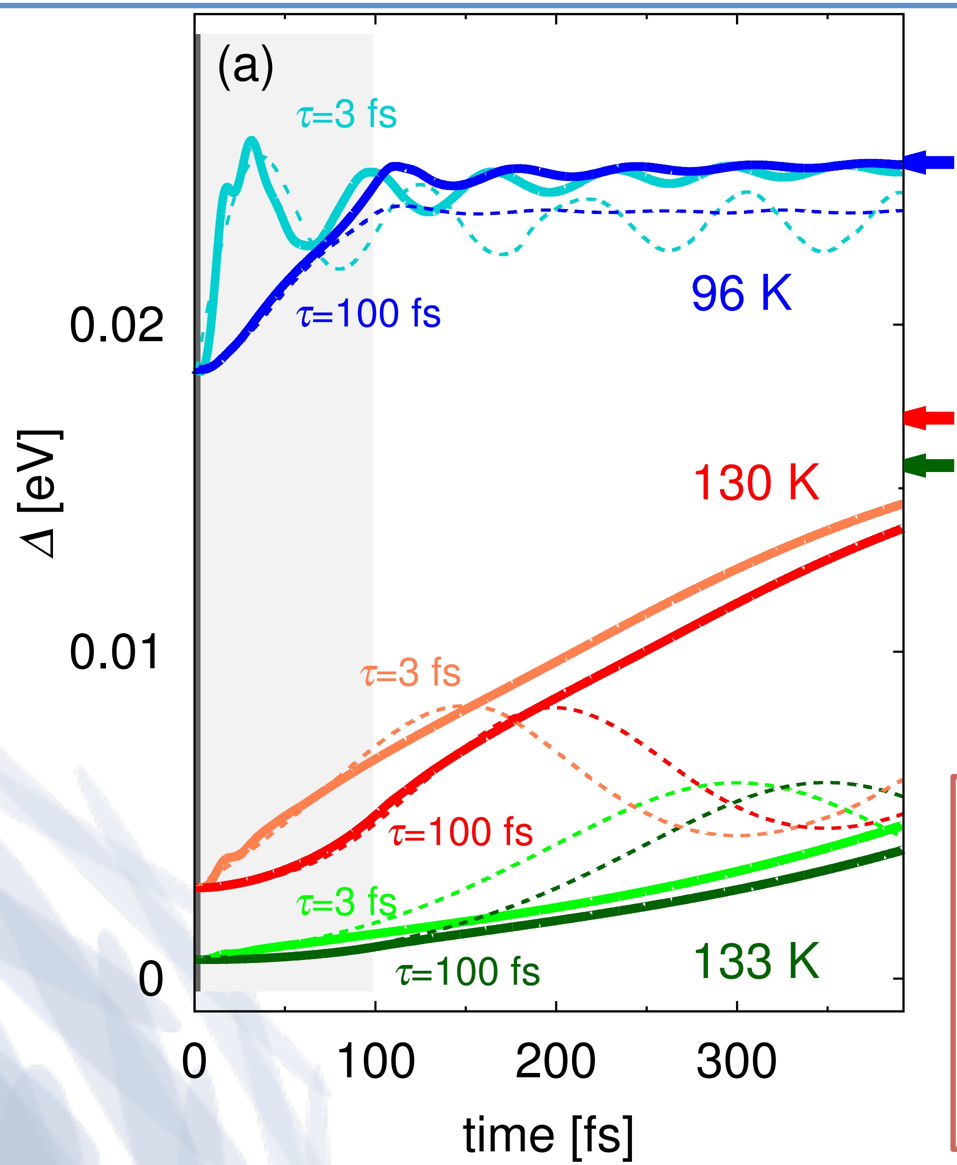


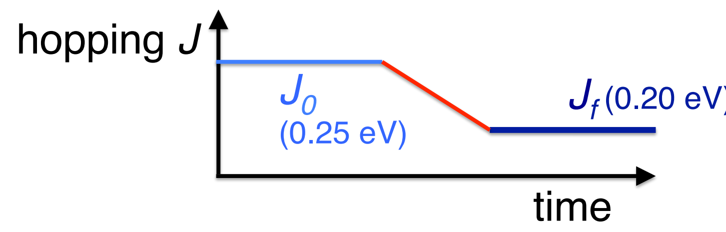


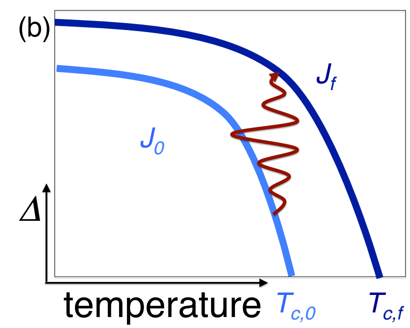
Equilibrium picture:

Enhancement of SC via enhanced DOS at Fermi energy

Superconductor evolution

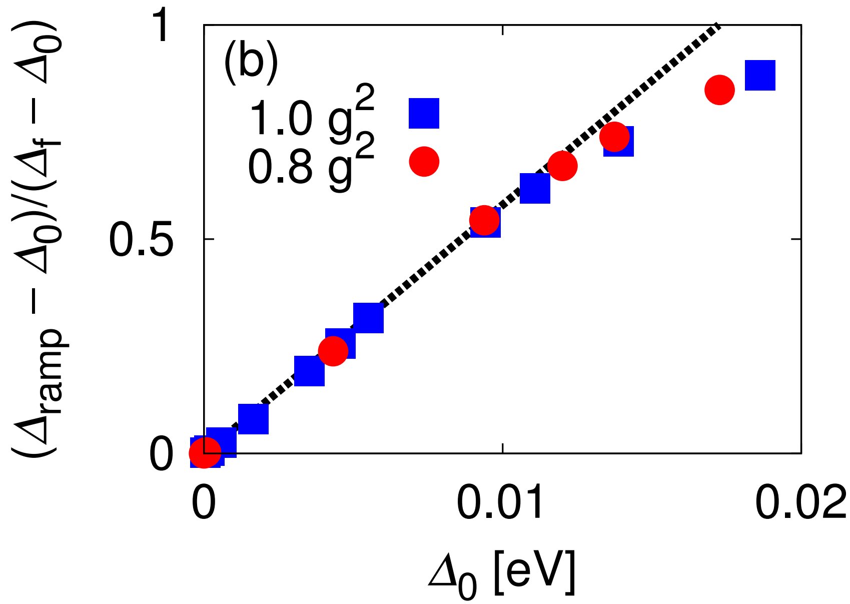


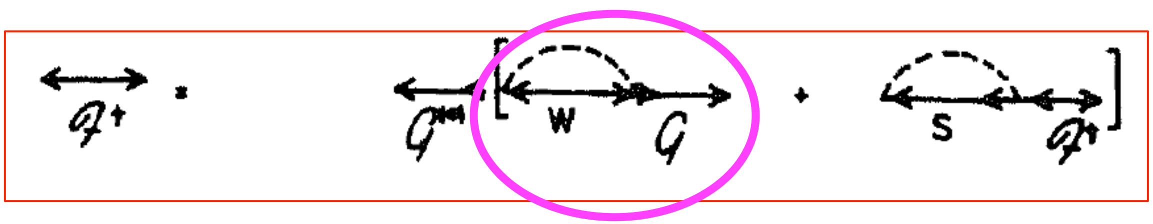




Enhancement of SC strongly depends on initial thermal state

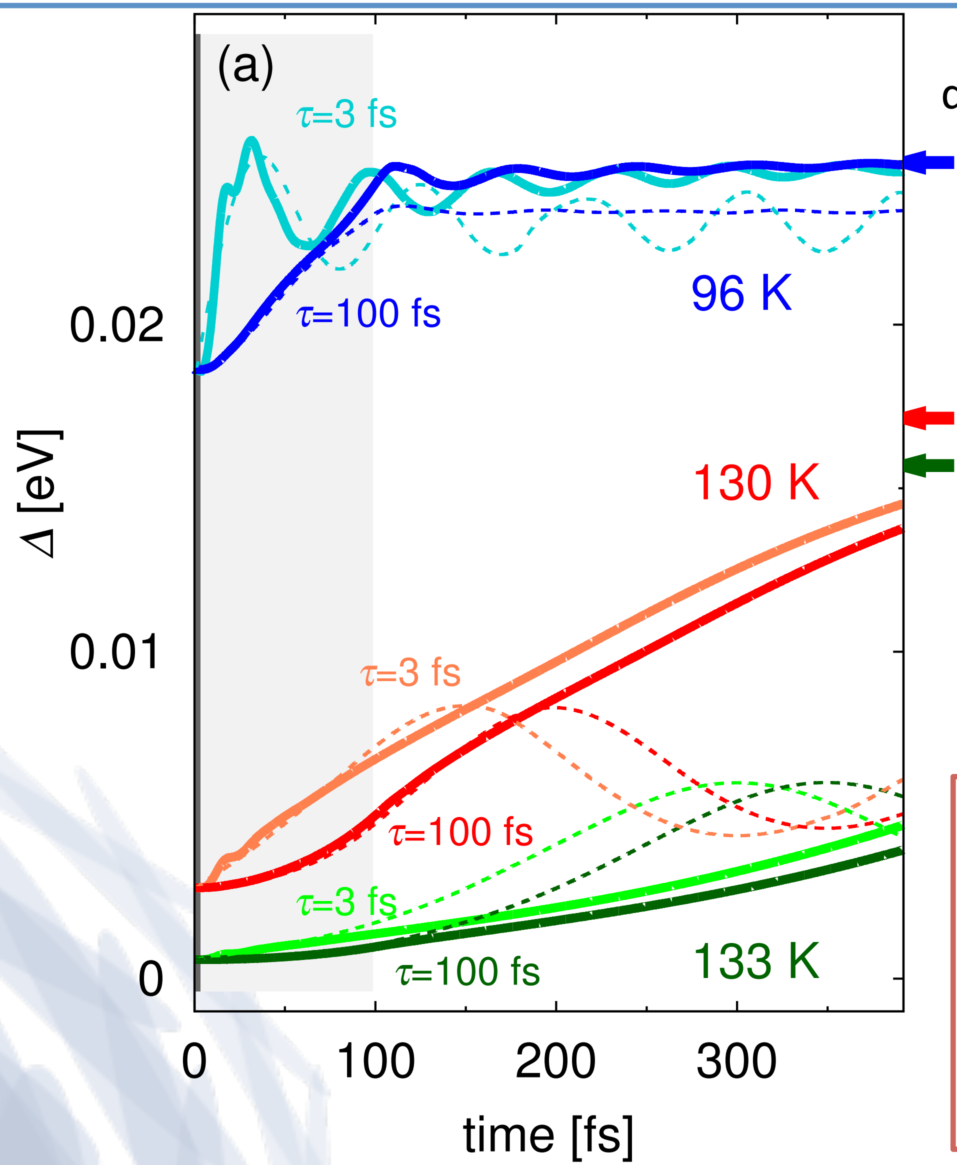
Enhancement during ramp



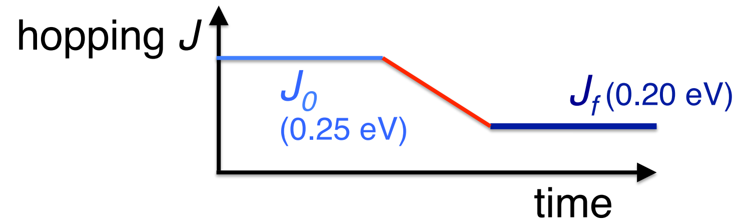


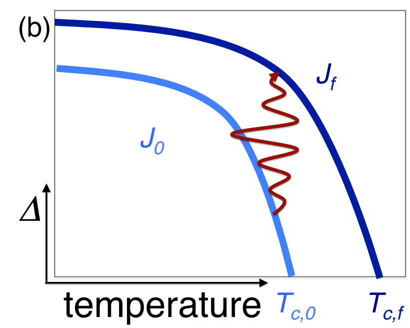
Order parameter enhancement ~Δ_0

Superconductor evolution



dashed: no dissipation (BCS only)





Dissipation helps enhancement for fast ramps

Summary part I

mpsd

- Amplitude mode oscillations in pumped SC

  PRB 92, 224517 (2015)

- Light-enhanced SC via nonlinear phononics

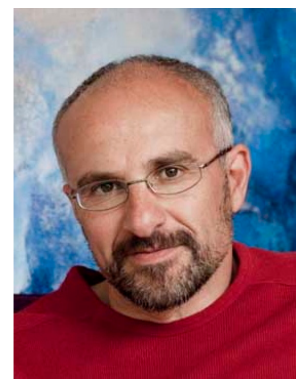
  PRB 93, 144506 (2016)


A. F. Kemper


T. P. Devereaux


B. Moritz


J. K. Freericks


A. Georges


C. Kollath

BERKELEY LAB

SLAC NATIONAL ACCELERATOR LABORATORY

GEORGETOWN UNIVERSITY

ÉCOLE POLYTECHNIQUE UNIVERSITÉ PARIS-SACLAY

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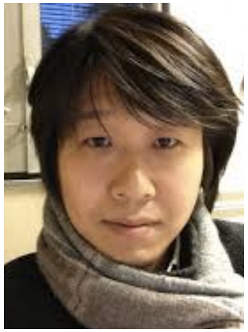
II. Theory of laser-controlled competing orders



Akiyuki Tokuno, Antoine Georges, Corinna Kollath
(Paris/Bonn)

arXiv:1611.04307

Ultrafast order

Why?

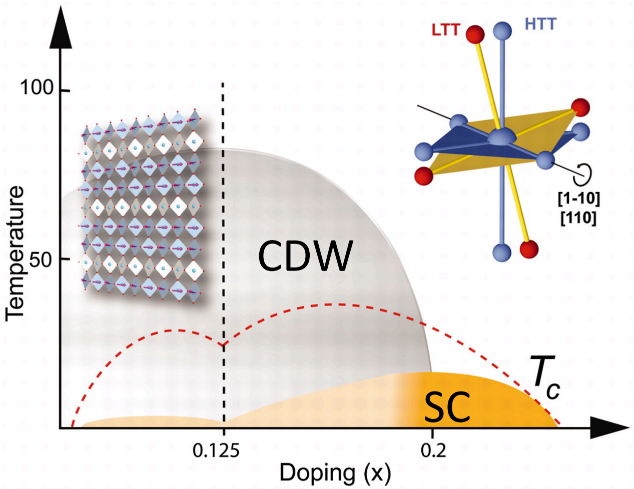
- understand ordering mechanisms
- control ordered states
- induce new states of matter

How?

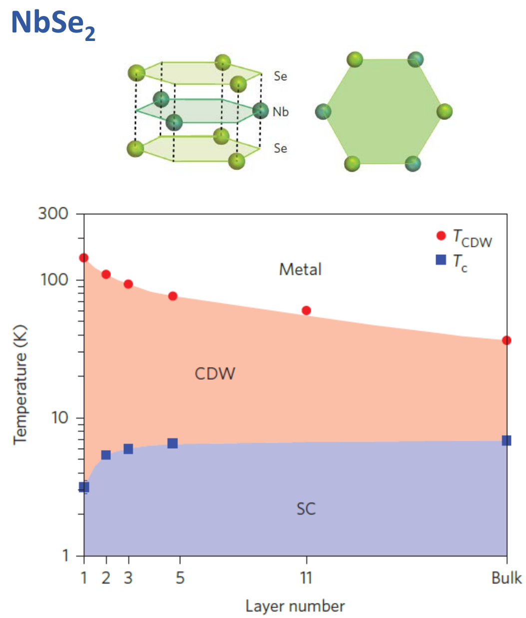
- resonance with something

Is there a generic mechanism to control ordered states?

Experimental motivation

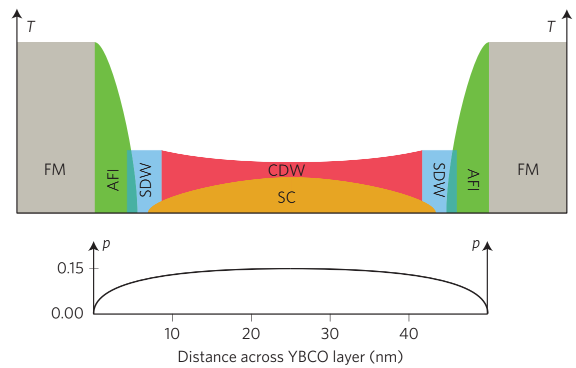


D. Fausti et al.,
Light-induced superconductivity in a stripe-ordered cuprate (LESCO),
Science, 331, 189 (2011)



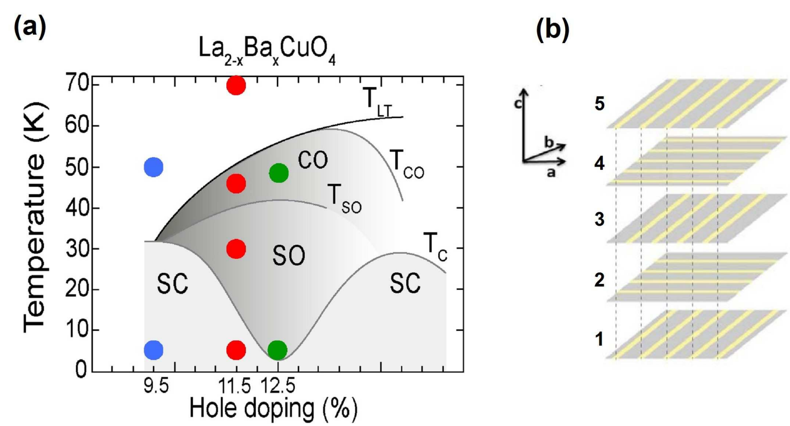
Nat. Nanotechnol. 10, 765 (2015)

YBCO-LCMO heterostructure



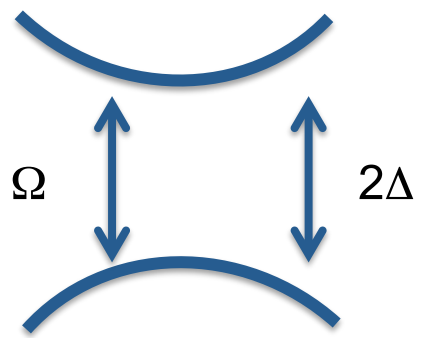
A. Frano et al.,,
Nat. Mater. 15, 831 (2016)

D. Nicoletti et al.,
Optically induced superconductivity in striped LBCO by polarization-selective excitation in the near infrared,
PRB 90, 100503 (2014)



Driven SC/CDW

CDW ~ A
1-photon resonance



Driven SC/CDW

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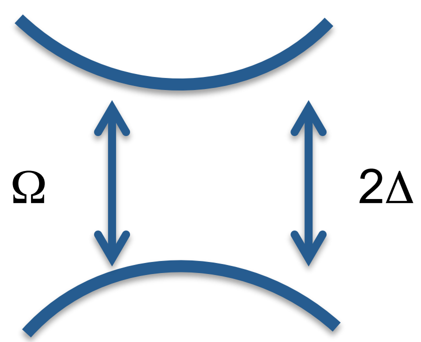
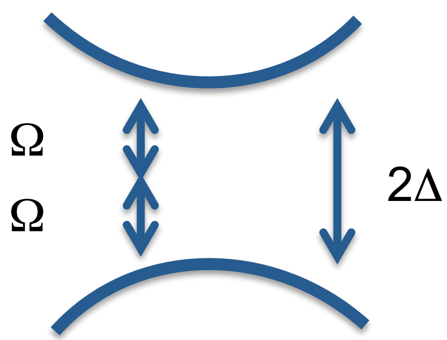
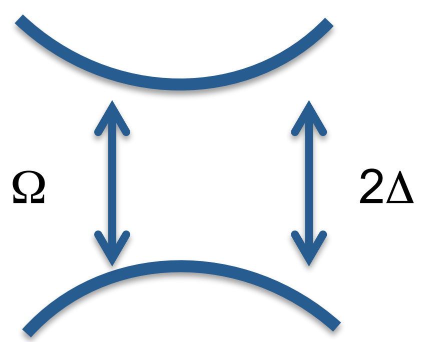


SC ~ A^2
2-photon resonance

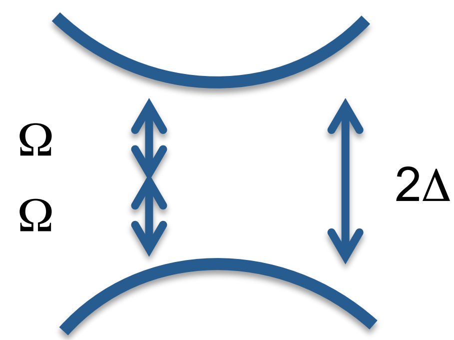


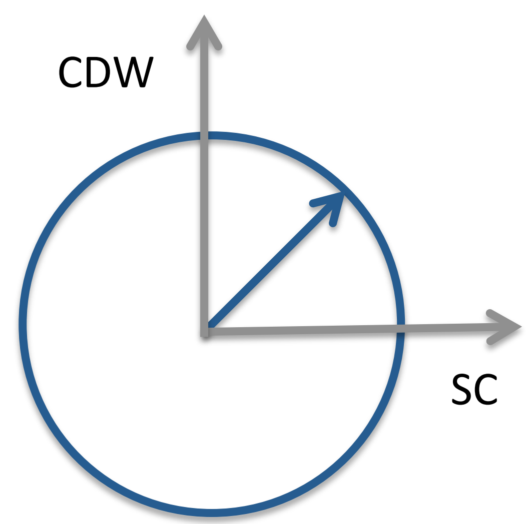
Driven SC/CDW

CDW ~ A
1-photon resonance



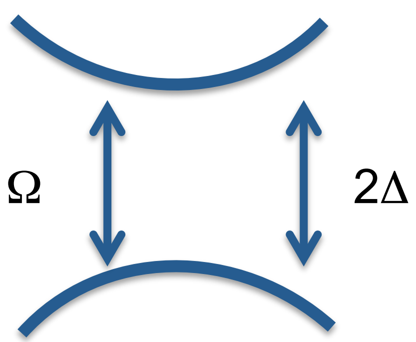
SC ~ A^2
2-photon resonance



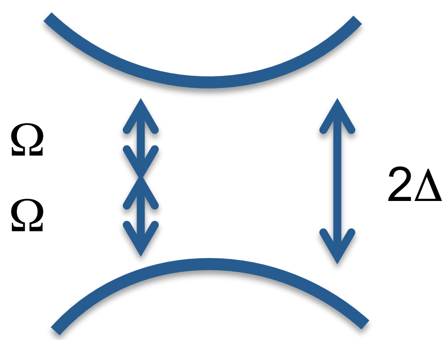


Driven SC/CDW

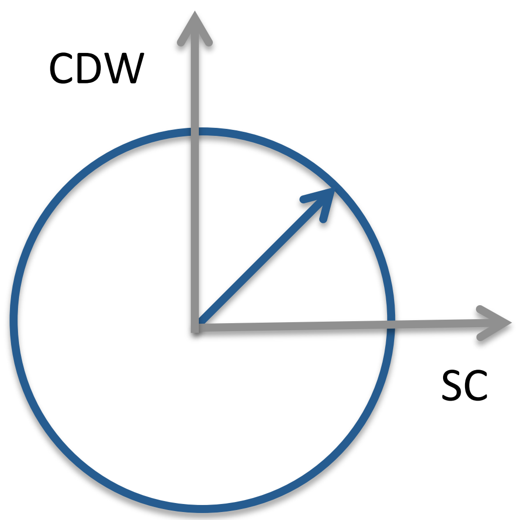
CDW ~ A
1-photon resonance



SC ~ A^2
2-photon resonance

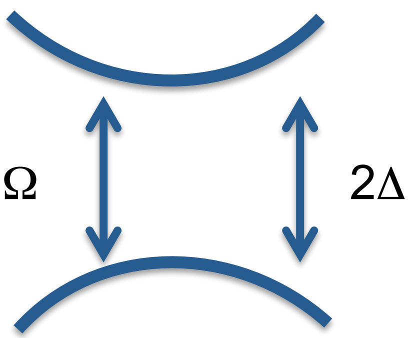


... laser lifts SC/CDW degeneracy

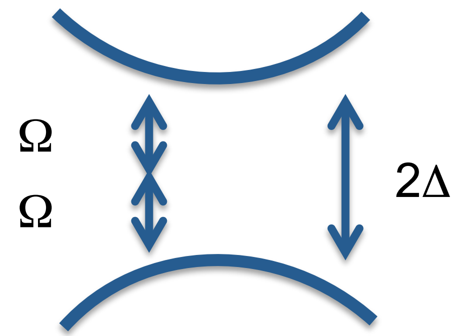


Driven SC/CDW

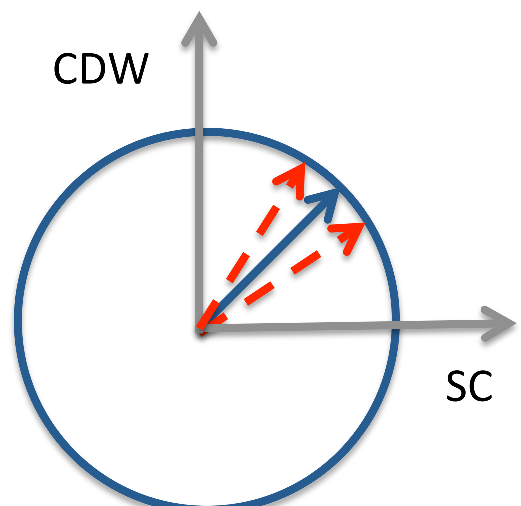
CDW ~ A
1-photon resonance



SC ~ A^2
2-photon resonance

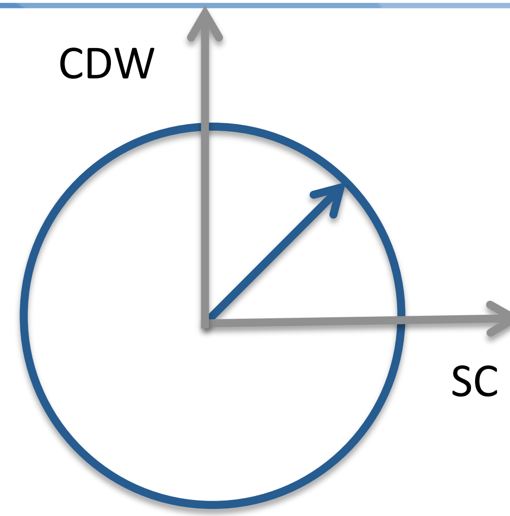


... laser lifts SC/CDW degeneracy
... Goldstone-like collective mode?



Competing orders

- attractive -U Hubbard model
- degeneracy of SC and CDW at perfect nesting
- SO(4) symmetry (SC, CDW, eta pairing)



VOLUME 63, NUMBER 19 PHYSICAL REVIEW LETTERS 6 NOVEMBER 1989

η Pairing and Off-Diagonal Long-Range Order in a Hubbard Model

Chen Ning Yang

C. N. Yang (1957 Nobel for parity violation in weak interaction)

S.-C. Zhang (Topological Insulators)

Reprinted from Mod. Phys. Lett. B4 (1990) 759–766

SO_4 SYMMETRY IN A HUBBARD MODEL

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and
S. C. ZHANG
IBM Research Division, Almaden Research Center, San Jose, CA 95120-6099, USA

Simplistic Model

$$H = \sum_{k\sigma} \epsilon(k) n_{k\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} = H_J + H_U,$$
$$\epsilon(k) = -2J(\cos(k_x) + \cos(k_y)),$$

attractive U + mean-field decoupling

$$\Delta_{SC} = U \sum_k f_k, \qquad f_k \equiv \langle c_{-k\downarrow} c_{k\uparrow} \rangle \qquad \text{(SC)},$$
$$\Delta_{CDW} = U \sum_k g_k, \qquad g_k \equiv \frac{1}{2} \sum_\sigma \langle c^\dagger_{k\sigma} c_{k+Q\sigma} \rangle \quad \text{(CDW)},$$
$$\Delta_\eta = U \sum_k \eta_k. \qquad \eta_k \equiv \langle c_{-(k+Q)\downarrow} c_{k\uparrow} \rangle \quad (\eta \text{ pairing}).$$

Mean-field Hamiltonian

$$H_{MF} = \sum_k \begin{pmatrix} c^\dagger_{k\uparrow} \\ c^\dagger_{k+Q\uparrow} \\ c_{-k\downarrow} \\ c_{-(k+Q)\downarrow} \end{pmatrix}^T \begin{pmatrix} \epsilon(k-A) & \Delta^*_{CDW} & \Delta_{SC} & \Delta_\eta \\ \Delta_{CDW} & \epsilon(k+Q-A) & \Delta_\eta & \Delta_{SC} \\ \Delta^*_{SC} & \Delta^*_\eta & -\epsilon(k+A) & -\Delta_{CDW} \\ \Delta^*_\eta & \Delta^*_{SC} & -\Delta^*_{CDW} & -\epsilon(k+Q+A) \end{pmatrix} \begin{pmatrix} c_{k\uparrow} \\ c_{k+Q\uparrow} \\ c^\dagger_{-k\downarrow} \\ c^\dagger_{-(k+Q)\downarrow} \end{pmatrix}$$

4x4 matrix: SO(4) algebra

$$\Delta_{SC} = U\sum_k f_k, \qquad f_k \equiv \langle c_{-k\downarrow} c_{k\uparrow}\rangle \qquad \text{(SC)},$$

$$\Delta_{CDW} = U\sum_k g_k, \qquad g_k \equiv \frac{1}{2}\sum_\sigma \langle c^\dagger_{k\sigma} c_{k+Q\sigma}\rangle \qquad \text{(CDW)},$$

$$\Delta_\eta = U\sum_k \eta_k. \qquad \eta_k \equiv \langle c_{-(k+Q)\downarrow} c_{k\uparrow}\rangle \qquad (\eta \text{ pairing}).$$

Mean-field equations

$$[G^<_k(t,t')]_{\alpha\beta} = +i\langle[\Psi^\dagger_k(t')]_\beta[\Psi_k(t)]_\alpha\rangle.$$

$$i\partial_t G^<_k(t,t) = [H_{MF}(k,t), G^<_k(t,t)].$$

eta pairing provides coupling

$$i\partial_t n_k = -\Delta_{SC}(f_k - f^*_k) + \Delta_{CDW}(g_k - g^*_k) - \Delta^*_\eta \eta_k + \Delta_\eta \eta^*_k,$$

$$i\partial_t f_k = \Delta_{SC}(1-(n_k + n_{-k})) + (\epsilon(k-A) + \epsilon(k+A))f_k + \Delta_{CDW}(\eta_k + \eta_{k+Q}) - \Delta_\eta(g^*_k + g^*_{-k}),$$

$$i\partial_t g_k = \Delta_{CDW}(n_k - n_{k+Q}) - 2\epsilon(k-A)g_k + \Delta_{SC}(\eta^*_k - \eta_{k+Q}) + \Delta_\eta f^*_k - \Delta^*_\eta f_{k+Q},$$

$$i\partial_t \eta_k = \eta_k(\epsilon(k-A) - \epsilon(k+A)) + \Delta_{CDW}(f_k + f_{k+Q}) - \Delta_{SC}(g_{-k} + g^*_k) - \Delta_\eta(n_k + n_{-(k+Q)} - 1).$$

nonlinear equations + self-consistency:

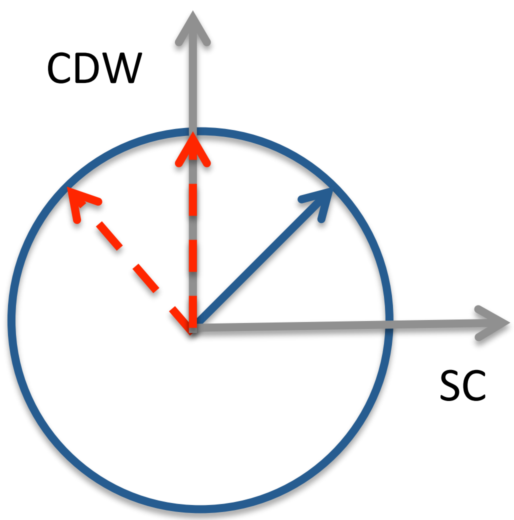
$$\Delta_{SC} = U\sum_k f_k,$$

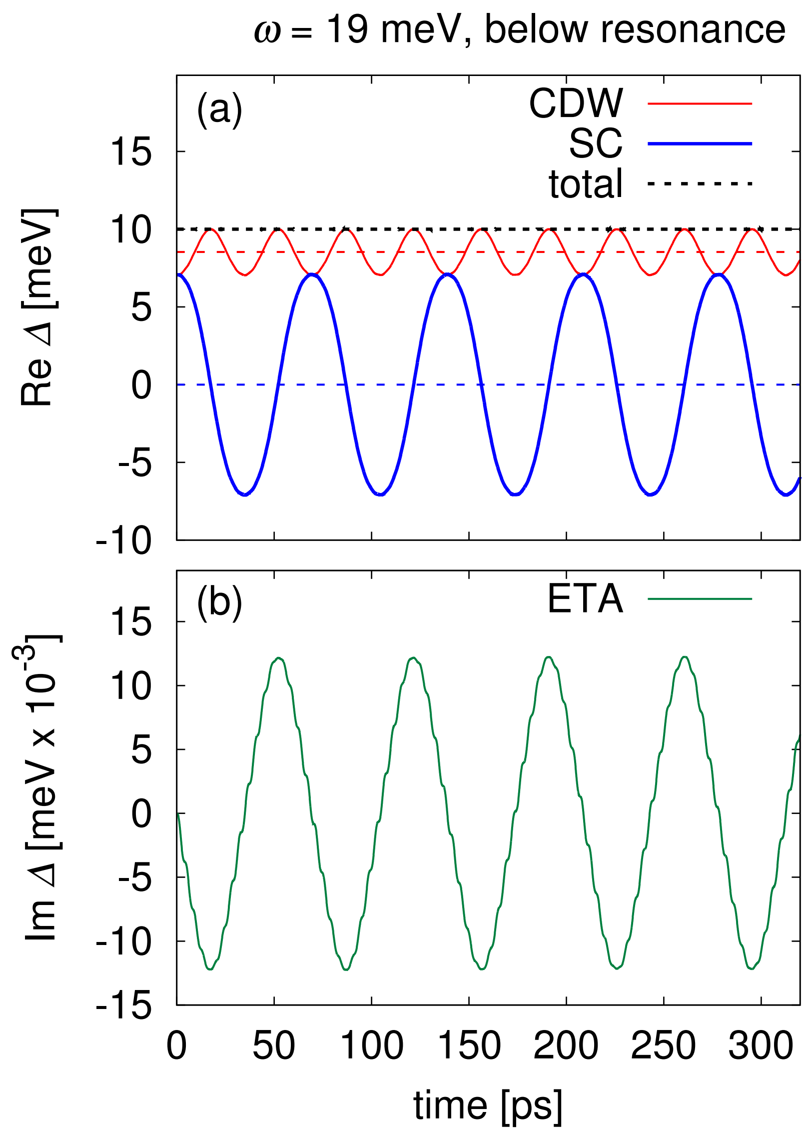
$$\Delta_{CDW} = U\sum_k g_k,$$

$$\Delta_\eta = U\sum_k \eta_k.$$

Gap resonance – cw driving

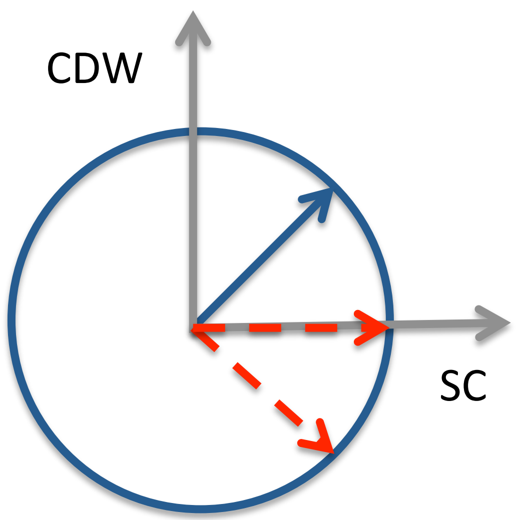
Below resonance:
SC down, CDW up

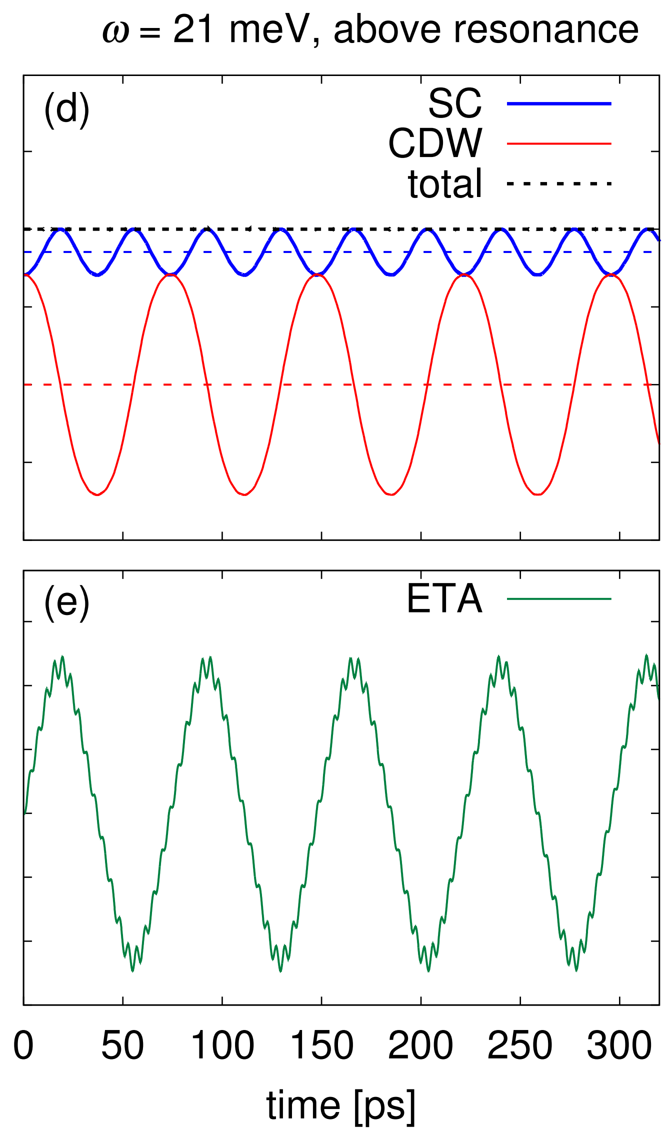




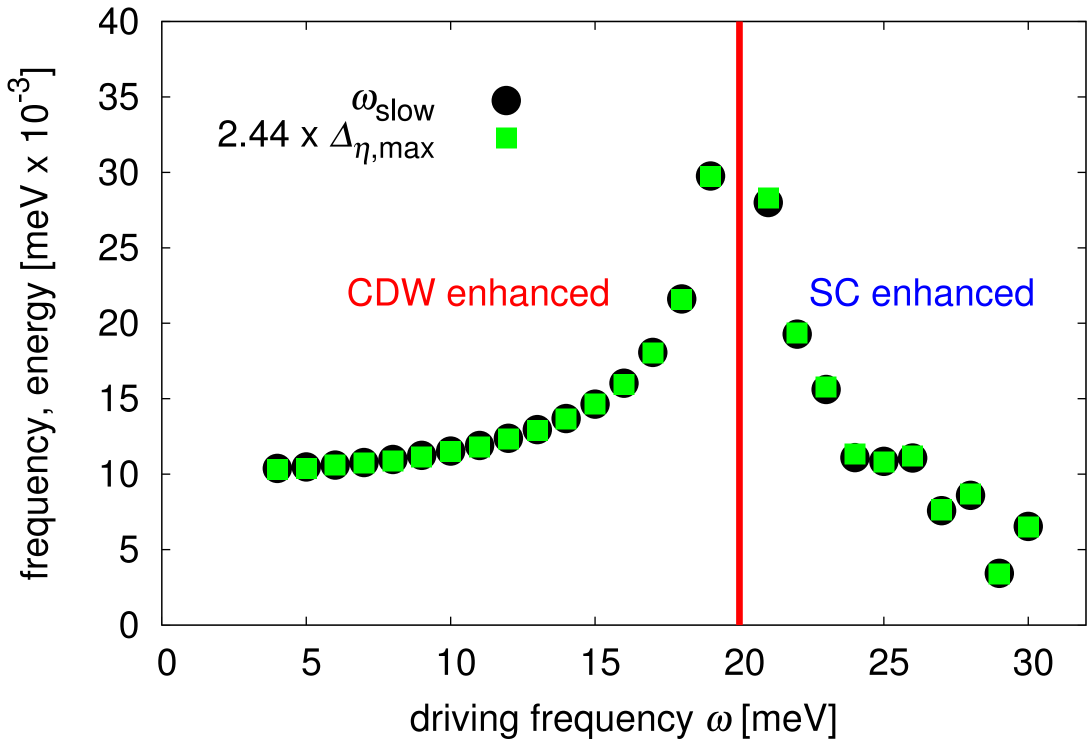
Gap resonance – cw driving

Above resonance:
SC up, CDW down





Gap resonance – cw driving



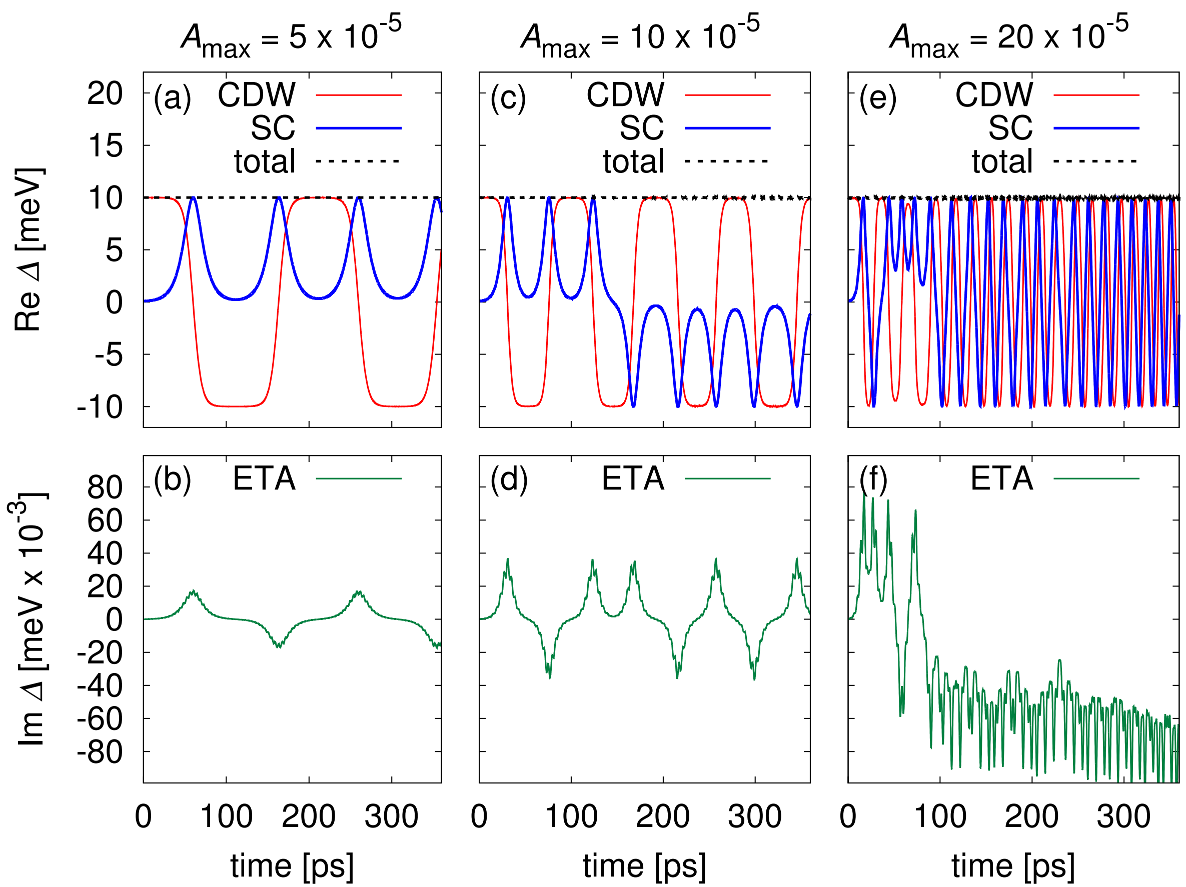
oscillation frequency set by light-induced eta pairing amplitude, which gives „mass“ to collective mode

resonant behavior at $\Omega=2\Delta$ = single-particle gap

Can we bring SC alive?

99% CDW initial state
Drive slightly above gap

SC comes alive!
Irregular behavior for stronger driving



Summary part II

- laser-controlled switching between SC/CDW
- light-induced eta pairing and a collective mode
- path to understanding of light-induced superconductivity

arXiv:1611.04307

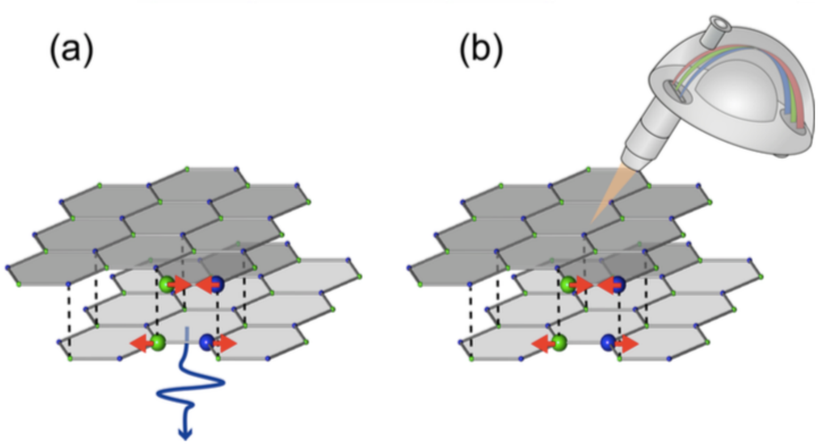
III. Dynamically enhanced coupling

Enhanced electron-phonon coupling in graphene with periodically distorted lattice

E. Pomarico,[1,2,*] M. Mitrano,[1,3] H. Bromberger,[1] M. A. Sentef,[1] A. Al-Temimy,[4] S. Forti,[4] C. Coletti,[4] A. Stöhr,[5] S. Link,[5] U. Starke,[5] C. Cacho,[6] R. Chapman,[6] E. Springate,[6] A. Cavalleri,[1,7] and I. Gierz[1,†]

arXiv:1607.02314

enhanced electron-phonon coupling in a periodically distorted graphene lattice driven on resonance with IR phonon

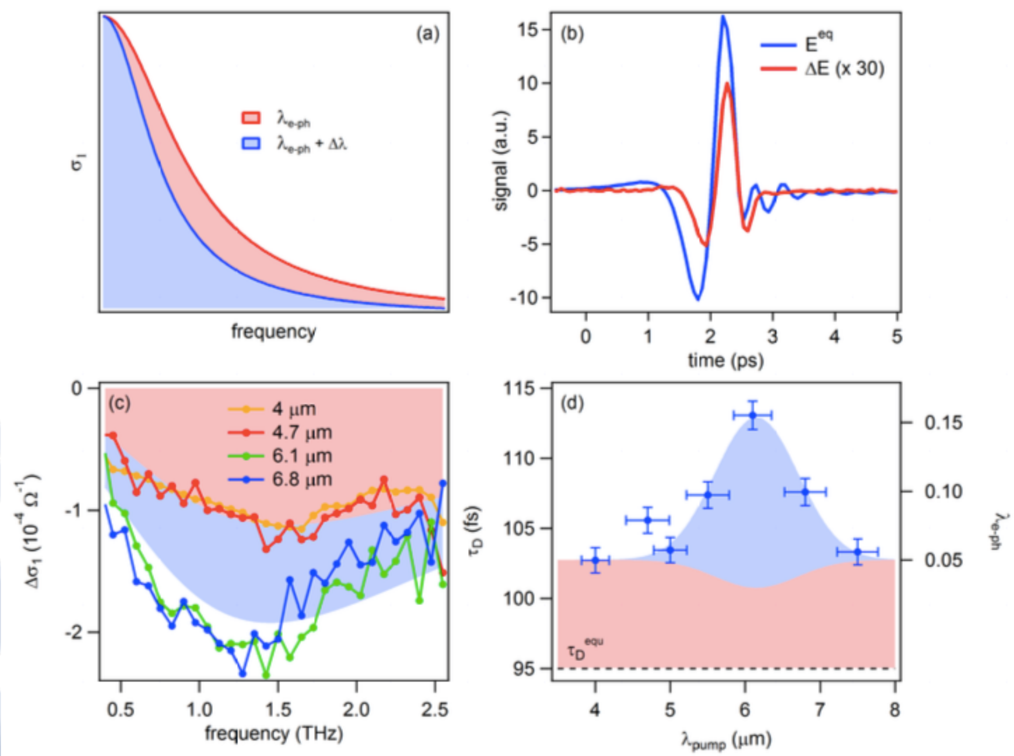


Dynamically enhanced coupling?

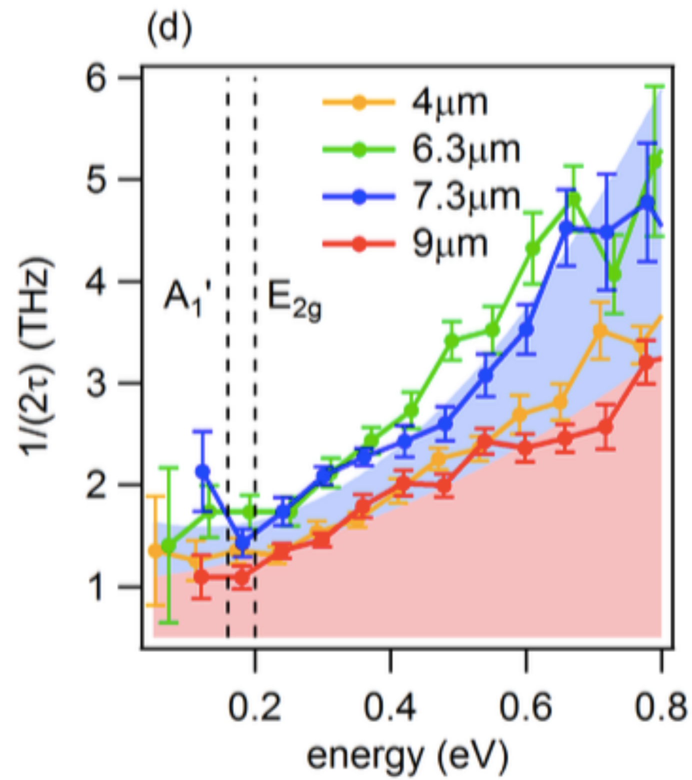
Enhanced electron-phonon coupling in graphene with periodically distorted lattice

arXiv:1607.02314

transient reduction of Drude weight



enhanced tr-ARPES relaxation



3-fold enhancement of effective $\lambda_{el\text{-}ph}$! Why?

Nonlinear electron-phonon interaction?

Hamiltonian involving nonlinear el-ph coupling:

$$H = H_{el} + \sum_i \omega_R b^\dagger_{R,i} b_{R,i} + \sum_i g_1 n_{el,i} x_{R,i} + \boxed{\sum_i g_2 n_{el,i} x_{R,i} x_{IR,i}} + H_{IR},$$

Coherently driven fast IR mode:

$$\langle x_{IR,i}(t)\rangle = x_{max} \cos \omega_{IR} t.$$

High-frequency limit (Floquet expansion):

$$\begin{aligned} H_{eff} &= \sum_i \frac{g_2 x_{max}}{\omega_{IR}} \frac{2\pi}{\omega_{IR}} \int_0^{\frac{2\pi}{\omega_{IR}}} \cos(\omega_{IR} t)^2 [x_{R,i}, n_{el,i} \omega_R b^\dagger_{R,i} b_{R,i}] \\ &= \sum_i \frac{g_2 x_{max} \omega_R}{2\omega_{IR}} n_{el,i} p_{R,i}. \end{aligned}$$

Induced additional linear term ~ amplitude of driven mode:

$$H_{eff,el-ph} = \sum_i (g_1 n_{el,i} x_{R,i} + \boxed{\frac{g_2 x_{max}}{2} n_{el,i} p_{R,i}})$$

similar idea in context of induced attraction: D. Kennes et al., arXiv:1609.03802

Summary part III

- Enhanced electron-phonon coupling in phononically driven bilayer graphene

arXiv:1607.02314

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