Theory of laser-driven nonequilibrium superconductivity

arXiv:1412.2762
arXiv:1505.07575

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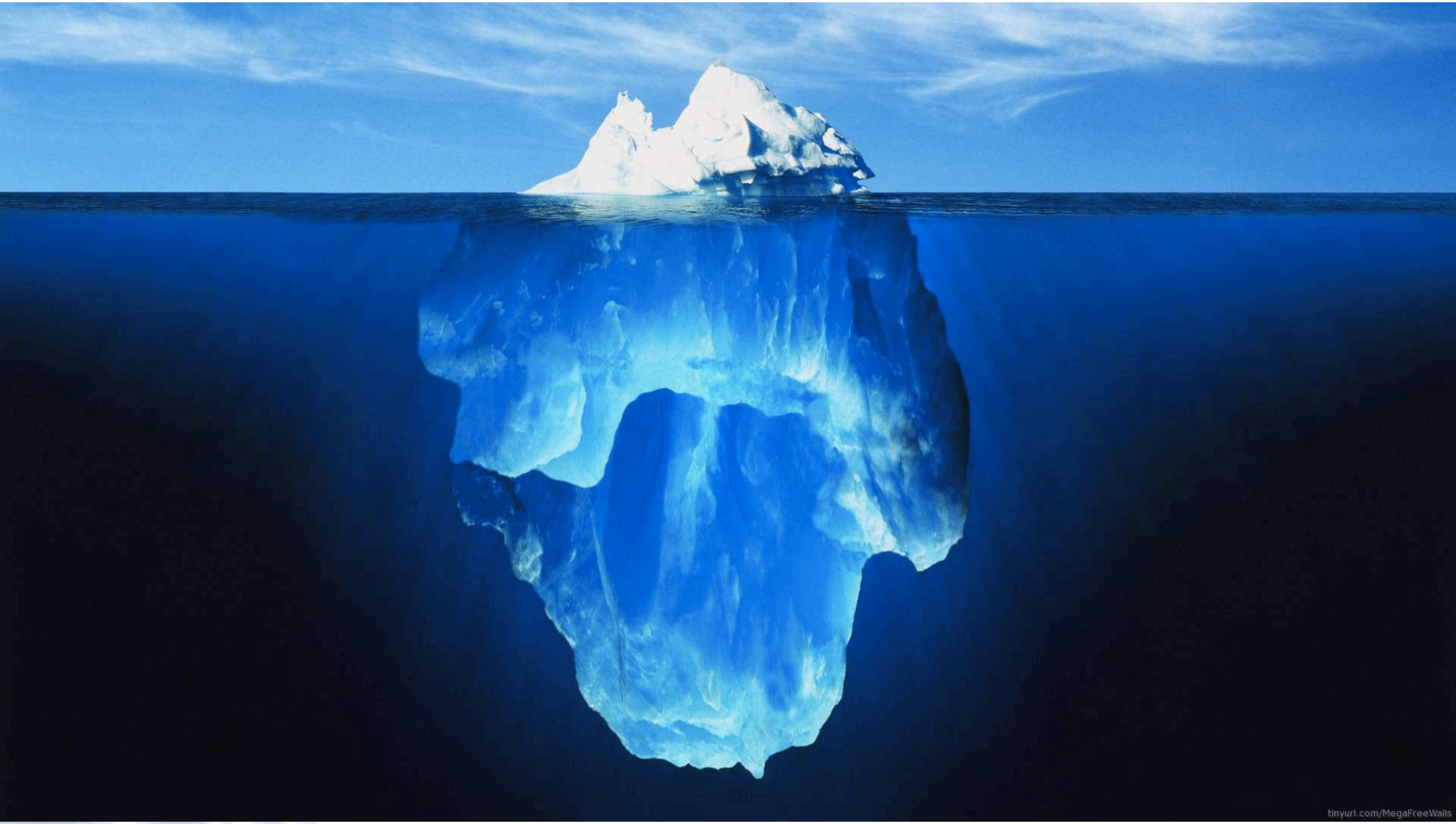
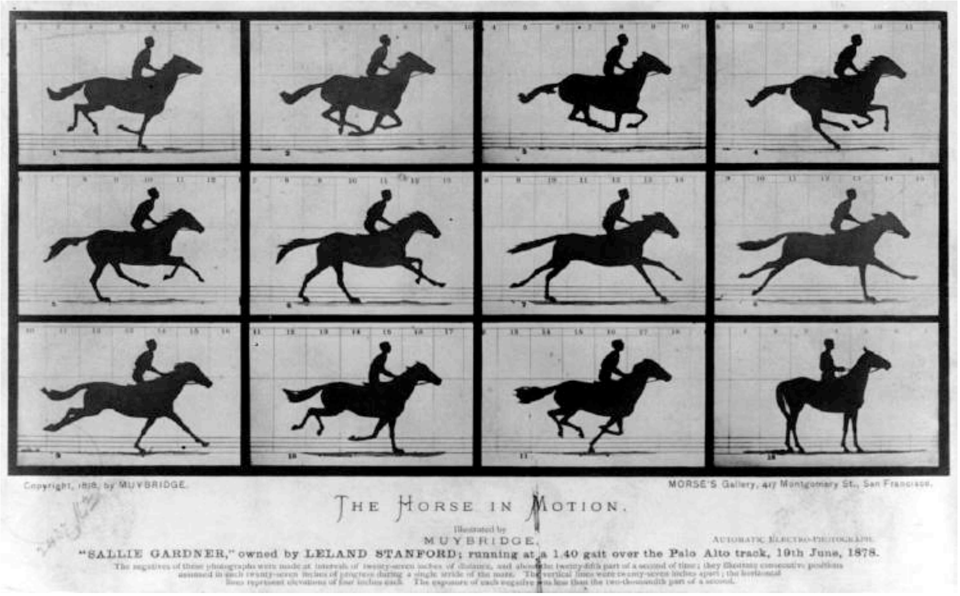
Nonequilibrium: The new frontier


tinyurl.com/MegaFreeWalls

Pump-probe spectroscopy (1887)

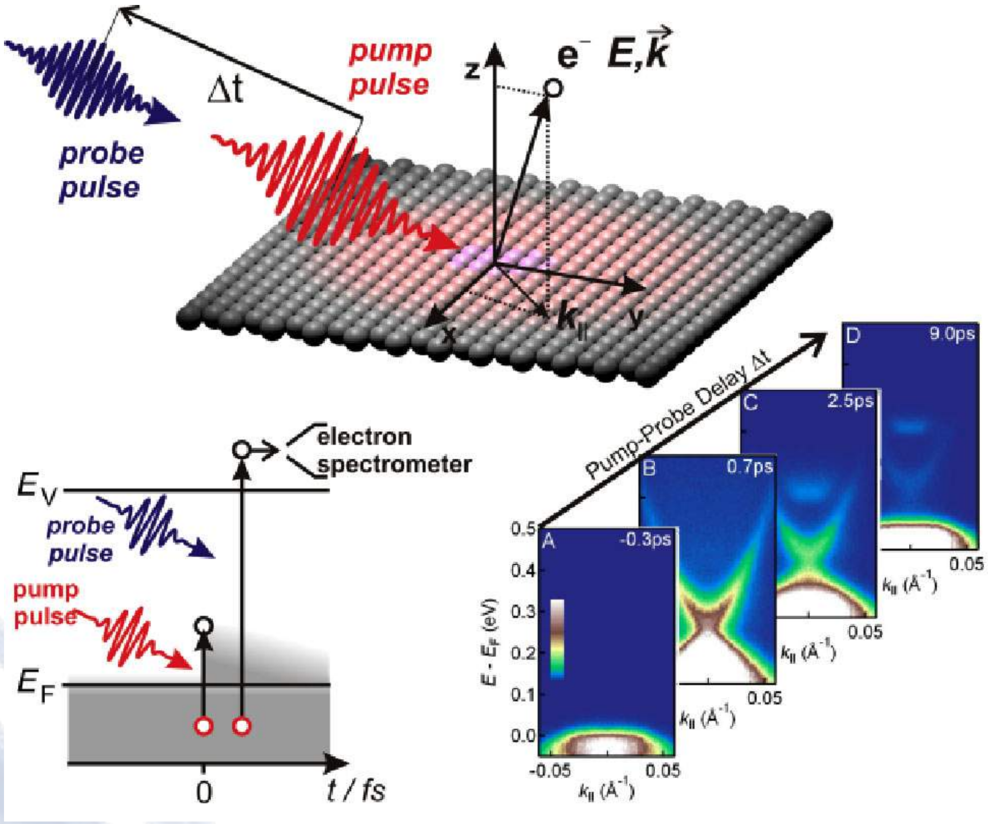
- stroboscopic investigations of dynamic phenomena



Muybridge 1887

Pump-probe spectroscopy (today)

- stroboscopic investigations of dynamic phenomena



TbTe3 CDW metal

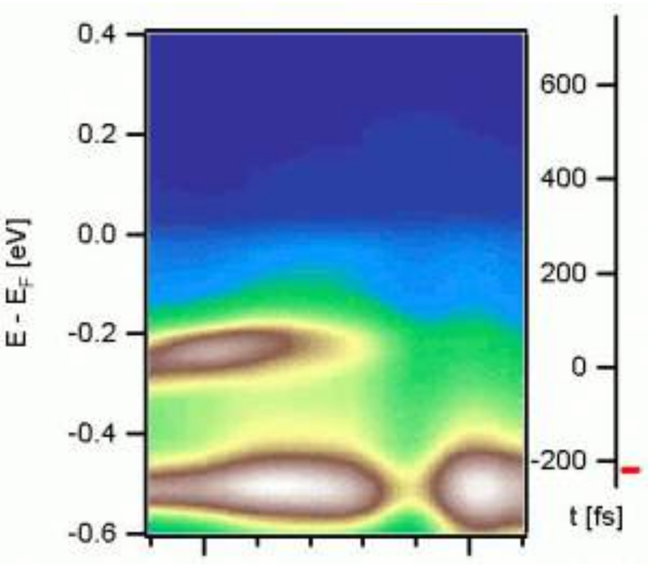


Image courtesy:
J. Sobota / F. Schmitt

Ultrafast Materials Science

Understanding the nature of quasi-particles

- Relaxation channels and dynamics

Understanding ordered phases

- Collective oscillations
- Competing order parameters
- Beyond the Landau paradigm of phase transitions

Creating new states of matter

- Photo-induced phase transitions
- Non-thermal phases

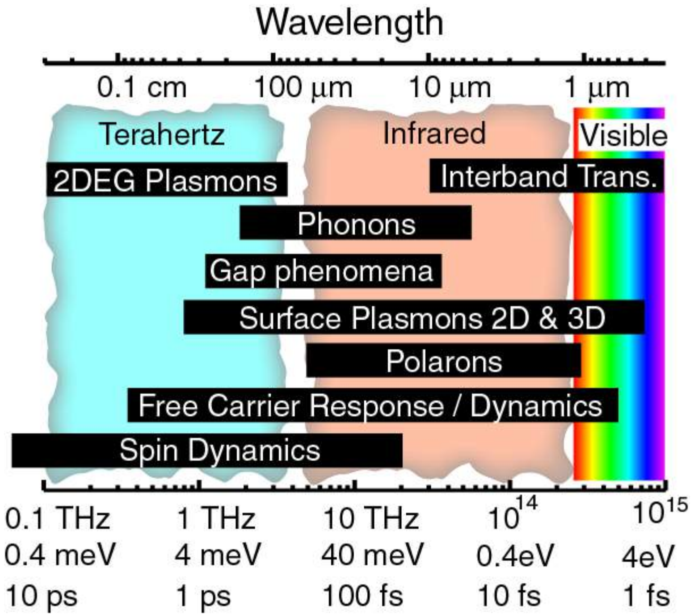


Image courtesy:
D. Basov

Outline

- NEGF, time-resolved photocurrent
- Ordered states: Driven superconductors
  - Higgs amplitude mode oscillations for optical pumping (1.5 eV laser)

    arXiv:1412.2762
  - light-enhanced superconductivity for phonon driving modeled as effective hopping ramp (nonlinear phononics)

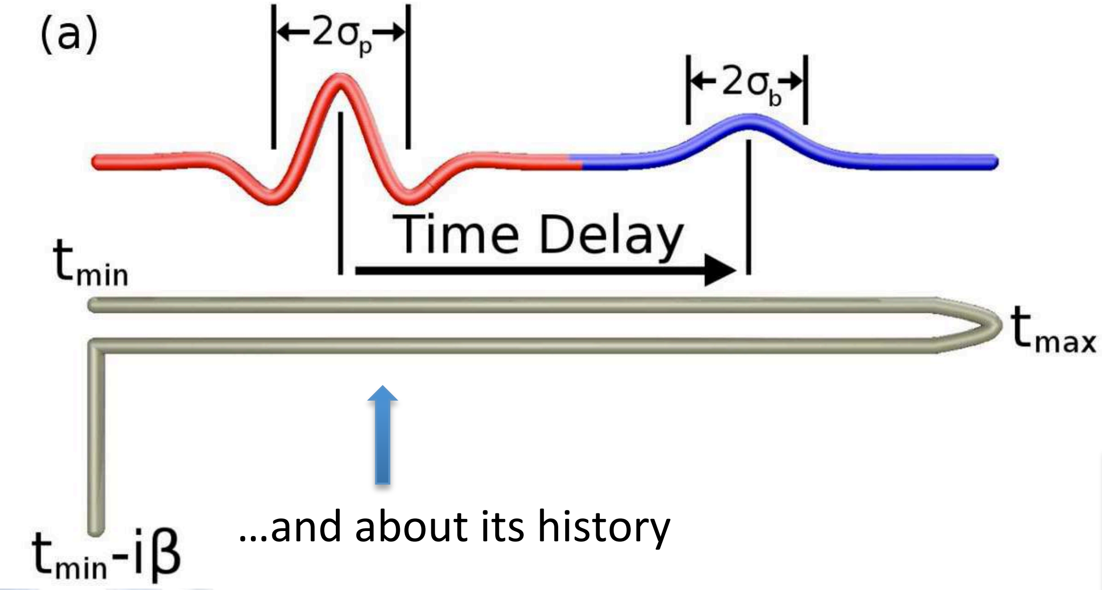
    arXiv:1505.07575

Non-Equilibrium Keldysh Formalism

$$G_{\mathbf{k}}(t,t') = G^0_{\mathbf{k}}(t,t') + \int dt_1\, dt_2\, G^0_{\mathbf{k}}(t,t_1)\Sigma(t_1,t_2)G_{\mathbf{k}}(t_2,t')$$

$$G_k(\omega) = G^0_k(\omega) + G^0_k(\omega)\underline{\Sigma(\omega)}G_k(\omega)$$

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



...and about its history

System knows about its thermal initial state...

same problem as in equilibrium (but worse):
use your favorite self-energy approximation, e.g. perturbation theory, nonequilibrium DMFT, ...

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

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

Equations of motion: Kadanoff-Baym

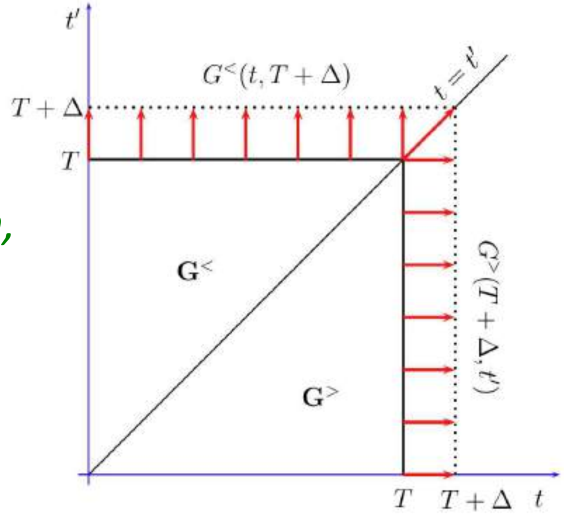
>,<,R,A are 4 Green's functions (2 independent)
Initial values obtained from Matsubara axis (equilibrium)

$$\left[i\partial_t - \epsilon(\mathbf{k}(t))\right] G^{\gtrless}_{\mathbf{k}}(t,t') = \int_0^t d\bar{t}\; \Sigma^R(t,\bar{t})\, G^{\gtrless}_{\mathbf{k}}(\bar{t},t') + \int_0^{t'} d\bar{t}\; \Sigma^{\gtrless}(t,\bar{t})\, G^{A}_{\mathbf{k}}(\bar{t},t')$$

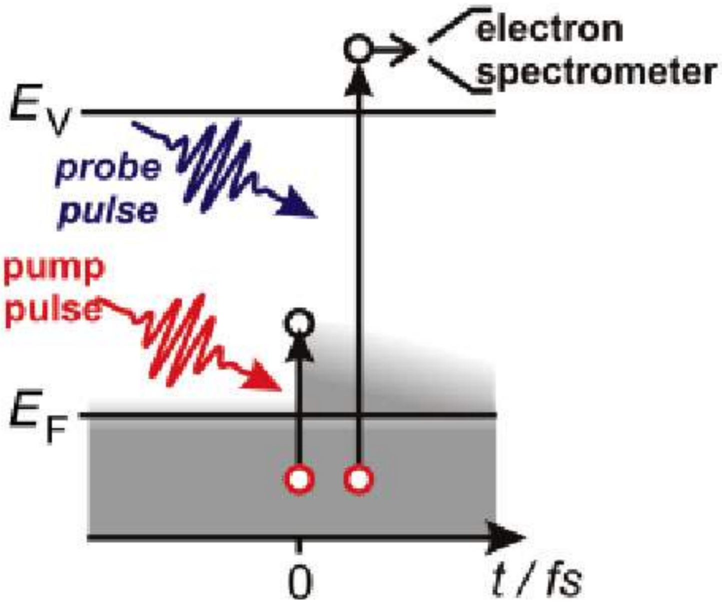
k indexes the quantum states

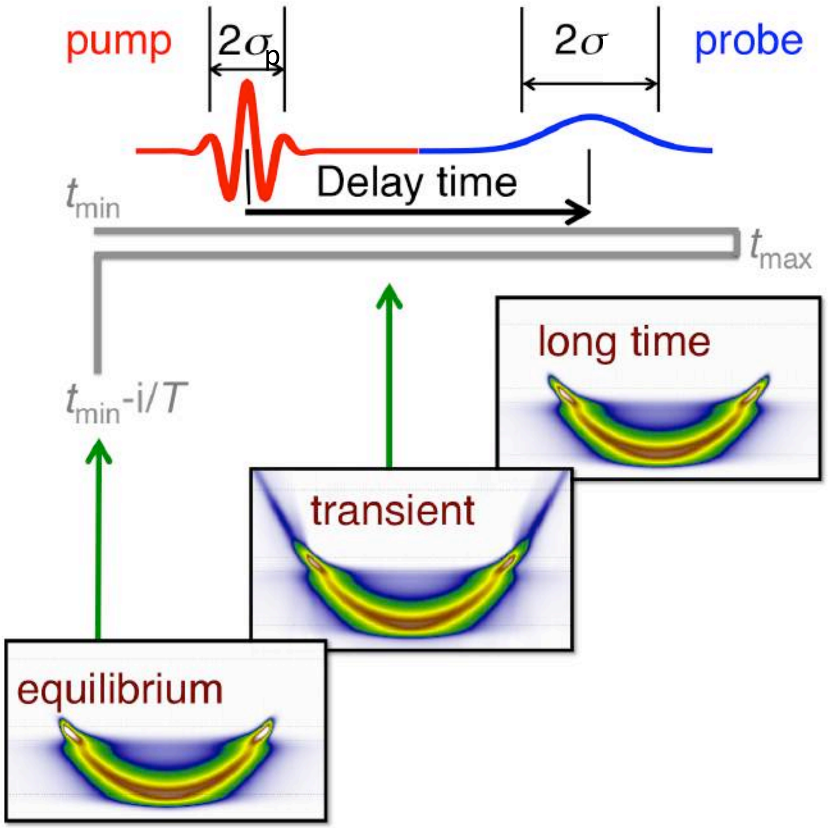
Σ integration kernel involves sum over all **k**

Time stepping method:
A.Stan, N.E.Dahlen, R. van Leeuwen,
J.Chem.Phys.130, 224101 (2009)



Pump-probe photoemission spectroscopy





$$A_{\mathbf{k}}(\omega, t_0) = \mathrm{Im}\, \frac{1}{2\pi\sigma^2} \int dt dt' \boxed{G^{<}_{\mathbf{k}}(t,t')} \boxed{e^{-(t-t_0)^2/2\sigma^2} e^{-(t'-t_0)^2/2\sigma^2}} e^{i\omega(t-t')}$$

M. Eckstein and M. Kollar, PRB (2008), J. K. Freericks et al., PRL (2009), J. K. Freericks et al., arXiv:1403.7585

+ gauge invariance (Bertoncini&Jauho Phys. Rev. B 44, 3655 (1991))

Model and Method

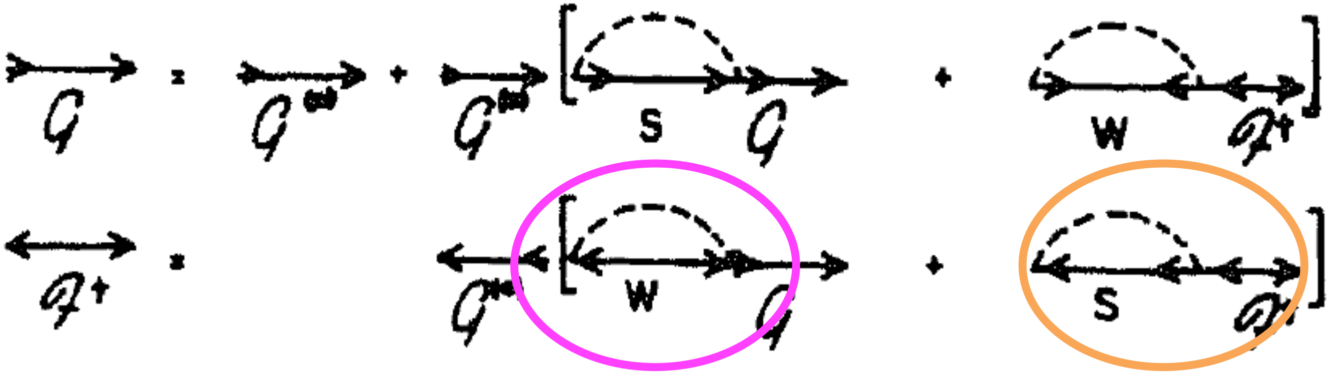
$$\mathcal{H} = \sum_{\boldsymbol{k}\sigma} \epsilon(\boldsymbol{k},t) c^{\dagger}_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma} + \sum_{\boldsymbol{q},\gamma} \Omega_{\gamma} b^{\dagger}_{\boldsymbol{q},\gamma} b_{\boldsymbol{q},\gamma} - \sum_{\boldsymbol{q},\gamma,\sigma} g_{\gamma} c^{\dagger}_{\boldsymbol{k}+\boldsymbol{q}\sigma}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

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

superconductor:

normal

anomalous

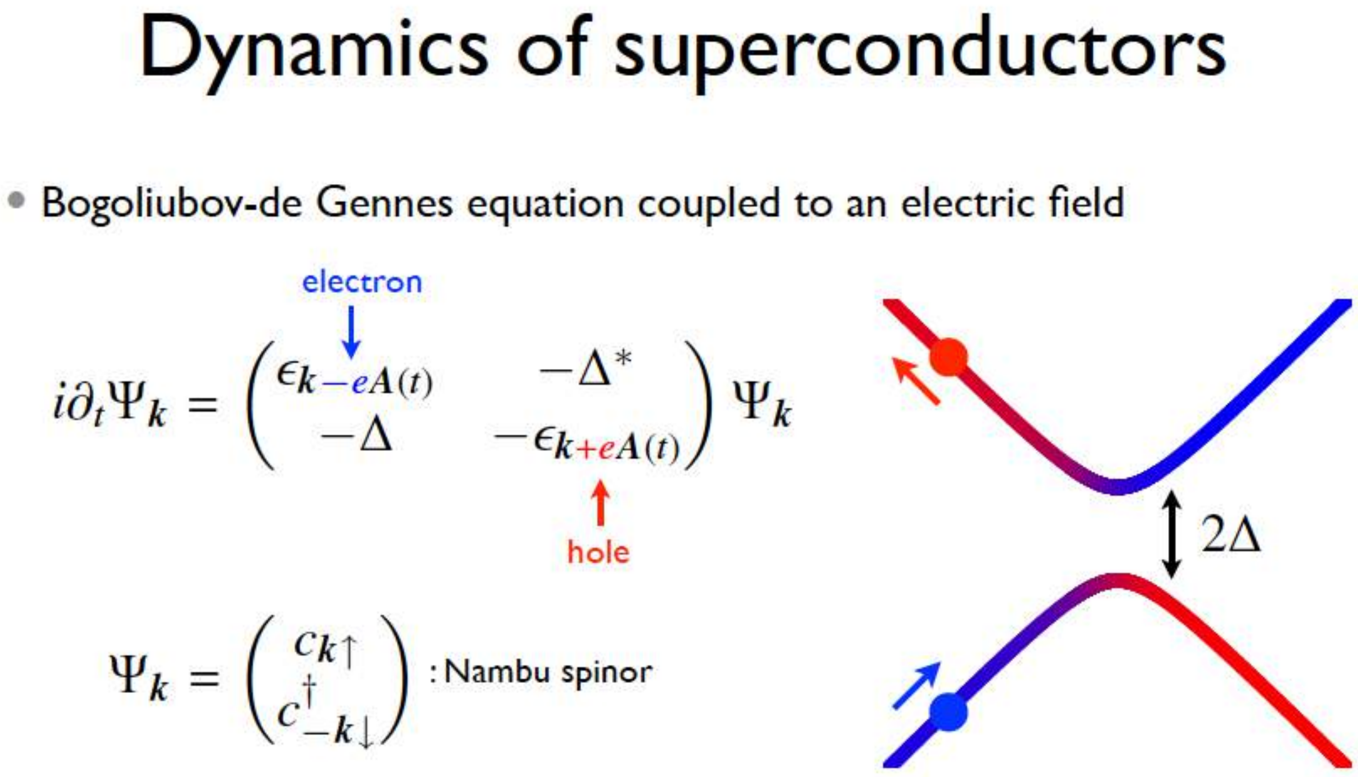


order parameter Δ, condensate dynamics

el-ph single-particle scattering

cf. textbooks (Mahan, AGD, ...) for Migdal-Eliashberg approx.

Higgs amplitude mode



Dynamics of superconductors

- Bogoliubov-de Gennes equation coupled to an electric field

$$i\partial_t \Psi_k = \begin{pmatrix} \epsilon_{k \overset{\text{electron}}{\overset{\downarrow}{-}} eA(t)} & -\Delta^* \\ -\Delta & -\epsilon_{k \underset{\text{hole}}{\underset{\uparrow}{+}} eA(t)} \end{pmatrix} \Psi_k$$

$$\Psi_k = \begin{pmatrix} c_{k\uparrow} \\ c^\dagger_{-k\downarrow} \end{pmatrix}$$: Nambu spinor

Higgs amplitude mode

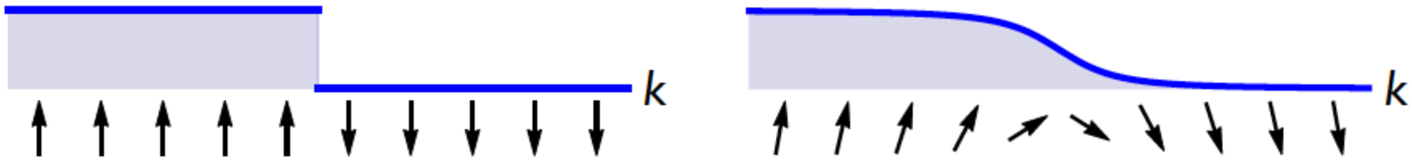
Anderson pseudospin

$$\boldsymbol{\sigma}_{\boldsymbol{k}} = \frac{1}{2}\Psi_{\boldsymbol{k}}^{\dagger} \cdot \boldsymbol{\tau} \cdot \Psi_{\boldsymbol{k}}$$

Anderson, Phys. Rev. 112, 1900 (1958)

$$\boxed{\partial_t \boldsymbol{\sigma}_{\boldsymbol{k}} = 2\boldsymbol{b}_{\boldsymbol{k}} \times \boldsymbol{\sigma}_{\boldsymbol{k}} \qquad \boldsymbol{b}_{\boldsymbol{k}} = \left(-\Delta', -\Delta'', \frac{\epsilon_{\boldsymbol{k}-e\boldsymbol{A}(t)} + \epsilon_{\boldsymbol{k}+e\boldsymbol{A}(t)}}{2}\right)}$$

Tsuji, Aoki, arXiv:1404.2711



normal state

BCS state

- Particle-hole symmetric by construction.
- Linear response vanishes.

Higgs amplitude mode

Light-pseudospin coupling

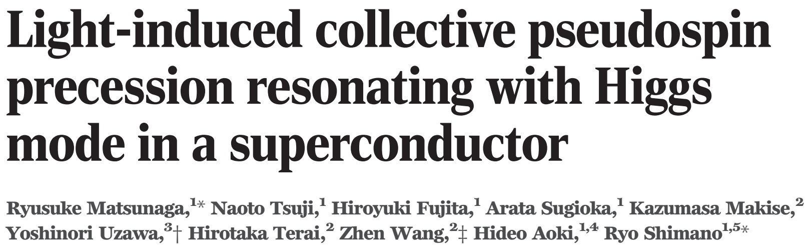
$$\boxed{\partial_t \boldsymbol{\sigma}_k = 2\boldsymbol{b}_k \times \boldsymbol{\sigma}_k \qquad \boldsymbol{b}_k = \left(-\Delta', -\Delta'', \frac{\epsilon_{k-eA(t)} + \epsilon_{k+eA(t)}}{2}\right)}$$

$$\epsilon(k-A) + \epsilon(k+A) = 2\epsilon(k) + \mathcal{O}(A^2),$$

A^2 coupling: „Anderson pseudospin resonance“ at 2 ω = 2 Δ

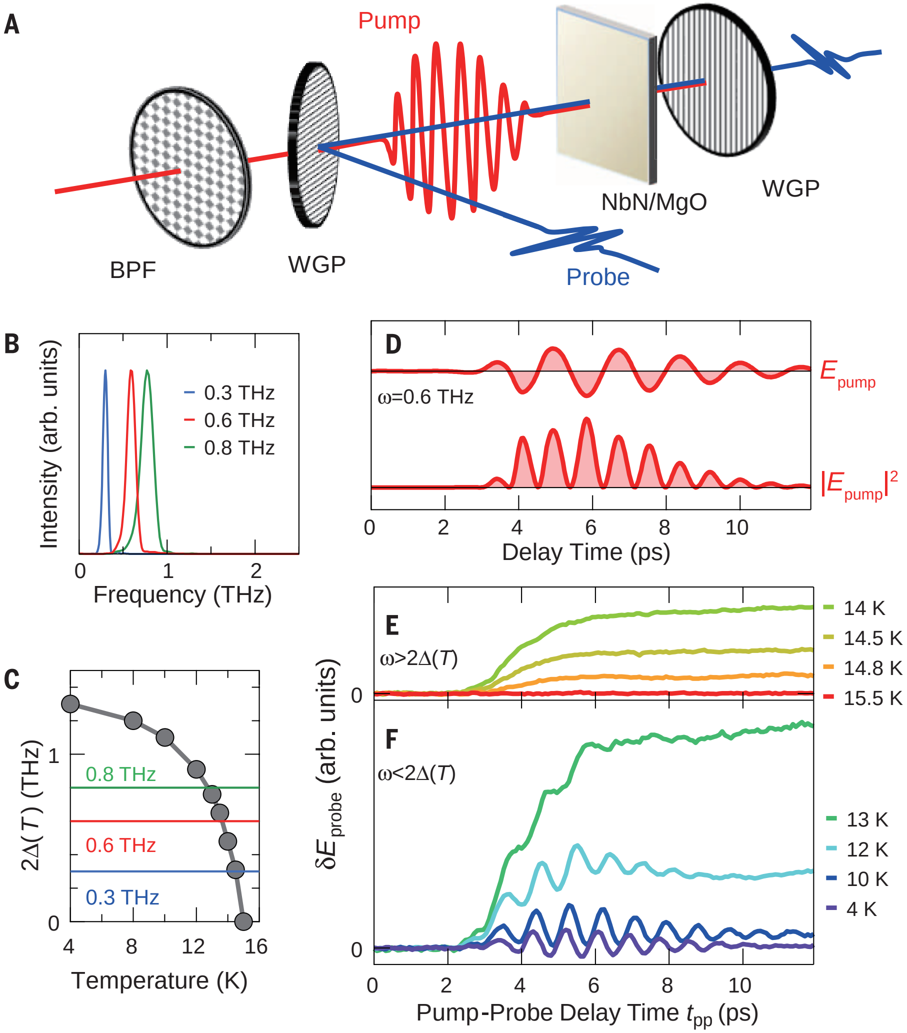
Tsuji & Aoki, arXiv:1404.2711
R. Matsunaga et al., Science 345, 1145 (2014)

Higgs amplitude mode



Light-induced collective pseudospin precession resonating with Higgs mode in a superconductor

Ryusuke Matsunaga,[1]* Naoto Tsuji,[1] Hiroyuki Fujita,[1] Arata Sugioka,[1] Kazumasa Makise,[2] Yoshinori Uzawa,[3]† Hirotaka Terai,[2] Zhen Wang,[2]‡ Hideo Aoki,[1,4] Ryo Shimano[1,5]*



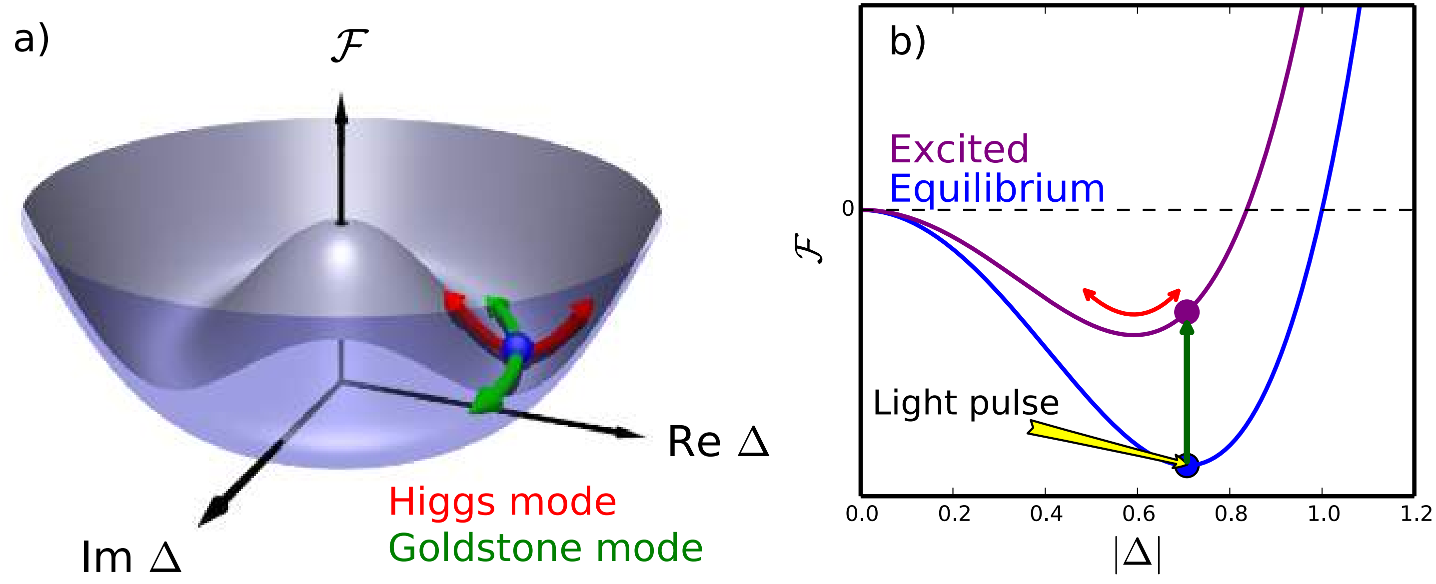
Matsunaga et al., Science 345, 1145 (2014); PRL 2012/2013

see also: Mansart et al., PNAS 110, 4539 (2013)

amplitude mode oscillations observed in pump-probe optics

what about pump-probe photoemission spectroscopy?

Higgs amplitude mode



amplitude mode cannot be directly accessed by single photons (coupling = 0 in linear response due to gauge invariance)

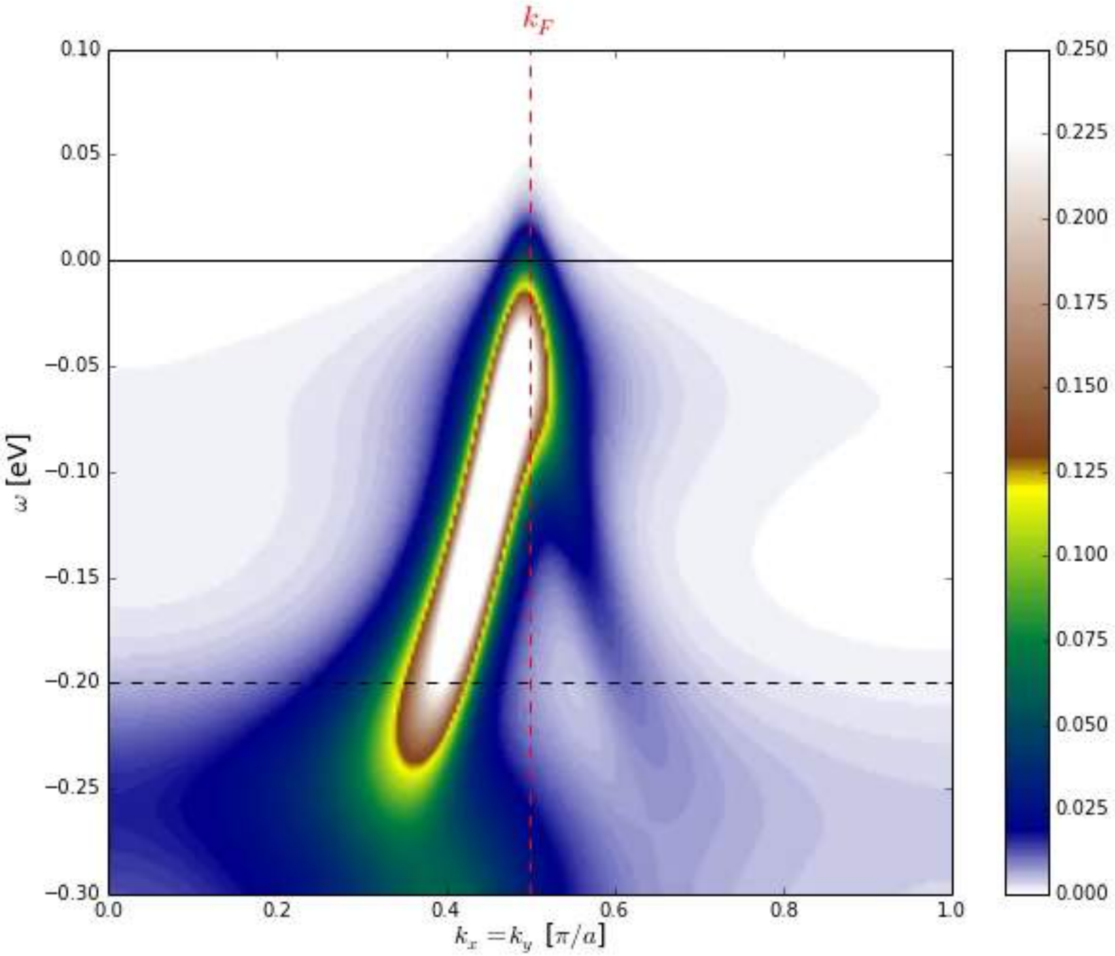
BUT: 2-photon nonlinear excitation works (Littlewood&Varma PRL 1981; Tsuji&Aoki arXiv:1404.2711)

seeing amplitude mode directly in time-resolved ARPES spectroscopy?

Include the effects of driving field through Peierls substitution

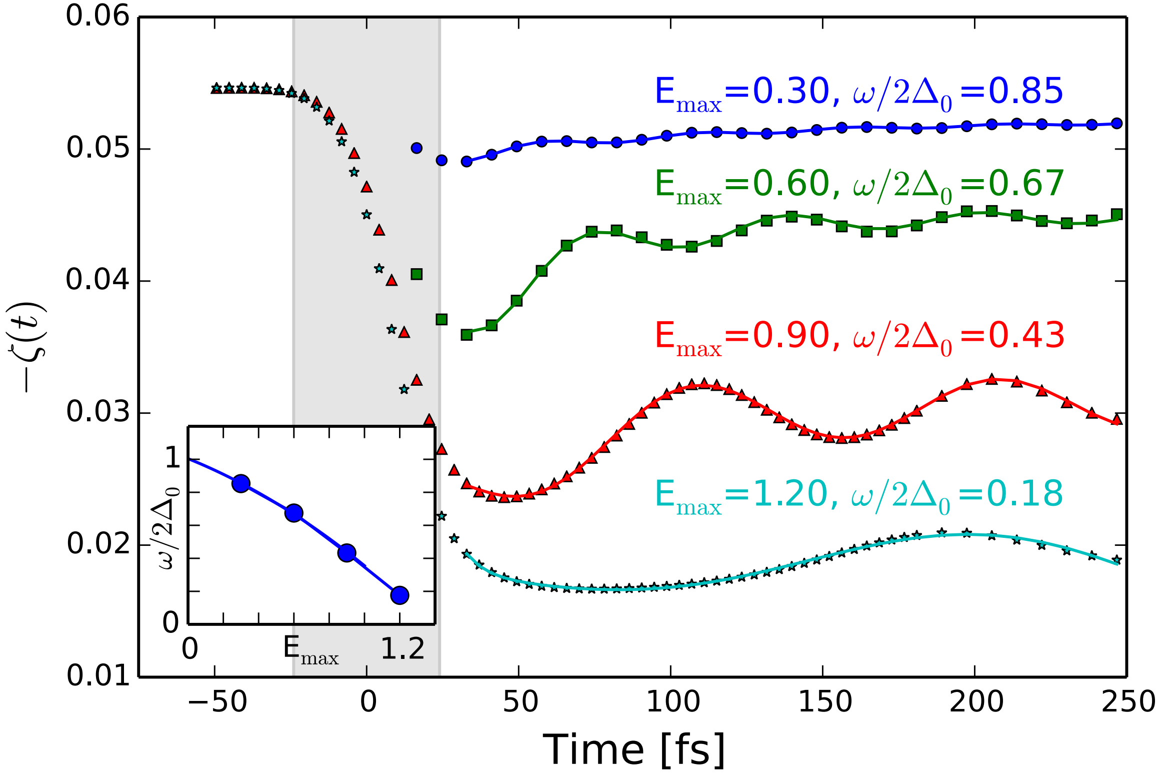
$$\boldsymbol{k} \to \boldsymbol{k} - e\mathbf{A}(t)$$

Oscillations in photocurrent



Amplitude mode oscillations

arXiv:1412.2762



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

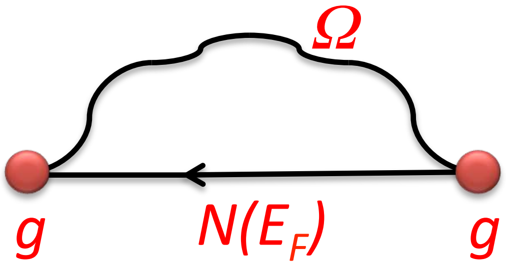
How to enhance boson-mediated SC?

- 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?

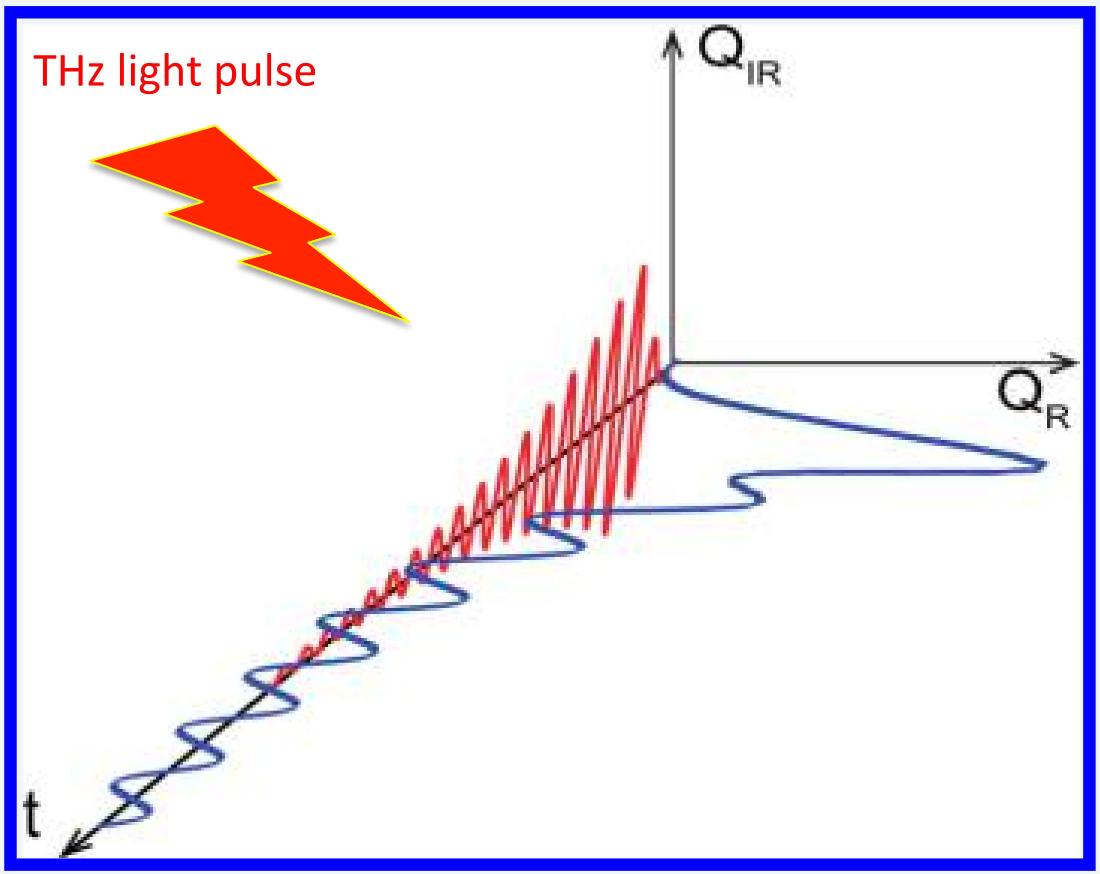
1. tune model parameters
   - e-boson coupling g
   - boson frequency Ω
   - electronic DOS $N(E_F)$

$\}$ α^2F – Eliashberg function

Gedankenexperiment (what if?)

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

Classical lattice dynamics



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

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

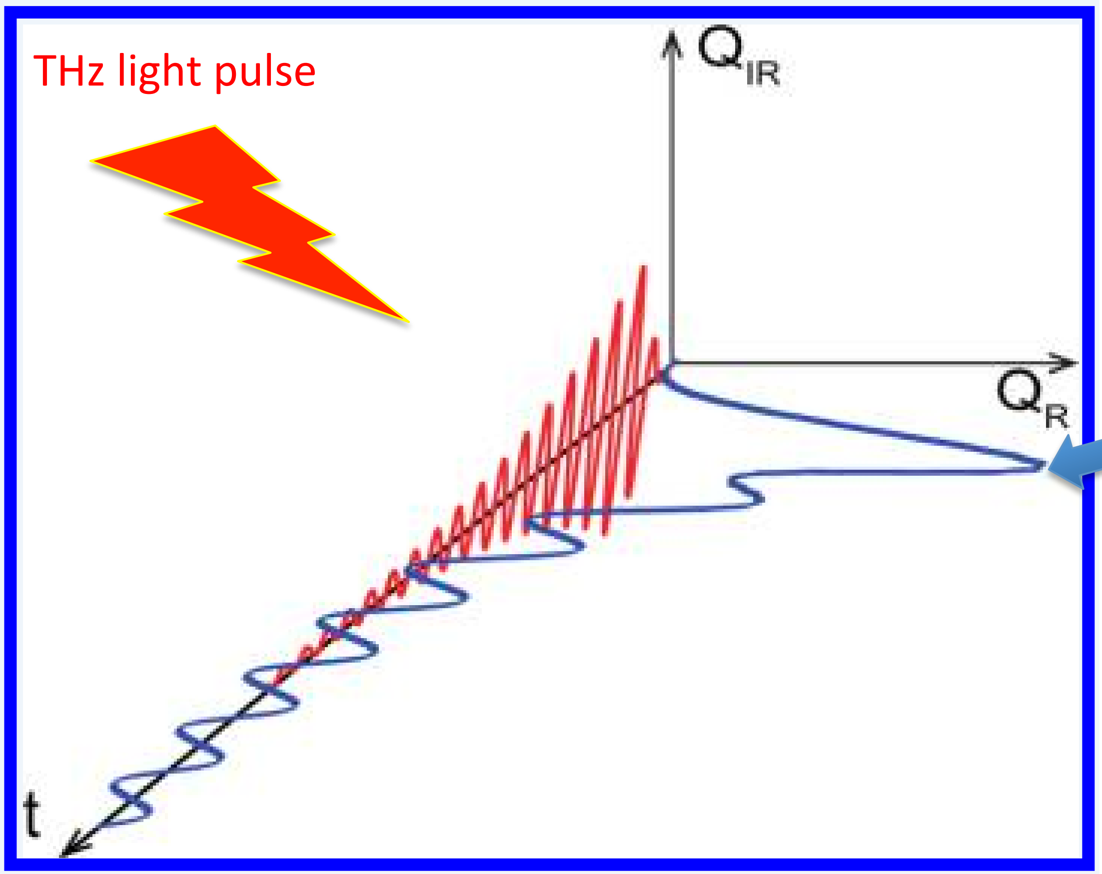
Rectification of a second (Raman) phonon via coherent driving of a first (IR) phonon

„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)

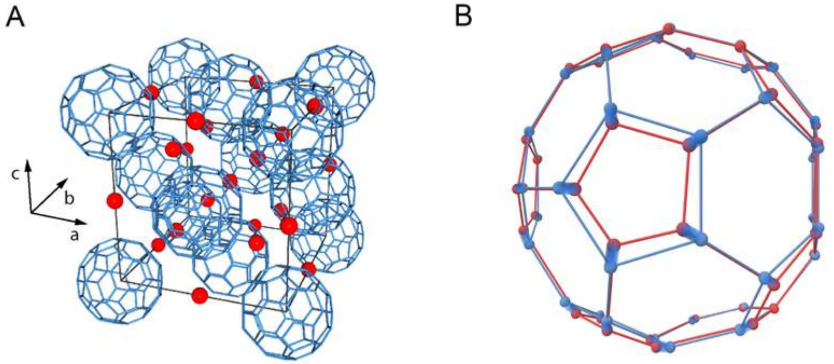
A. Subedi, A. Cavalleri, A. Georges, PRB 89, 220301R (2014)

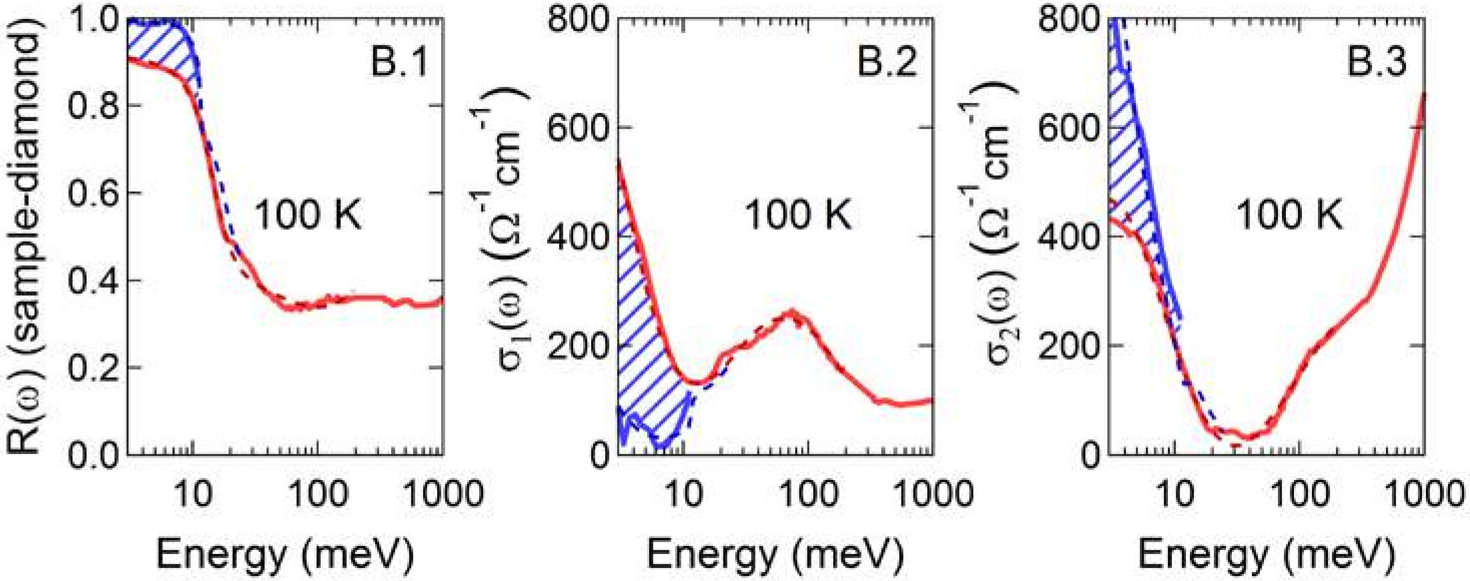
Experimental motivation

„An optically stimulated superconducting-like phase in K3C60 far above equilibrium Tc“

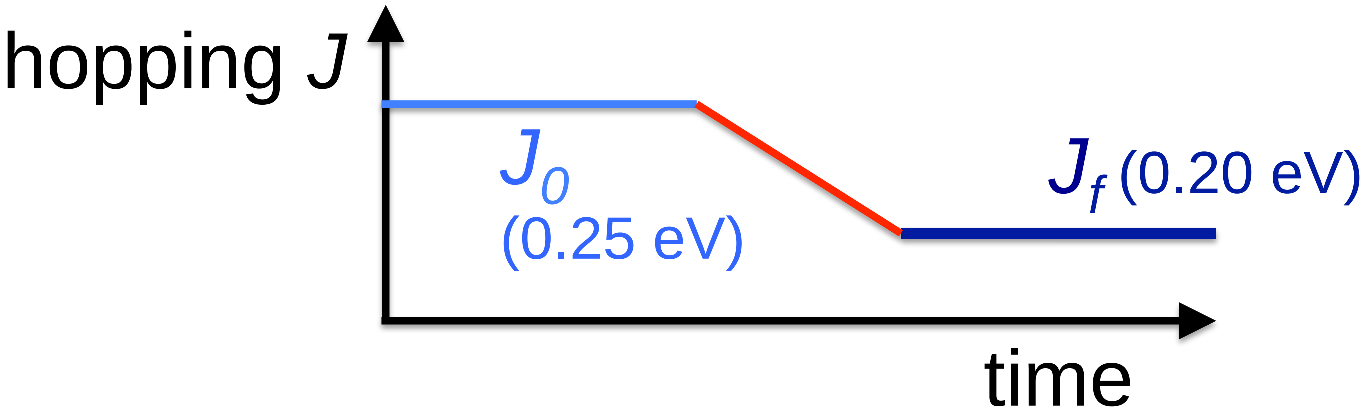
M. Mitrano et al., arXiv: 1505.04529

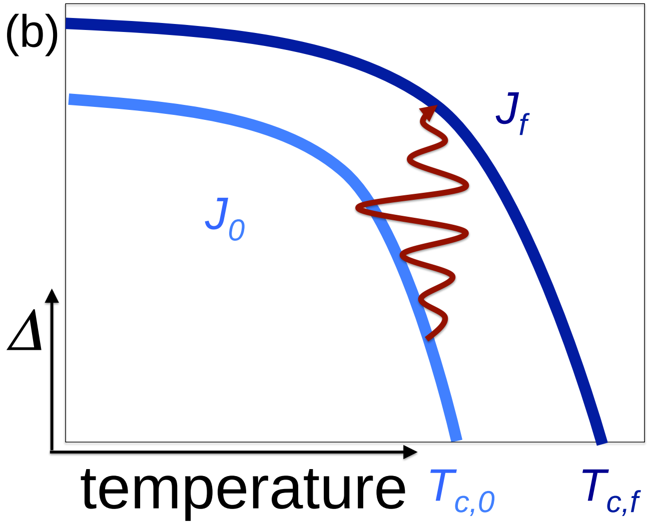
cf. Alice Cantaluppi‘s talk





Simplest model: hopping ramp

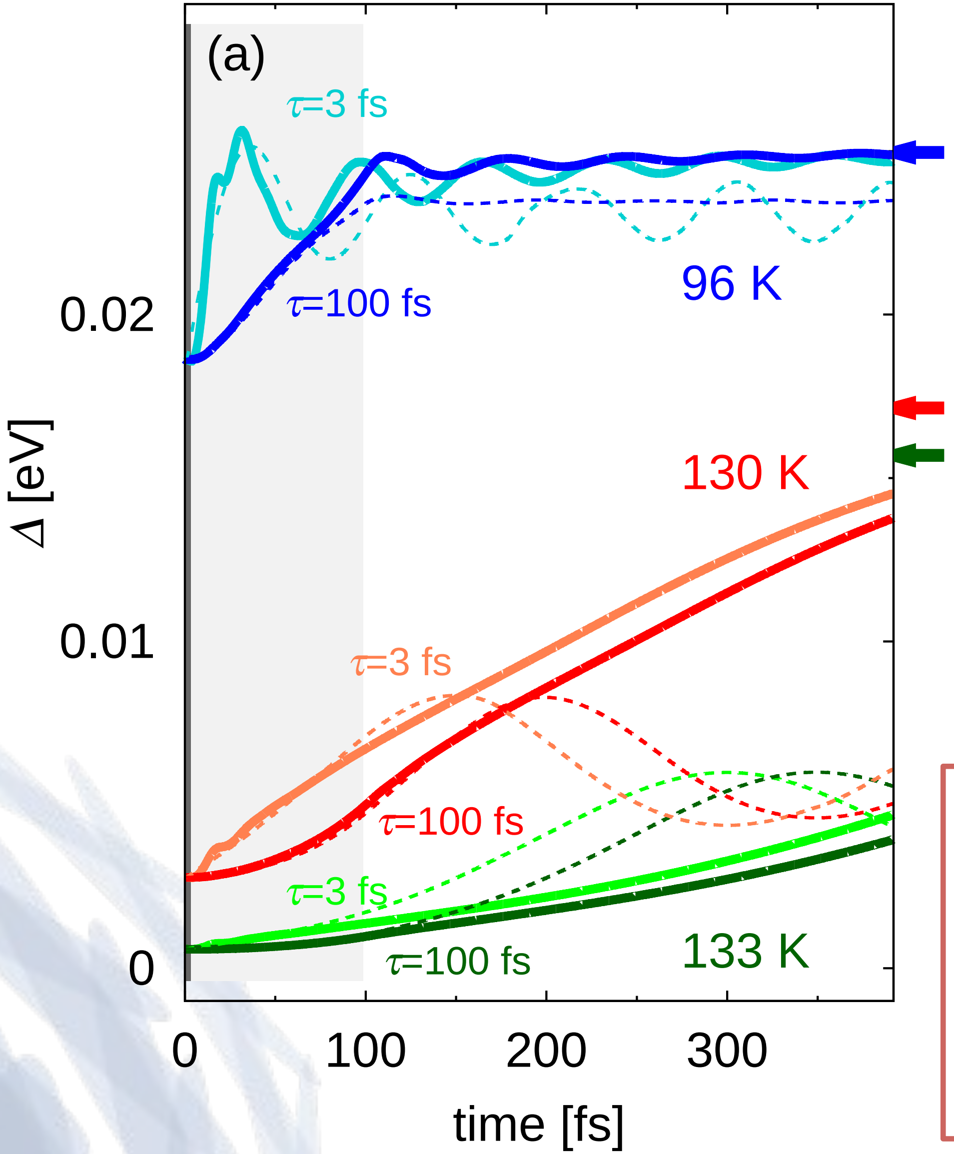


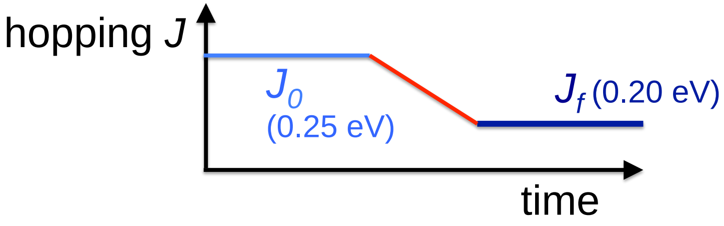


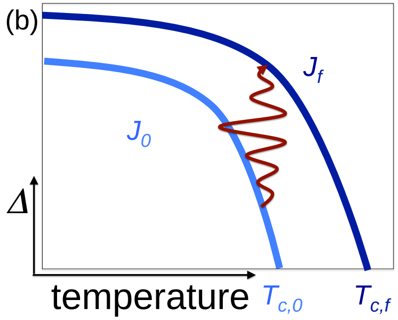
Equilibrium picture:

Enhancement of SC via enhanced DOS at Fermi energy

Superconductor evolution

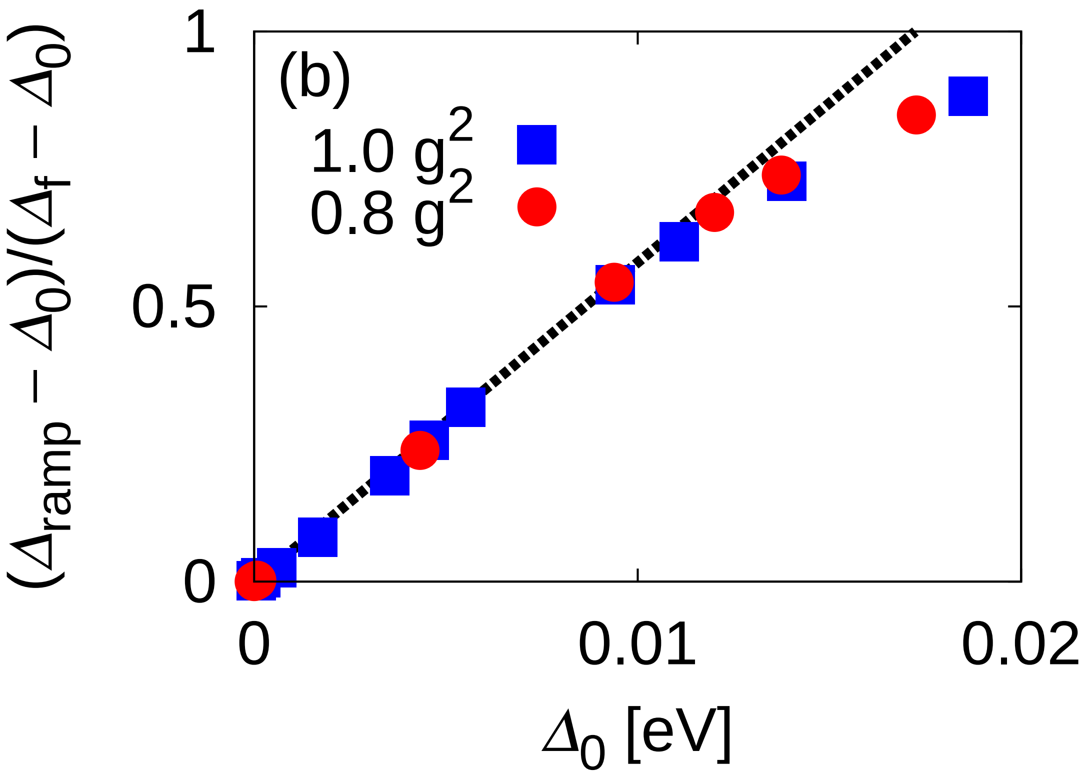


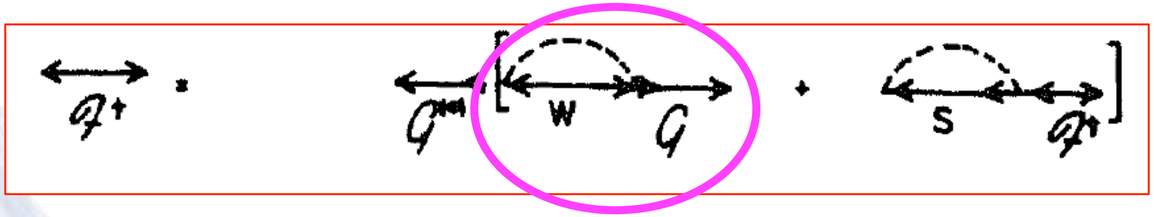




Enhancement of SC strongly depends on initial thermal state

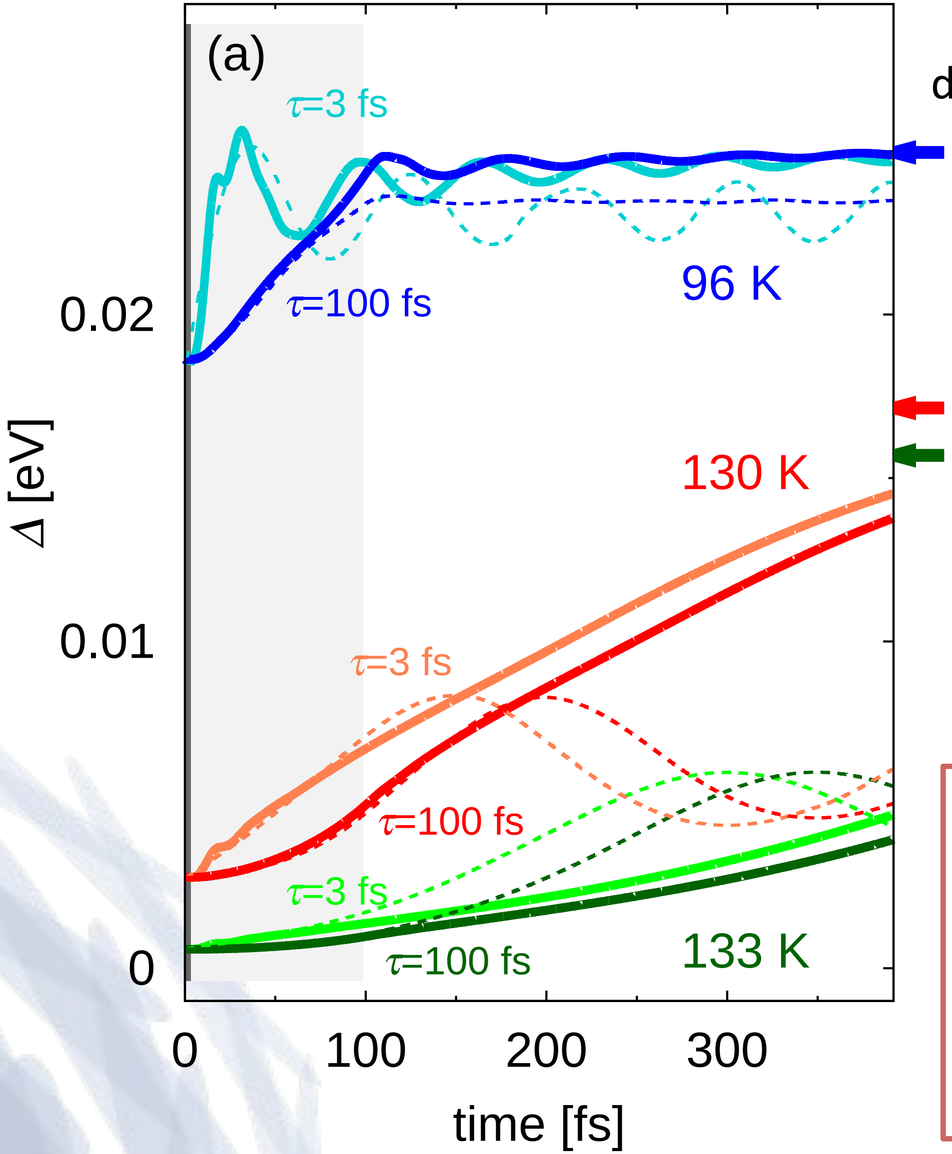
Enhancement during ramp



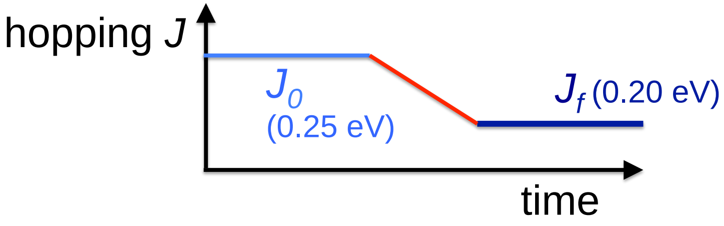


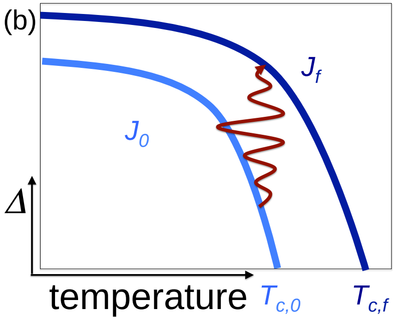
Order parameter enhancement ~Δ_0

Superconductor evolution



dashed: no dissipation (BCS only)





Dissipation helps enhancement for fast ramps

Summary: NEGF at work!

- Amplitude mode oscillations in pumped SC

  arXiv:1412.2762

- Light-enhanced SC via nonlinear phononics

  arXiv:1505.07575


A. F. Kemper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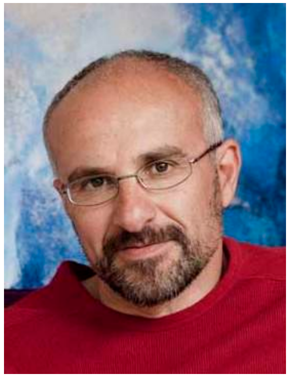
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