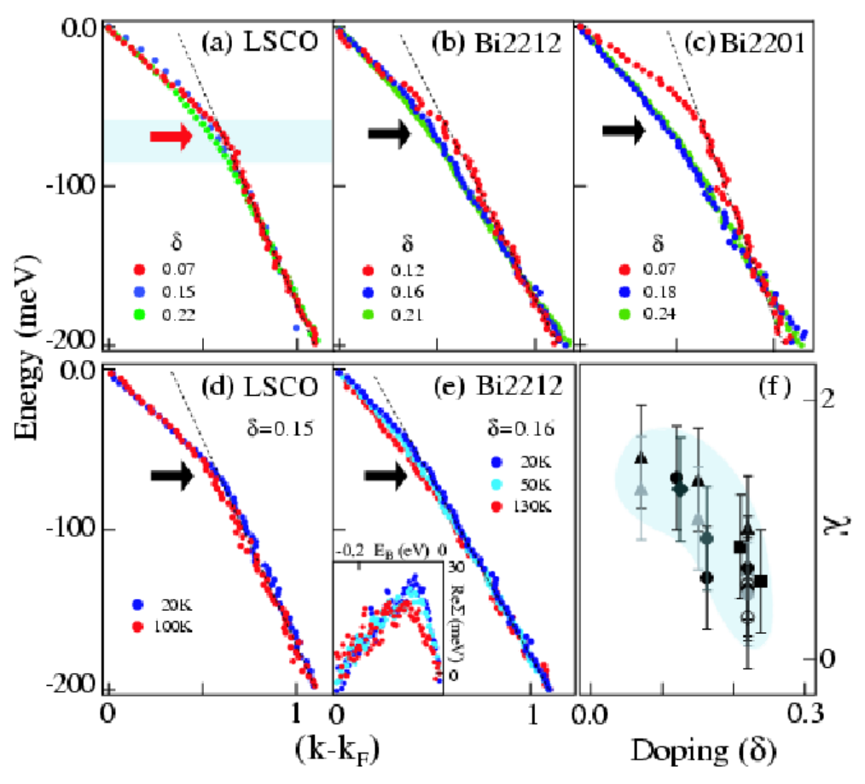
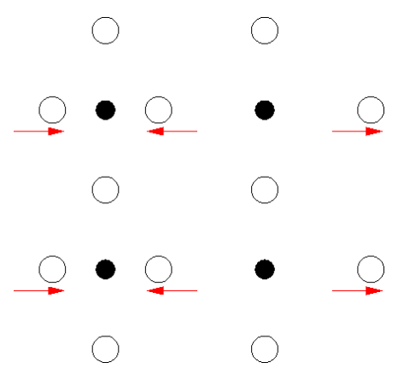
Electron-phonon coupling to breathing phonons in cuprates

Oliver Rösch and Olle Gunnarsson
Max-Planck-Institut für Festkörperforschung, D-70569 Stuttgart

MAX-PLANCK-INSTITUT
für Festkörperforschung

Kink in electron dispersion



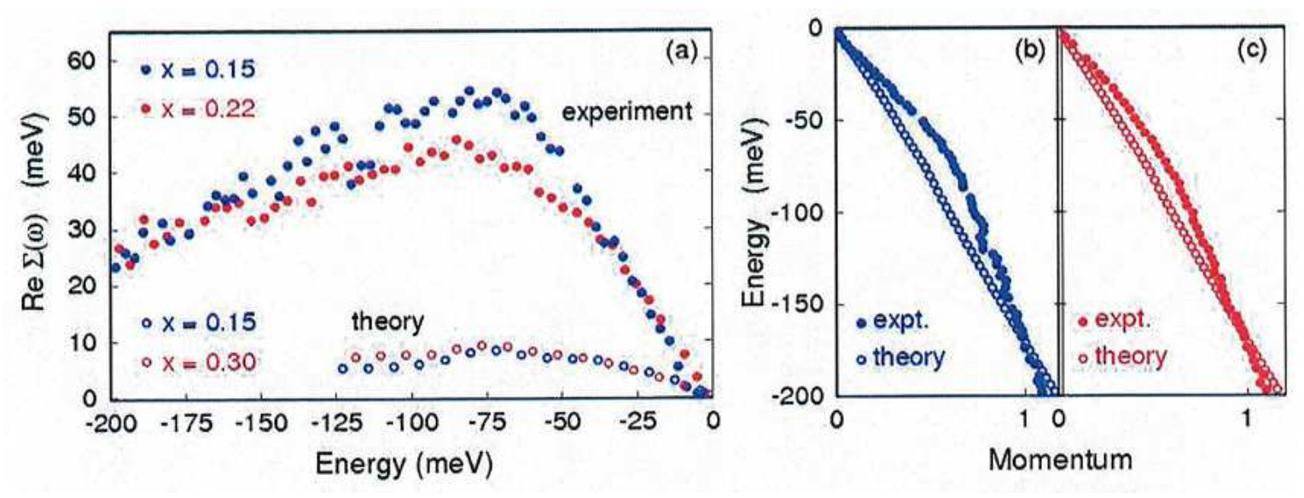


Kink in ARPES QP dispersions at $\sim$ 70 meV

Strong interaction with (half-breathing) phonon mode?

Lanzara, Nature **412**, 510.

DFT: Electron-phonon coupling and dispersion kinks



$La_{2-x}Sr_xCuO_4$

Giustino, Cohen Louie, Nature **452**, 975.

Small DFT kink mainly due to breathing phonons.

But, DFT kink almost an order of magnitude smaller than experiment.

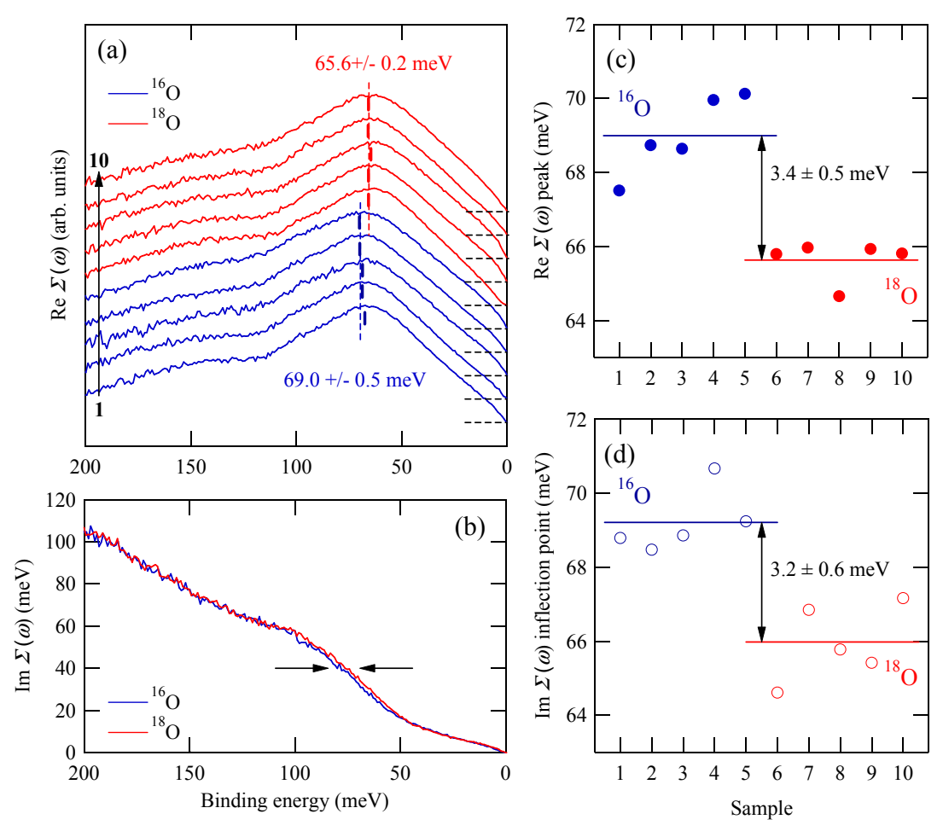
Electron-phonon interaction not responsible for kink?

Zone-boundary half-breathing phonon: $\lambda \sim 0.01.$

Heid, Bohnen, Zeyher, Manske, PRL **100**, 137001.

Bohnen, Heid, Krauss, Europhys. Lett **64**, 104.

Isotope shift of kink



$Bi_2Sr_2CaCu_2O_{8+\delta}$
Dessau group,

arXiv:0808.1323.

Kink energy 69 meV,

Isotope shift:

3.4 ± 0.5 meV (Re Σ).

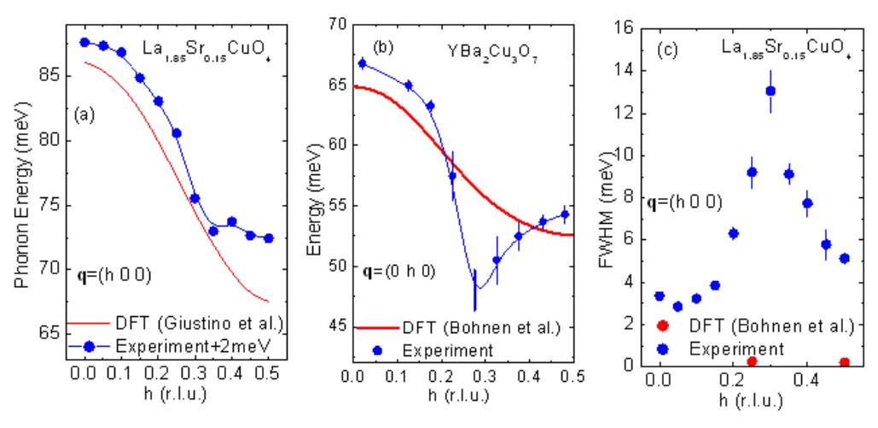
3.2 ± 0.6 meV (Im Σ).

For for phonon with energy 69 meV such isotope shift (3.9 meV) expected.

Substantial coupling to phonon with energy ~ 70 meV.

Isotope effect also seen in penetration depth and STM (shift 3.7 meV).

Half-breathing phonon. Neutron scattering



Reznik, Sangiovanni, Gunnarsson and Devereaux, Nature **455**, E6.

Reznik *et al.*, Nature **440**, 1170.

Reznik *et al.*, J. Low Temp. Phys. **147**, 353.

LDA widhts: Bohnen ($YBa_2Cu_3O_7$)

Giustino, Cohen Louie, Nature **452**, 975

Very strong anomaly at $\mathbf{q} \approx (0.3, 0, 0)$ in both dispersion and width.

Reduced with temperature $\Rightarrow$ Not anharmonic effects or impuritites.

LDA usually describes phonons very well, but here strongly underestimates width.

Anomalously strong coupling.

Electron-phonon coupl. Undoped La_2CuO_4. Shell model

Find the electron-phonon coupling strength to a Zhang-Rice singlet.

1. Use shell model to describe electrostatic coupling to phonons.

Phonon eigenvectors $\Rightarrow$ Potential on a singlet due to a phonon.

Screening only by the "shells".

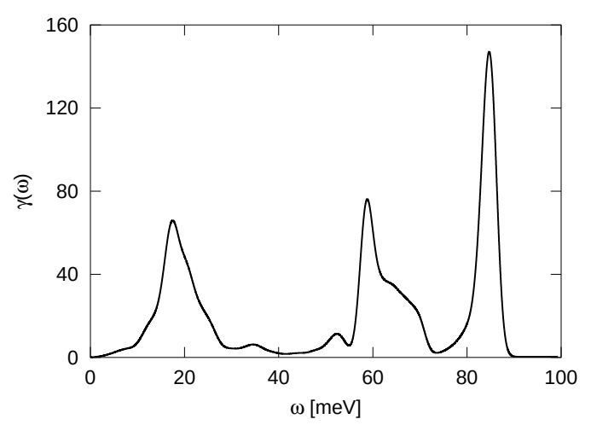
LDA too effective screening.

2. Add coupling due to modulation of t_{pd} and $\varepsilon_d - \varepsilon_p$ (breathing phonons).

Coupling to (half-)breathing modes (80 meV), O_z modes (60-70 meV) and La (Cu) modes (20 meV).

Total $\lambda \sim 1.2$. Breathing $\lambda \sim 0.4$.

$$\gamma(\omega) \equiv \sum_{\mathbf{q}\nu} \frac{|g_{\mathbf{q}\nu}|^2}{(\omega_{\mathbf{q}\nu} N)} \delta(\omega - \omega_{\mathbf{q}\nu}).$$



Sufficient to explain experimentally observed polaronic effects for undoped cuprates.

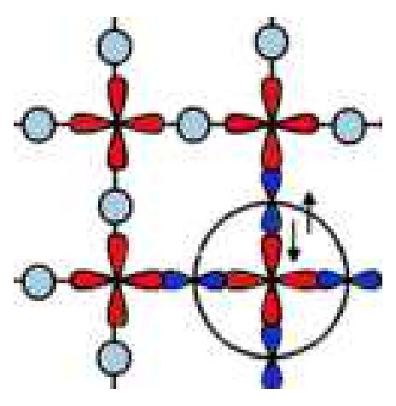
Rösch, Gunnarsson, Zhou, Yoshida, Sasagawa, Fujimori, Hussain, Shen, Uchida, PRL **95**, 227002.

Three-band (Emery) model

Important physics in CuO_2 plane.

Include one Cu x^2-y^2-3d and two O $2p$ orbital/cell.

$$H = \sum_{i\sigma} \varepsilon_i^d n_{i\sigma}^d + \sum_{j\sigma} \varepsilon_j^p n_{j\sigma}^p + U \sum_i n_{i\uparrow}^d n_{i\downarrow}^d - \sum_{<i,j>\sigma} t_{ij}^{pd} (d_{i\sigma}^\dagger p_{j\sigma} + H.c.)$$



t-J model

Undoped system: One hole per Cu site. AF coupling.

Doped system: Additional holes mainly on O sites.

Form Zhang-Rice singlets from Cu and O holes.

$$H_{eff} = J \sum_{<i,j>} \left(\vec{S}_i \cdot \vec{S}_j - \frac{1}{4} n_i n_j \right) + \sum_{i \neq j, \sigma} t_{ij} \tilde{c}_{i\sigma}^\dagger \tilde{c}_{j\sigma}$$

Origin of strong electron-phonon coupling

Zhang-Rice singlet: Nominally d^1p^1.

Coherent hopping Cu x^2-$y^2 \leftrightarrow$ O $2p \Rightarrow$

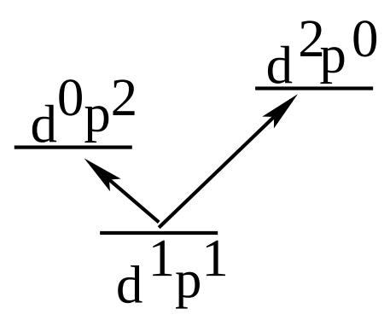
$E^{Z-R} \approx -4t_{pd}^2 \left(\frac{2-1}{\varepsilon_p} + \frac{2}{U-\varepsilon_p} \right)$.

Large singlet energy (~ 5 eV).

Due to singlet character, coupling to two config.

For rigid lattice uninteresting constant.

Phonons modulate singlet energy via t_{pd}.



$$\frac{1}{\sqrt{2}}(|p\uparrow\rangle|d\downarrow\rangle - |p\downarrow\rangle|d\uparrow\rangle)$$

Strong coupling because Zhang-Rice singlet energy large.

Rösch and Gunnarsson, PRL **92**, 146403.

HF Solution of three-band model

Consider three-band model with frozen phonons
in Hartree-Fock (HF) mean-field approximation.

Simulates LDA in paramagnetic doped system,
but is able to give AF solution in undoped case

Downfold to one-band model.

Project out O-2p levels, get effective Cu-3d model.

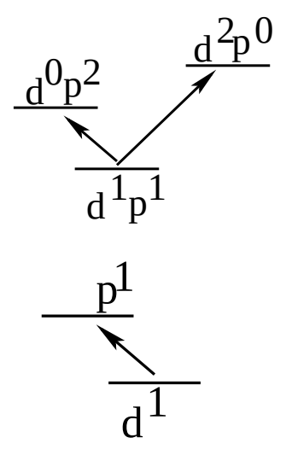
This allows direct comparison with $t-J$ model.

Phonon softening in HF solution (linear response)

Softening given by Re $\Pi_{\mathbf{q}}(\omega) \approx g_{\mathbf{q}}^2 \times \frac{1}{\pi} \int d\omega' \frac{\text{Im}\, \chi_{\mathbf{q}}(\omega')}{\omega - \omega'}$

$\Pi_{\mathbf{q}}(\omega) \approx g_{\mathbf{q}}^2 \chi_{\mathbf{q}}(\omega)$: phonon self-energy
$\chi_{\mathbf{q}}(\omega)$: charge correlation function

source	$t-J$	HF	ratio
coupling g^2	$[\frac{2-1}{\varepsilon_p} + \frac{2}{U-\varepsilon_p}]^2$	$\frac{1}{\varepsilon_p^2}$	≈ 3
sum rule for Im χ	$\approx 2\pi\delta$	$\approx \pi$	$\approx 2\delta$
$< 1/\omega >_{\text{Im}\,\chi}$			≈ 1
screening	≈ 1	≈ 0.5	≈ 2
product			$\approx 12\delta$

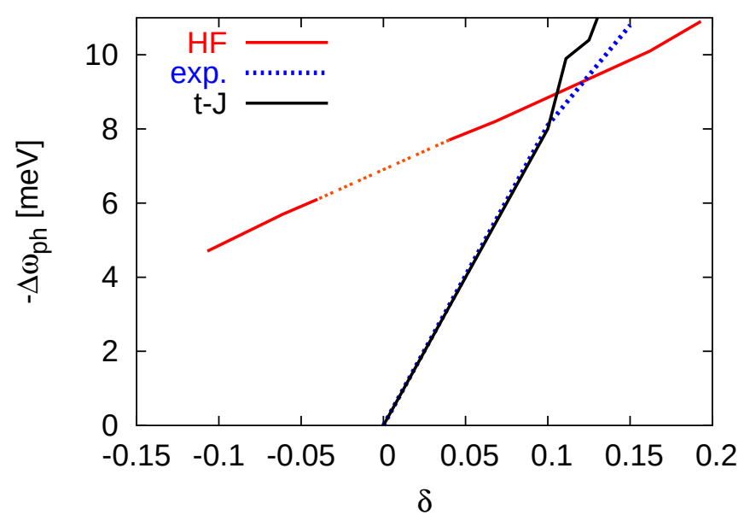


Large enhancement of the coupling for the half-breathing phonon.

$\Rightarrow$ Softening for $\approx 10-15\%$ doping is of right size
but due to different reasons than in $t-J$ model

O. Rösch and O. Gunnarsson, PRB **70**, 224518.

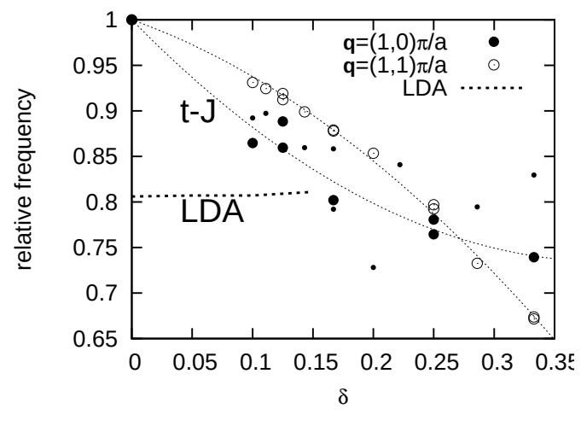
Doping dependence of softening

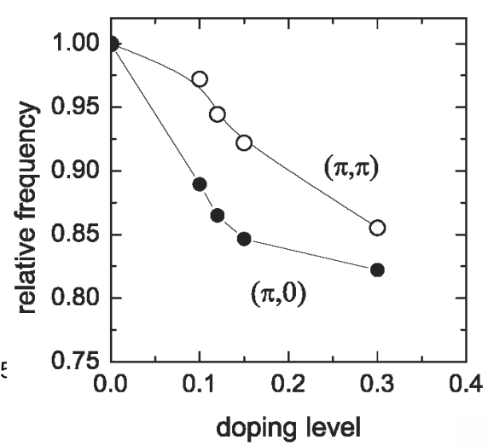


$$\Delta\omega_{ph} = \omega_{ph}^{\text{Para}}(\delta) - \omega_{ph}^{\text{AF}}(\delta = 0).$$

HF doping dependence much weaker than experiment.

LDA: Even weaker doping dependence.





LDA=$\frac{\omega_{LDA}(x)}{\omega_{exp}(x=0)}$.

LDA: Zhang, Louie, Cohen, PRL **98**, 067005

t-J: Rösch and Gunnarsson, PRL **92**, 146403; Rösch, thesis.

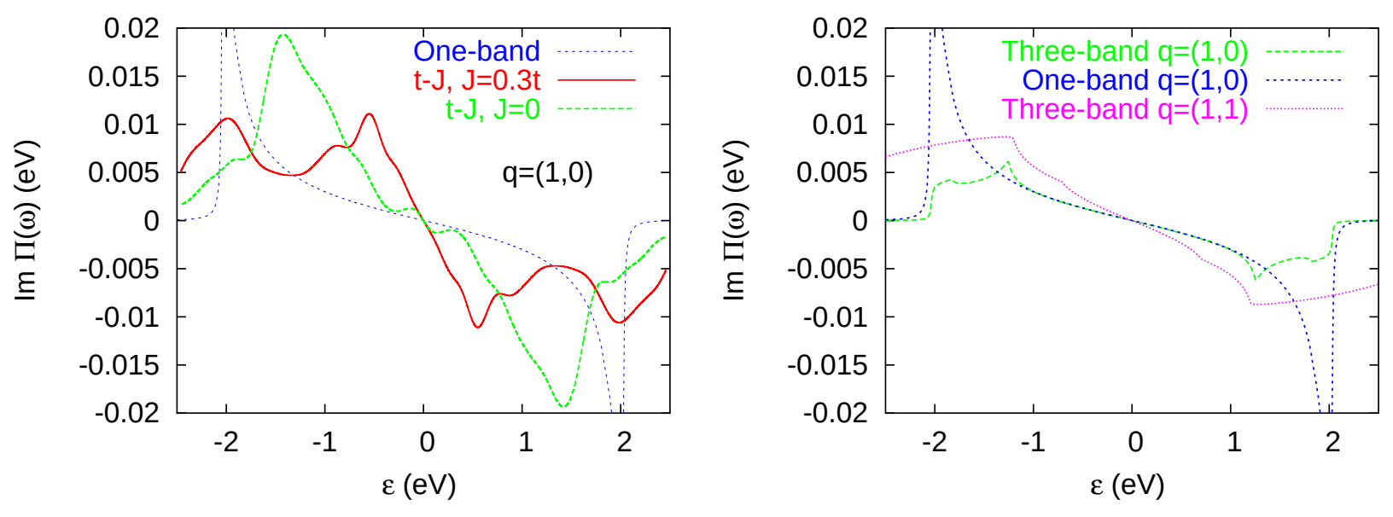
Exp. (right), Pintschovius phys. stat. sol (b) **242**, 30.

Many-body treatment: Reasonable doping dependence for both half- and full-breathing phonons.

:

Line width in HF solution

HF softening OK for $\delta \sim 0.10 - 0.15$, but width much smaller than exp.
Real and imaginary part of self-energy related. Contradiction?



t-J calculation for 4×4 cluster (details of Im Π not reliable).

- Linewidth (0.4 meV) smaller than in t-J model (3 meV) (many low-lying excitations in t-J model).
- Full-breathing mode softens more than half-breathing mode, contrary to exp.

O. Rösch and O. Gunnarsson, PRB **70**, 224518.

Summary

- LDA suggests very weak coupling to half-breathing phonon.
- Many-body treatment (t-J model) suggests much stronger coupling.
- Experimental evidence for substantial coupling.
- LDA fails to describe dispersion of half-breathing phonon.
- t-J model gives proper dispersion and much larger width.