Workshop ”Strong Correlations and ARPES”, Dresden

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Electron-phonon interaction in undoped cuprates and its effect on ARPES spectra

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- Property-dependent apparent electron-phonon coupling
- Polaronic behavior in undoped cuprates

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Advanced Materials IMPRS

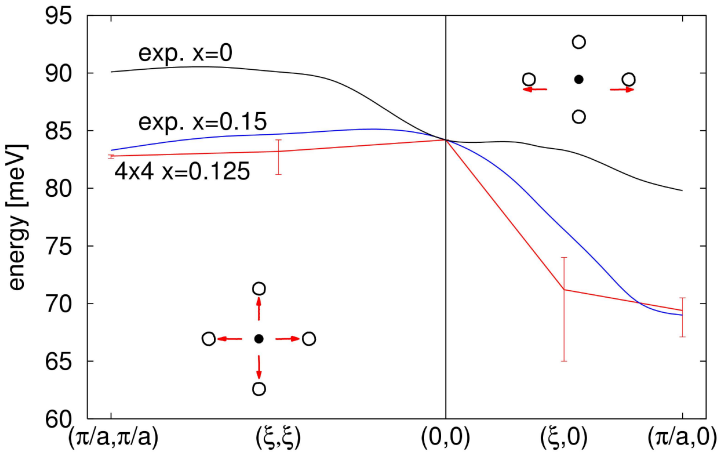
Electron-phonon coupling in high-T_c cuprates

- Phonon properties: anomalous softening of O half-breathing mode.

  Described by t-J model with electron-phonon interaction

  derived from three-band model.

  $\longrightarrow$ Rösch & Gunnarsson, PRL **92**, 146403 ('04); PRB **70**, 224518 ('04)



Phonon line width

$\Rightarrow \lambda \approx 0.2 - 0.3$

- Electronic properties: kink in ARPES dispersions at about 70 meV.

  Interaction with phonon mode? $\lambda \approx 1$

Apparent electron-phonon coupling

Electron-phonon coupling usually studied

for non-interacting electrons.

- $2\,\mathrm{Im}\,\Pi(\omega_{ph}) = 2\pi\omega_{ph}^2 \mathrm{N}(0)\lambda$ (phonon self-energy, weak coupl.)
- $\mathrm{Re}\,\Sigma(\omega) = -\lambda\omega$ if $|\omega| \ll \omega_{ph}$ (electron self-energy, weak coupl.)

With λ obtained from one experiment (e.g. phonon width),

another experiment (e.g. ARPES) can be predicted.

Similar relations are often implicitly assumed

for strongly correlated systems.

If this is not valid, different experiments may appear contradictory.

Sum rules: Phonon self-energy

Consider t-J model with on-site el-ph coupling.

Phonon self-energy: $\Pi(\mathbf{q},\omega) \approx (|g_{\mathbf{q}}|^2/N)\chi(\mathbf{q},\omega)$

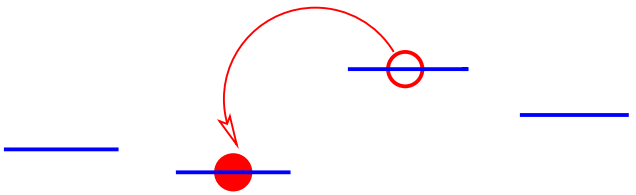
($\chi(\mathbf{q},\omega)$: charge response function)

Sum rule at doping δ (Khaliullin & Horsch, PRB **54**, R9600 (1996))

$$\frac{1}{\pi N}\sum_{\mathbf{q}\neq 0}\int_{-\infty}^{\infty} d\omega\, |\mathrm{Im}\,\chi(\mathbf{q},\omega)| = 2\delta(1-\delta)N \Rightarrow \Pi \to 0 \text{ as } \delta \to 0$$

System responds to phonons by transferring singlets to sites with lower singlet energies.

But there is only fraction δ singlets available.



Similar reduction of electron self-energy for low doping?

Sum rules: Electron self-energy

Σ_{ep}: Electron self-energy due to electron-phonon interaction

Sum rule for undoped system

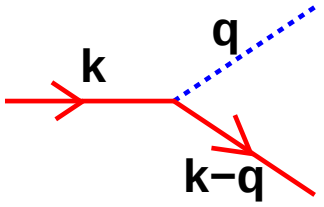
$$\frac{1}{\pi}\int_{-\infty}^{0} d\omega \, \mathrm{Im}\, \Sigma_{ep}(\mathbf{k}, \omega - i0^+) = \frac{1}{N}\sum_{\mathbf{q}} |g_{\mathbf{q}}|^2 \equiv \overline{g}^2$$

$\mathbf{k}$-indep. !

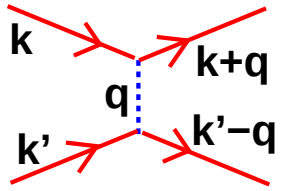
Identical to lowest-order result for non-interacting electrons.

In contrast to phonon self-energy no suppression by correlations.

Singlet created in PES easily scattered by phonons as other singlets block only fraction δ states.

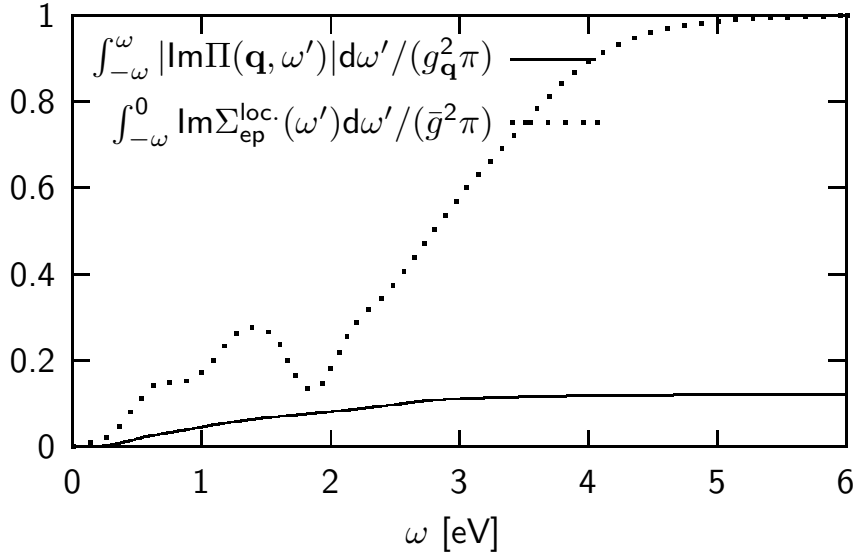


Similarly, phonon-induced singlet-singlet interaction should be effective for small δ because of few restrictions for scattering.



(O. Rösch, O. Gunnarsson, Phys. Rev. Lett. **93**, 237001 (2004))

Sum rules: Numerical example



$4 \times 3,\ \mathbf{q} = (\pi, 0)$

Π for $\delta = 1/12$

$\Sigma_{ep}^{loc.}$ for $\delta = 0$

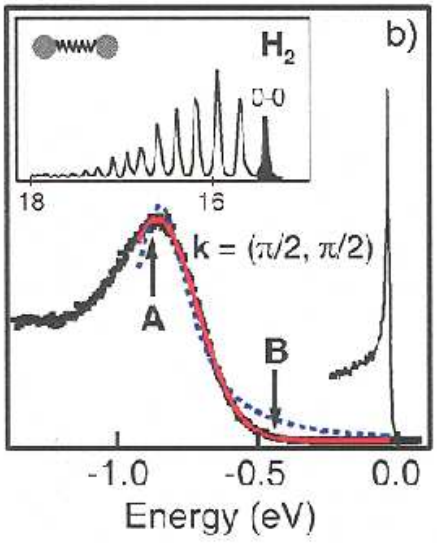
(Dimensionless) Im Σ_{ep} integrates to unity, Im Π integrates to $\approx 2\delta$.

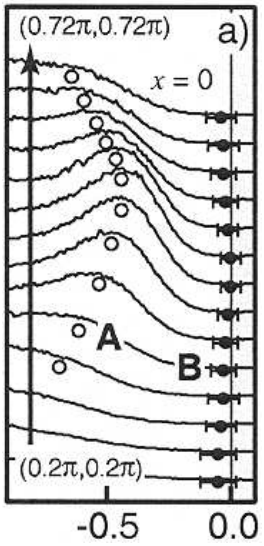
$$\lambda^{\Sigma} = -\left.\frac{d\mathrm{Re}\ \Sigma_{ep}(\omega)}{d\omega}\right|_{\omega=0} = \frac{1}{\pi}\int d\omega \frac{\mathrm{Im}\ \Sigma_{ep}(\omega)}{\omega^2} \approx 0.6$$

$$\lambda^{\Pi} = \frac{2\mathrm{Im}\ \Pi(\omega_{ph})}{2\pi\omega_{ph}^2 N(0)} = -\alpha\frac{\mathrm{Re}\ \Pi(\omega_{ph})}{\omega_{ph}} \approx 0.2$$

Fits with expectation from sum-rules: $\frac{\lambda^{\Sigma}}{\lambda^{\Pi}} = \frac{1}{c\delta}$ where $c \approx 2 - 4$.

Undoped cuprates: Polaronic behavior





undoped $CaCuO_2Cl_2$

(K.M. Shen *et al.*,

PRL **93**, 267002 (2004))

Gaussian line shape unlike quasi-particle (QP) peak.

Chemical potential pinned well above broad peak.

Polaronic behavior.

QP at $\varepsilon \approx 0$ with strongly suppressed weight & dispersion.

Broad side band develops.

Strong coupling to bosons. Phonons? Spin fluctuations?

La_2CuO_4: El.-ph. coupling from shell model

Use shell model to describe phonons. Calculate change of electrostatic potential due to phonon modes $\Rightarrow$ coupling to singlets.

Add coupling due to modulation of t_{pd} as for half-breathing mode.

$$H_{ep} = \frac{1}{\sqrt{N}} \sum_{\mathbf{q}\nu i} g_{\mathbf{q}\nu}(1 - n_i)\sqrt{2\omega_{\mathbf{q}\nu}} Q_{\mathbf{q}\nu} e^{i\mathbf{q}\mathbf{R_i}}$$

Dimensionless coupling $\lambda = 2 \sum_{\mathbf{q}\nu} \frac{|g_{\mathbf{q}\nu}|^2}{8t\omega_{\mathbf{q}\nu} N} = 1.2$

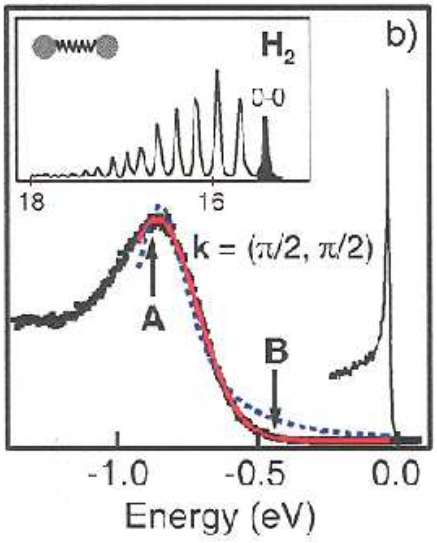
Holstein-t-J model: Polaronic behavior for $\lambda > 0.4$

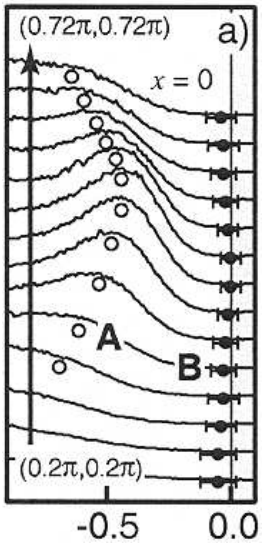
(e.g., Mishchenko & Nagaosa, PRL **93**, 036402 (2004)).

Phonons sufficient to put undoped cuprates well onto polaronic side.

Strong correlations important ($\lambda > 1.2$ needed for Holstein model).

Undoped cuprates: Polaronic behavior





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Gaussian line shape unlike quasi-particle (QP) peak.

Chemical potential pinned well above broad peak.

Polaronic behavior.

QP at $\varepsilon \approx 0$ with strongly suppressed weight & dispersion.

Broad *phonon* side band disperses like QP in t-J model *without* phonons.

(Mishchenko & Nagaosa, PRL **93**, 036402 (2004))

Adiabatic approximation

Ground state: $\langle Q|E_0\rangle \approx \phi_0(Q)|\Phi_0(Q)\rangle$.

$$g(\mathbf{k},z) = \langle E_0|c^\dagger_{\mathbf{k}}\tfrac{1}{z-H}c_{\mathbf{k}}|E_0\rangle$$
$$= \int dQdQ'\langle E_0|Q\rangle\langle Q|c^\dagger_{\mathbf{k}}\tfrac{1}{z-H}c_{\mathbf{k}}|Q'\rangle\langle Q'|E_0\rangle$$

$$H = H_{el} + H_{ep}(Q) + \tfrac{1}{2}\kappa Q^2 + \tfrac{1}{2M}\hat{P}^2 \equiv \mathcal{H}(Q) + \tfrac{1}{2M}\hat{P}^2.$$

Neglect $\frac{1}{2M}\hat{P}^2$. Then there is only a contribution for $Q = Q'$.

$$g(\mathbf{k},z) \approx \int dQ\, |\phi_0(Q)|^2 G(\mathbf{k},z,Q)$$

$$G(\mathbf{k},z,Q) = \langle \Phi_0(Q)|c^\dagger_{\mathbf{k}}\tfrac{1}{z-\mathcal{H}(Q)}c_{\mathbf{k}}|\Phi_0(Q)\rangle$$

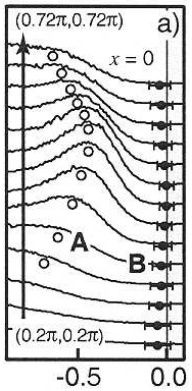
$G(\mathbf{k},z,Q)$ purely electronic, weighted by $|\phi_0(Q)|^2$.

Undoped system: No el.-ph. coupling in *initial* state.

$|\phi_0(Q)|^2$ has Gaussian bell shape centered on $Q = 0$.

$\Rightarrow$ Spectrum *without* el-ph. coupling [$G(\mathbf{k},z,Q=0)$]

but broadened due to contributions from $Q \neq 0$.



(O. Rösch, O. Gunnnarsson, Eur. Phys. J. B **43**, 11 (2005))

Method for calculating spectra for undoped systems

Adiabatic approximation: $g(\mathbf{k}, z) \approx \int dQ \, |\phi_0(Q)|^2 G(\mathbf{k}, z, Q)$

For undoped system $|\phi_0(Q)|^2 \sim e^{-\omega_{ph} Q^2}$ is known.

Use as weight for Monte-Carlo sampling over Q.

For each Q only $G(\mathbf{k}, z, Q)$ for distorted lattice

without (dynamical) electron-phonon coupling is needed.

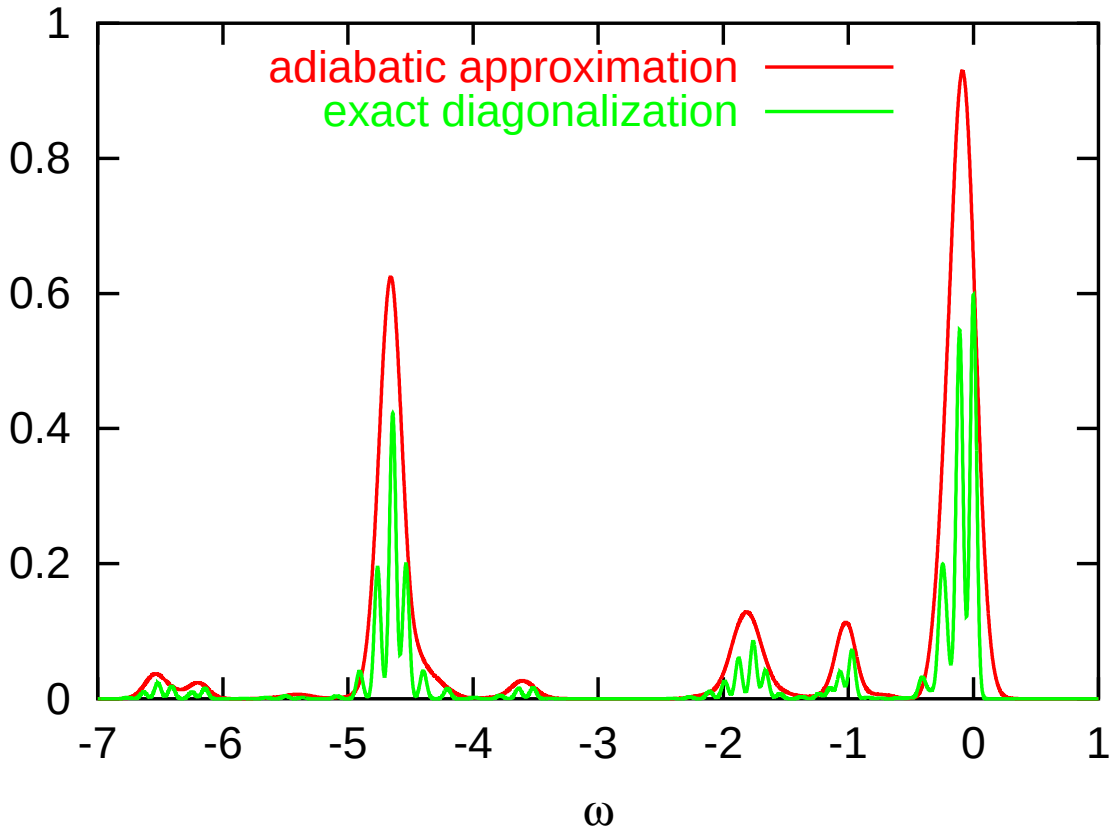
No blow-up of Hilbert space even for strong coupling.

Easy to add temperature dependence: $e^{-\omega_{ph} Q^2} \longrightarrow e^{\frac{-\omega_{ph} Q^2}{2n(T)+1}}$.

Adiabatic approximation: Example

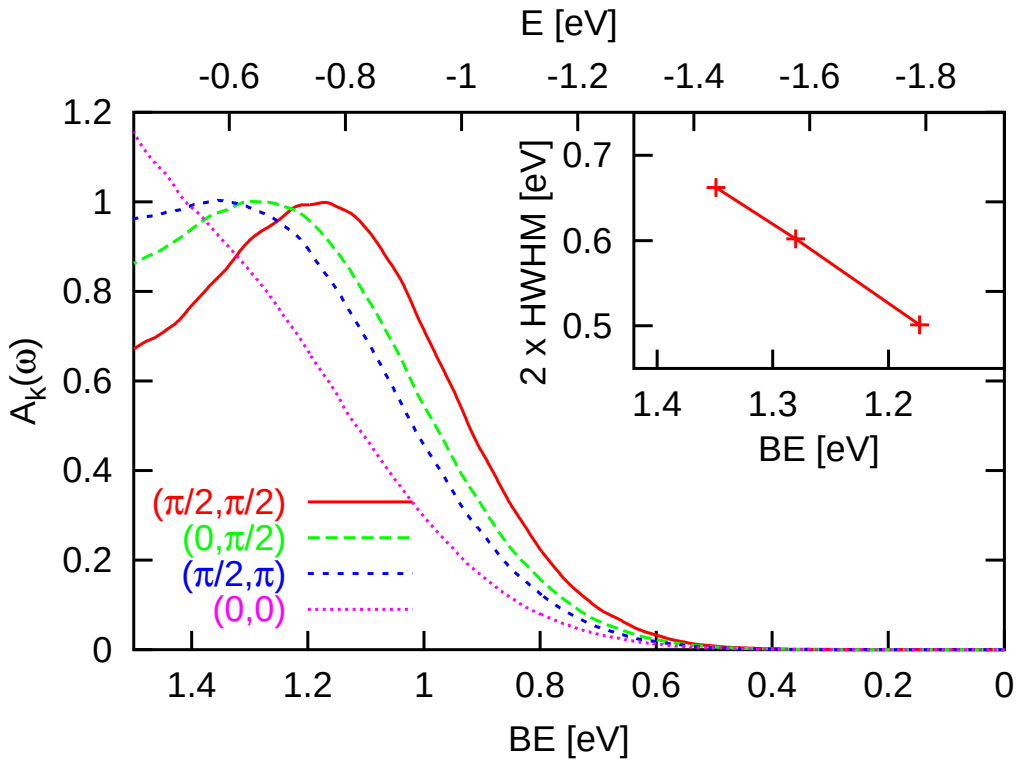
ARPES ($\mathbf{k} = (3,1)\frac{\pi}{5}$) from undoped 10-site Holstein-t-J model

($t = 1,\ J = 0.4,\ \omega_{ph} = 0.1,\ g = \sqrt{0.05}$)



Width of phonon side band

La_2CuO_4. 4×4 t-J cluster with 21 phonon modes & $\mathbf{q}$-dependent couplings.



Width $\geq$ 500 meV. Increases with binding energy.

In good agreement with experimental findings

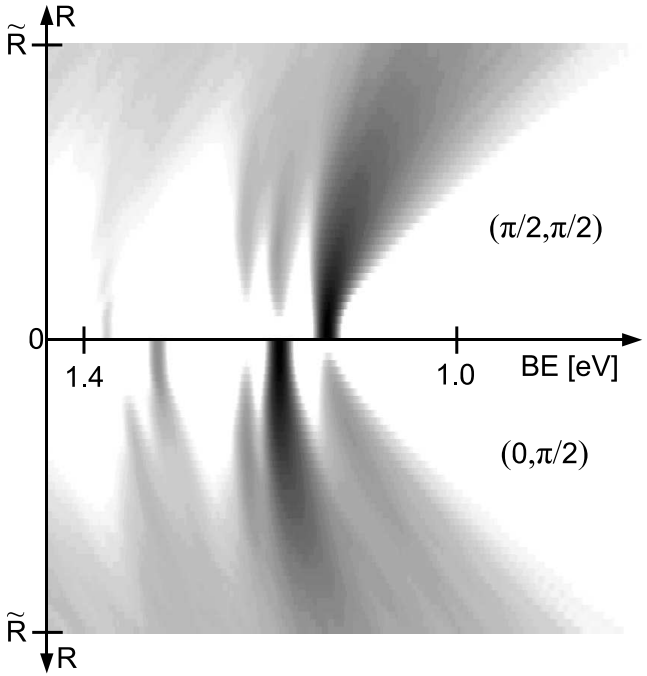
for La_2CuO_4 (480 meV at $(\pi/2, \pi/2)$).

Increase of width with binding energy

rescale: $R_{\mathbf{q}\nu}=\sqrt{\omega_{\mathbf{q}\nu}/(2n_{\mathbf{q}\nu}(T)+1)}\;Q_{\mathbf{q}\nu}$

$\Rightarrow A_{\mathbf{k}}(\omega) \propto \int dR\; R^{d-1}e^{-R^2} \times \int d\Omega\; \mathrm{Im}\; G(\mathbf{k},\omega+i0^+,\mathbf{Q}(\mathbf{R}))$:

sample directions for fixed $R=|\mathbf{R}|$ followed by integration over R



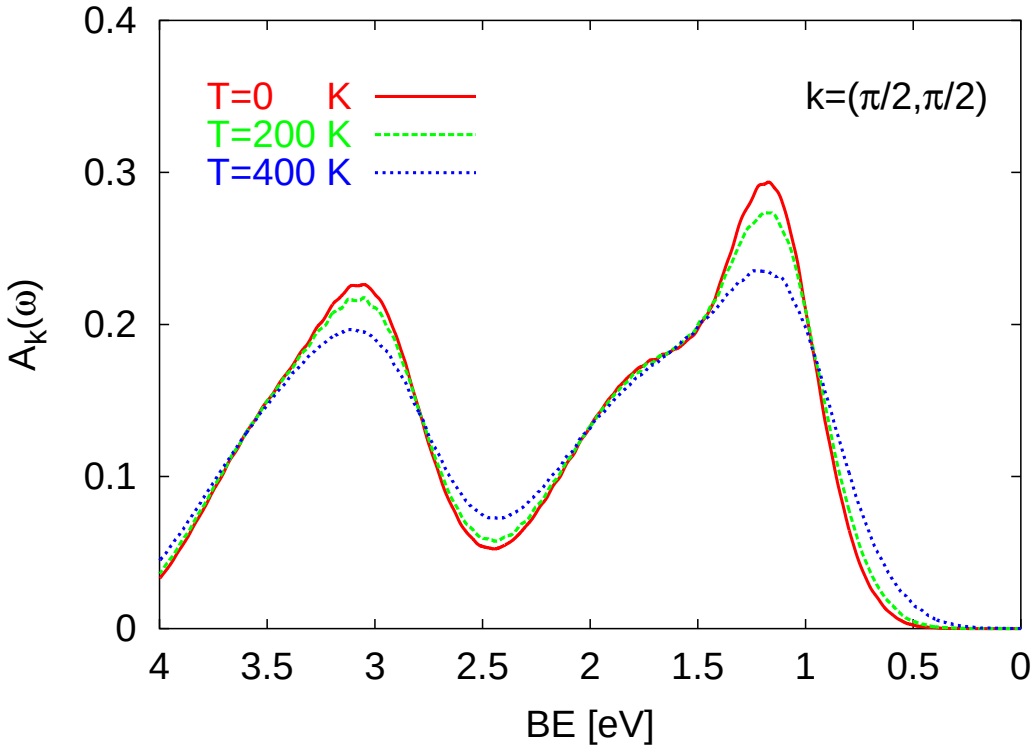
($\mathbf{q}=(0,0)$)-coupling not included

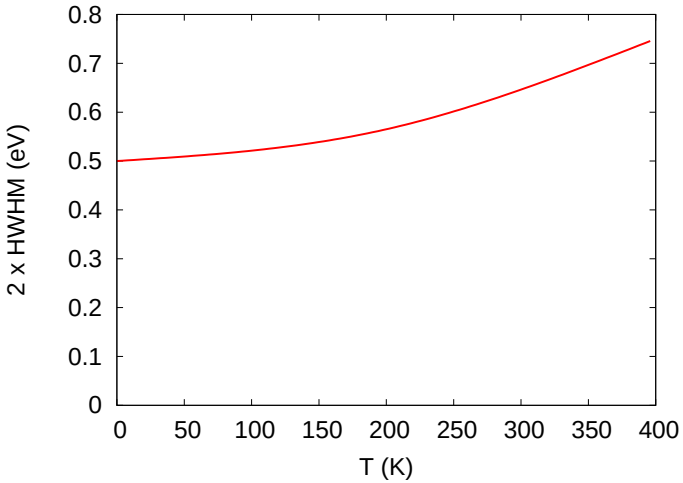
$R^{d-1}e^{-R^2}$ peaks strongly around $\tilde{R}=\sqrt{(d-1)/2}$.

$R/\tilde{R} \approx$ relative coupling strength

Extra contributions due to non-conservation of electronic momentum for $R\neq 0$ depend on binding energy.

Temperature dependence of width





Moderate T dependence.

Mainly due to 20 meV modes.

La_2CuO_4. 4×4 t-J cluster with 21 phonon modes & $\mathbf{q}$-dependent couplings.

Summary

- Apparent electron-phonon coupling in strongly correlated materials depends on property studied.

- Electron-phonon interaction in undoped cuprates results in polaronic behavior.

- Adiabatic approximation explains why phonon side band in undoped system follows quasi-particle dispersion of purely electronic model.

- Model gives correct width of side band which increases with binding energy and shows moderate temperature dependence.

Sum-rule for Σ_{ep}: Derivation

$$G(\mathbf{k},z) = \frac{a_{\mathbf{k}}}{z-\varepsilon_{\mathbf{k}}-\Sigma(\mathbf{k},z)}. \qquad A(\mathbf{k},\omega) = \mathrm{Im}\ \mathrm{G}(\mathbf{k},\omega - \mathrm{i}0^+)/\pi.$$

$$\Sigma(\mathbf{k},z) \overset{|z|\to\infty}{\longrightarrow} \frac{b_{\mathbf{k}}}{z}. \qquad b_{\mathbf{k}} = \int d\omega\ \mathrm{Im}\ \Sigma(\mathbf{k},\omega - \mathrm{i}0^+)/\pi.$$

$$G(\mathbf{k},z) = \frac{a_{\mathbf{k}}}{z}\left(1 + \frac{\varepsilon_{\mathbf{k}}}{z} + \frac{\varepsilon_{\mathbf{k}}^2+b_{\mathbf{k}}}{z^2} + \ldots\right)$$

$$= \frac{a_{\mathbf{k}}}{z}\left(1 + \frac{\langle\omega\rangle_{\mathbf{k}}}{z} + \frac{\langle\omega^2\rangle_{\mathbf{k}}}{z^2} + \ldots\right).$$

$$\langle\omega^n\rangle_{\mathbf{k}} = \frac{\int d\omega\ \omega^n A(\mathbf{k},\omega)}{\int d\omega\ A(\mathbf{k},\omega)} \qquad \text{here}: \int d\omega\ \omega^n A(\mathbf{k},\omega) = \langle 0|c_{\mathbf{k}}^\dagger H^n c_{\mathbf{k}}|0\rangle$$

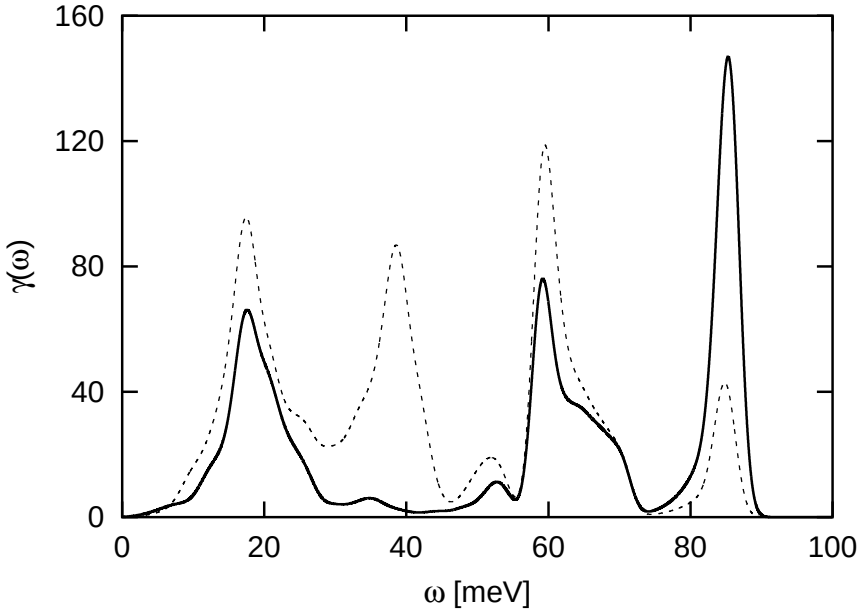
Observed kink strength $\frac{1+\lambda_{el}+\lambda_\Sigma}{1+\lambda_{el}} = 1 + \frac{\lambda_\Sigma}{1+\lambda_{el}} < 1 + \lambda_\Sigma$

can underestimate coupling from phonon.

La_2CuO_4: El.-ph. coupling from shell model

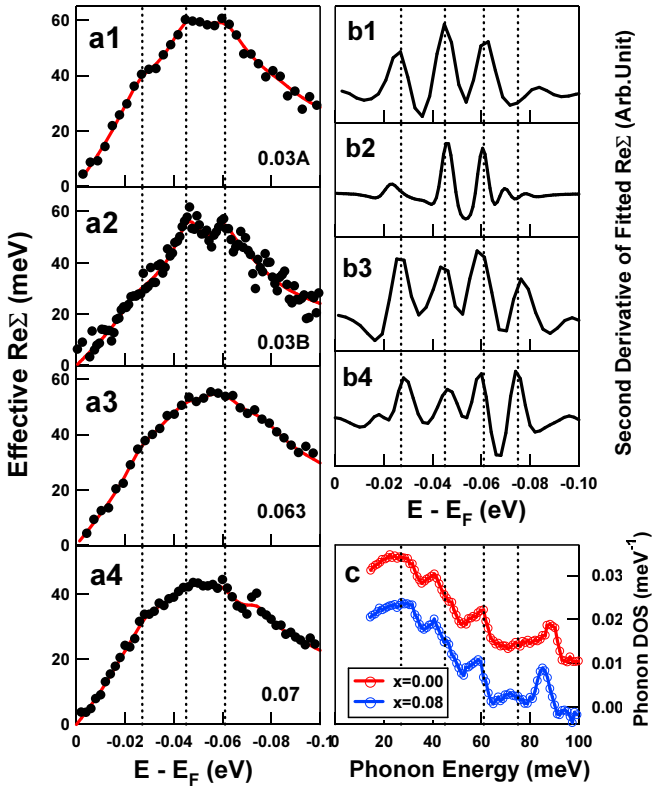
Spectral distribution of coupling:

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



dashed line for coupling to holes

in non-bonding O p orbitals

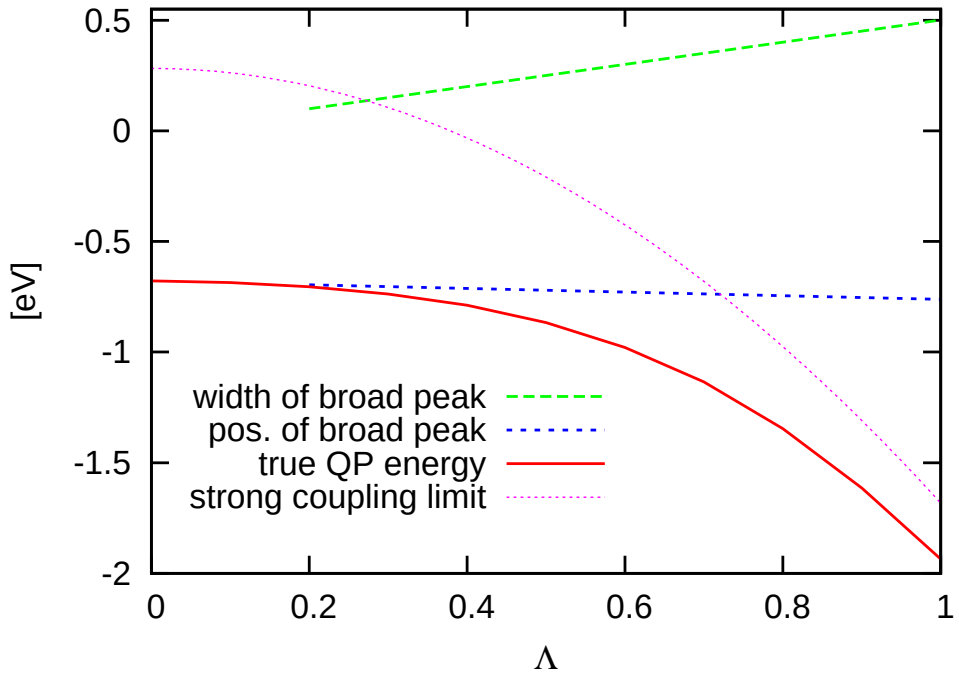


X. J. Zhou *et. al.*,

cond-mat/0405130.

Dependence on coupling strength

$$g_{\mathbf{q}\nu} \longrightarrow \Lambda g_{\mathbf{q}\nu}$$



Binding energy

(1.17 eV f. $\Lambda = 1$)

approx. $\sim \Lambda^2$,

width

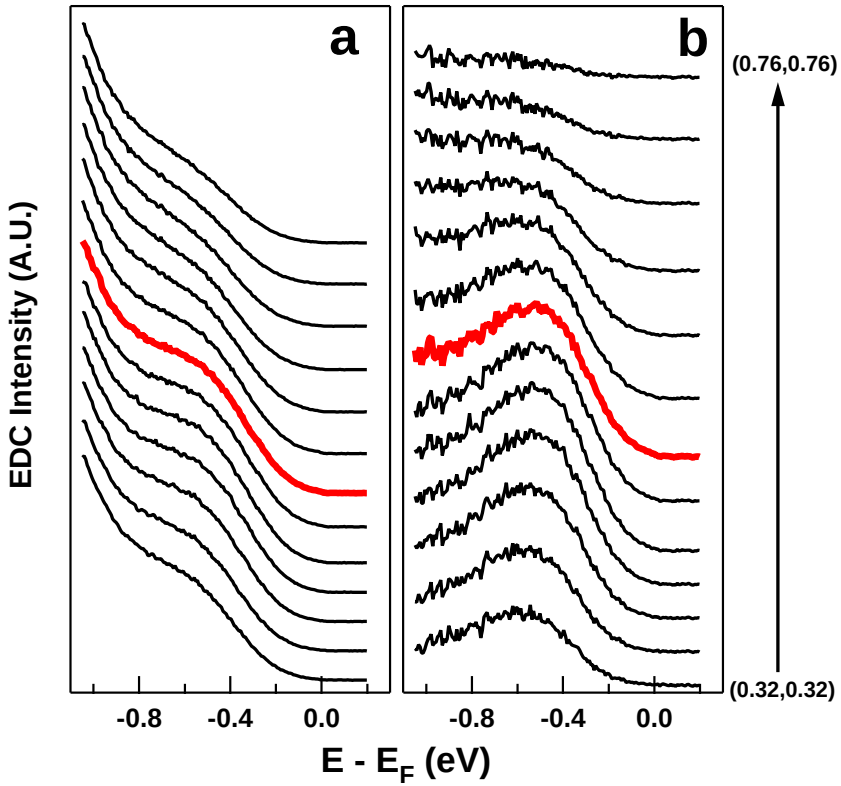
(0.50 eV f. $\Lambda = 1$)

approx. $\sim \Lambda$.

La_2CuO_4. 4×4 t-J cluster with 21 phonon modes & $\mathbf{q}$-dependent couplings,

$$\mathbf{k} = (\pi/2, \pi/2).$$

La_2CuO_4: Experimental spectra



Photoemission spectra along nodal direction in 1^{st} BZ,

for (b) 'background' spectrum near (π, π) was subtracted.

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