Electron-phonon coupling in cuprates

Olle Gunnarsson

- Property-dependent apparent electron-phonon coupling.
- Vertex corrections.
- Undoped cuprates: Polaronic behavior.

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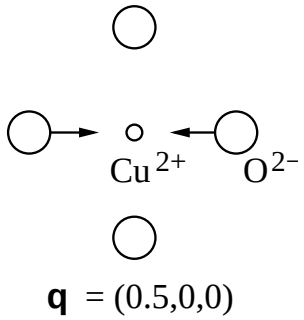
Important effects of electron-phonon coupling

- Kink in nodal direction of photoemission spectrum.

(Lanzara *et al.*, Nature **412**, 510 (2001)).

- Anomalous softening, broadening of half-breathing phonon.

(Pintschovius phys. stat. sol. **242**, 30 (2005)).



Interplay with Coulomb interaction important

- LDA underestimates width of half-breathing phonon by one order of magnitude.

(Bohnen, Heid and Krauss, Europhys. Lett. **64**, 104 (2003)).

Here use t-J model or Hubbard model.

t-J model

t-J model with phonons can be derived from the three-band model.

- Electron-phonon coupling mainly due to modulation of t_{pd}.

- One-site term order of magnitude larger than off-site term (neglected).

(Rösch and Gunnarsson, PRL **92**, 146403 (2004)).

Apparent el-ph coupling

Electron-phonon coupling usually studied for non-interacting electrons.

- $\Sigma_{ep}(\omega) = \begin{cases} -\lambda\omega, & \text{if } |\omega| \ll \omega_{ph}; \\ 0, & \text{if } |\omega| \gg \omega_{ph} \end{cases}$ (electron self-energy, weak coupl.)
- 2 Im $\Pi(\omega_{ph}) = 2\pi\omega_{ph}^2 N(0)\lambda$ (phonon self-energy, weak coupl.)

If λ determined from one experiment (e.g., phonon width), another experiment (e.g., PES) can be predicted.

Similar relations are often implicitly assumed for strongly correlated systems.

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

Sum rule. Phonon self-energy. t-J model

$$\Pi(\mathbf{q},\omega) = \frac{(g_{\mathbf{q}}^2/N)\chi(\mathbf{q},\omega)}{1+(g_{\mathbf{q}}^2/N)\chi(\mathbf{q},\omega)D_0(\mathbf{q},\omega)}.$$

Π phonon self-energy, χ charge response function,

D_0 noninteracting phonon Green's function.

Sum-rule: (δ doping).

$\frac{1}{\pi N}\sum_{\mathbf{q}\neq 0}\int_{-\infty}^{\infty}|\mathrm{Im}\chi(\mathbf{q},\omega)|d\omega = 2\delta(1-\delta)N \sim \delta N$. (Khaliullin and Horsch)

As $\delta \to 0, \chi \to 0$

$$\frac{1}{\pi N}\sum_{\mathbf{q}\neq 0}\frac{1}{g_{\mathbf{q}}^2}\int_{-\infty}^{\infty}|\mathrm{Im}\Pi(\mathbf{q},\omega)|d\omega \approx 2\delta(1-\delta)\sim \delta.$$

As $\delta \to 0, \Pi \to 0.$

Natural: For zero doping all states filled. No response possible.

Is the electron self-energy reduced in a similar way?

Sum rule. Electron self-energy

Define Green's function

$G(\mathbf{k},z)=\frac{a(\mathbf{k})}{z-\varepsilon(\mathbf{k})-\Sigma(\mathbf{k},z)};\qquad \Sigma(\mathbf{k},z)\,_{|z|\to\infty}\overrightarrow{}\frac{b(\mathbf{k})}{z}.$

$\langle\omega^n\rangle_{\mathbf{k}}=\int_{-\infty}^{\infty}\omega^n A(\mathbf{k},\omega)d\omega/a(\mathbf{k})\qquad A(\mathbf{k},\omega)=\frac{1}{\pi}\mathrm{Im}G(\mathbf{k},\omega-i0^+).$

$\frac{1}{\pi}\int_{-\infty}^{\infty}\mathrm{Im}\Sigma(\mathbf{k},\omega-i0^+)d\omega=b(\mathbf{k})=\langle\omega^2\rangle_{\mathbf{k}}-(\langle\omega\rangle_{\mathbf{k}})^2.$

Undoped t-J model with on-site coupling

($\Sigma_{ep}=\Sigma-\Sigma(g=0)$):

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

Identical to the lowest order result for noninteracting electrons (but valid for any $\bar{g}$).

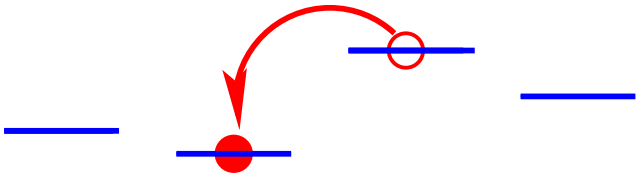
$\mathbf{k}$-independent! Nontrivial. Not valid for off-site coupling.

In contrast to phonon self-energy, correlation does not suppress Σ_{ep}.

O. Rösch and O. Gunnarsson, PRL **93**, 237001 (2004).

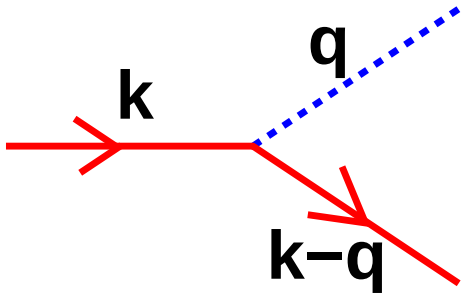
Phonon self-energy:

System responds to phonons by transferring singlets to sites with lower singlet energies. But there are only fraction δ singlets available.



Electron self-energy

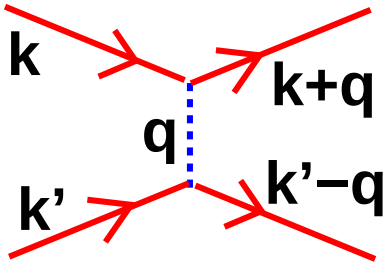
Singlet created in PES. Is easily scattered by phonons to other states as only fraction δ blocked by other singlets.



Strong asymmetry between carriers and phonons.

Phonon induced carrier-carrier interaction:

One singlet emits a phonon, which is absorbed by another singlet. Both scattering processes allowed in limit $\delta \longrightarrow 0$. No suppression of carrier-carrier interaction.



Strong interaction without soft phonons possible.

O. Rösch and O. Gunnarsson, PRL **93**, 237001 (2004).

Relation between Hubbard and t-J models

Consider large U limit, half-filling and symmetric parameters.

$$A_{\rm H}(\mathbf{k},\omega) = A_{t\text{-}J}(\mathbf{k},\omega+\tfrac{U}{2}) + A_{t\text{-}J}(-\mathbf{k},\tfrac{U}{2}-\omega).$$

Define self-energies

$$G_{\rm H}(\mathbf{k},z) = \int d\omega \frac{A_{\rm H}(\mathbf{k},\omega)}{z-\omega} \equiv \frac{1}{z-\Sigma_{\rm H}(\mathbf{k},z)}.$$

$$G_{t-J}(\mathbf{k},z) = \int d\omega \frac{A_{t-J}(\mathbf{k},\omega)}{z-\omega} \equiv \frac{0.5}{z-\Sigma_{t-J}(\mathbf{k},z)}.$$

This requires

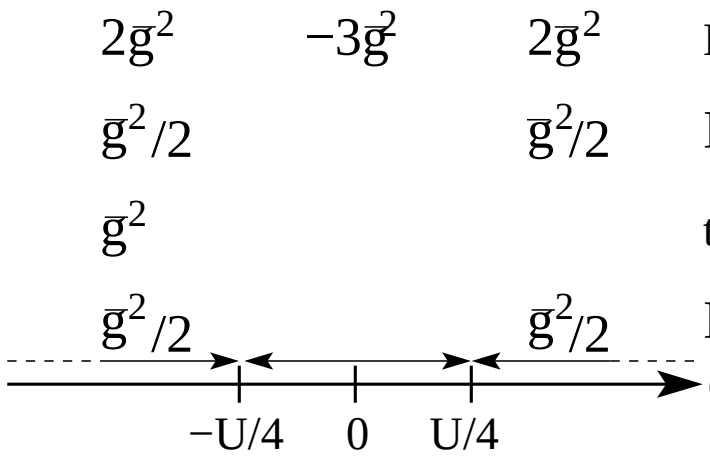
$$\Sigma_{\rm H}(\mathbf{k},z) \approx 2\Sigma_{t\text{-}J}(\mathbf{k},z+\tfrac{U}{2}) + \frac{U^2}{4z}.$$

Then Im $\Sigma_{\rm H}(\mathbf{k},z) = 2{\rm Im}\Sigma_{t\text{-}J}(\mathbf{k},z+\frac{U}{2})$, which gives the sum rule

$$\tfrac{1}{\pi}\int_{-\infty}^{-U/4} {\rm Im}\Sigma^{\rm ep}_{\rm H}(\mathbf{k},\omega-i0^+)d\omega = 2\bar{g}^2.$$

Integration only over the photoemission part. Twice the value for the t-J model.

Sum rules. Hubbard model. El.-ph. part of electron self-energy



Sum rule for Im Σ over photoem. and inverse photoem. parts, each $2\bar{g}^2$.

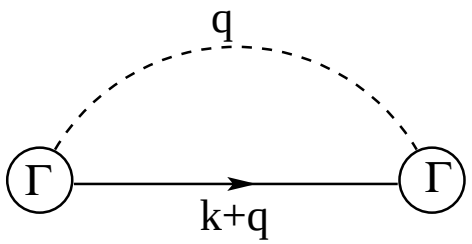
Total sum rule just $\bar{g}^2$.

Im $\Sigma(\mathbf{k}, \omega)$ has large positive contribution $U^2/4$ at $\omega = 0$.

The electron-phonon interaction slightly reduces this by $-3\bar{g}^2$.

Calculate lowest order diagram in electron-phonon interaction, neglecting vertex corrections ($\Gamma = 1$).

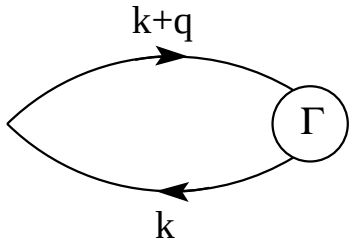
Sum rule over photoemission spect. violated by factor 4.



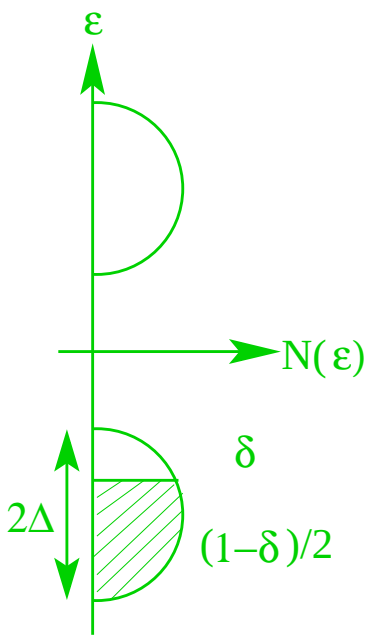
Vertex corrections important for electron-phonon part of electron self-energy.

Vertex corrections phonon self-energy. Large U

In limit of weak electron-phonon coupling, phonon self-energy given by density-density correlation function. Neglect vertex corrections ($\Gamma = 1$).



Assume that doping δ results in a weight $\sim \delta$ on the inverse photoemission side close to Fermi energy. Assume that this weight and photoemission spectrum within energy range 2Δ.



Exact sum rule fulfilled

$\frac{1}{\pi N^2} \sum_{\mathbf{q}} \int_{-2\Delta}^{2\Delta} |\mathrm{Im}\chi_{\mathrm{H,No\ vert.}}(\mathbf{q},\omega)| d\omega = 2\delta(1-\delta)$

Sufficient to use dressed electron Green's functions.

Neglect of vertex corrections violates sum rule for electron-phonon contribution to electron but not phonon self-energy.

q-dependence

$\frac{1}{\pi N^2}\sum_{\mathbf{q}\neq\mathbf{0}}\int_{-2\Delta}^{2\Delta}|\mathrm{Im}\chi_{\mathrm{H}}(\mathbf{q},\omega)|d\omega = 2\delta(1-\delta).$

$\frac{1}{\pi}\int_{-2\Delta}^{2\Delta}|\mathrm{Im}\chi_{\mathrm{H,No\ vert.}}(\mathbf{q},\omega)|d\omega = 2\sum_{\mathbf{k}}[w_{\mathrm{P}}(\mathbf{k})w_{\mathrm{IP}}(\mathbf{k+q})+w_{\mathrm{P}}(\mathbf{k+q})w_{\mathrm{IP}}(\mathbf{k})]$

$\frac{1}{\pi N^2}\sum_{\mathbf{q}}\int_{-2\Delta}^{2\Delta}|\mathrm{Im}\chi_{\mathrm{H,No\ vert.}}(\mathbf{q},\omega)|d\omega = 2\delta(1-\delta).$

Calculate $w_{\mathrm{P}}(\mathbf{k})$ and $w_{\mathrm{IP}}(\mathbf{k})$ for $\sqrt{18}\times\sqrt{18}$ t-J model with two holes.

$\frac{1}{\pi N}\int_{-2\Delta}^{2\Delta}|\mathrm{Im}\chi_{\mathrm{H}}(\mathbf{q},\omega)|d\omega$

$\mathbf{q}/\frac{\pi}{3}$	$(0,0)$	$(1,1)$	$(2,0)$	$(2,2)$	$(3,1)$	$(3,3)$
No vert.	0.1660	0.1848	0.1927	0.2103	0.2025	0.2285
Exact	28.44	0.2100	0.1961	0.2191	0.2085	0.2212
Ratio		0.8804	0.9825	0.9597	0.9714	1.0330

Even $\mathbf{q}$-dependence rather well described.

Two-site model

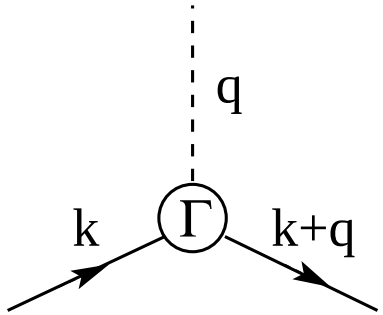
Consider a two-site model:

$$H = t(n_+ - n_-) + U\sum_{i=1}^{2} n_{i\uparrow}n_{i\downarrow} + \omega_{ph}b^\dagger b + g(c_+^\dagger c_- + c_-^\dagger c_+)(b + b^\dagger).$$

Huang, Hanke, Arrigoni, Scalapino (PRB **68**, 220507 (2003)):

$$\Gamma(k,q) = \frac{G_2(k,q)}{G(k+q)G(k)}.$$

$$G_2(k,q) = \int_0^\beta d\tau e^{i(\omega_n+\omega_m)} \int_0^\beta d\tau' e^{-i\omega_m\tau'}$$
$$\times \sum_{pq\sigma'} \langle T_\tau c^\dagger_{p+q\sigma'}(\tau') c_{p\sigma'} c_{k+q\sigma}(\tau) c^\dagger_{p\sigma}(0)\rangle.$$



$$\Gamma(\omega', +, \omega, -) = \frac{\omega'(\omega+\omega')+\omega t+(U/2)^2}{(\omega'+t)(\omega+\omega'-t)}.$$ (ω'=electron; ω=phonon).

$$\omega' \approx \pm\frac{U}{2} \Rightarrow \Gamma(\omega', +, \omega, -) = 2.$$

Fixes up electron self-energy sum rule in photoemission and inverse photoemission ranges.

Small q and ω

Huang, Hanke, Arrigoni, Scalapino (PRB **68**, 220507 (2003)):

Koch, Zeyher (PRB **70**, 094510 (2004)):

$\sqrt{Z(p)Z(p+q)}\Gamma(p,q)$ reduced in static case (phonon frequency zero).

Fermi liquid arguments (Grilli, Castellani PRB **50**, 16880 (1994)):

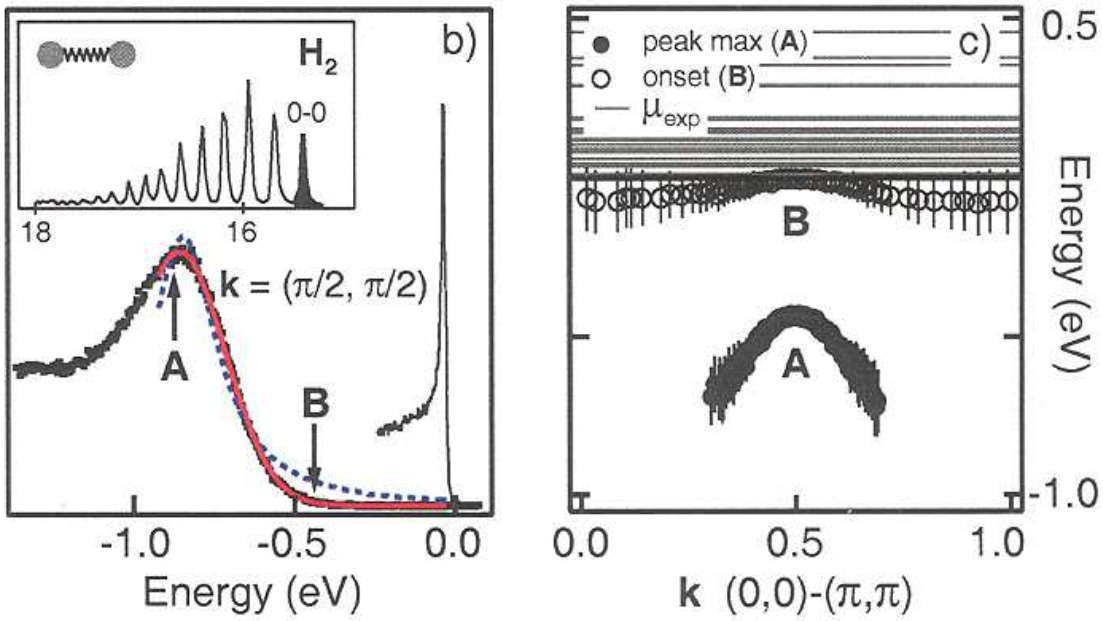
Small $|\mathbf{q}|$ and ω:

$\sqrt{Z(p)Z(p+q)}\Gamma(p,q)$ reduced for $\omega = 0$ but not for $|\mathbf{q}| = 0$.

Here integration over all $\mathbf{q}$ and ω and study of $\Gamma(p,q)$.

Vertex corr. give enhancement of electron but not phonon self-energy sum rule.

Polaronic behavior



Undoped $CaCuO_2Cl_2$.

K.M. Shen *et al.*, PRL **93**, 267002 (2004).

Spectrum *very* broad, even at top of band (insulator!).

Shape Gaussian, not like a quasi-particle.

Chemical potential always well above broad peak A, although expected to be anywhere in the gap depending on sample preparation.

Polaronic behavior. Broad boson side band.

Quasi-particle (≈ 0 weight, small dispersion) at $\varepsilon \approx 0$.

Strong coupling to bosons. Phonons, spin fluctuations?

Electron-phonon coupling. Undoped system. Shell model

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

Zhang-Rice singlet is an additional hole in a linear combination of four O holes.

Use a shell model to describe phonons.

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

Screening by the ”shells”, but otherwise no screening.

Add coupling due to modulation of t_{pd} and $\varepsilon_d - \varepsilon_p$ as in the treatment of the half-breathing mode.

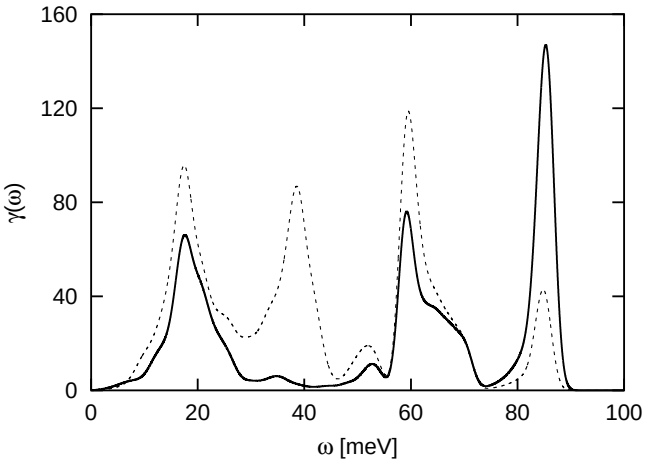
Electron-phonon coupling strength. La_2CuO_4

$$H_{ep} = \frac{1}{\sqrt{N}} \sum_{\mathbf{q}\nu i} M_{\mathbf{q}\nu i}(1-n_i)(b_{\mathbf{q}\nu} + b^{\dagger}_{-\mathbf{q}\nu})$$

Dimensionless coupling $\lambda = 2\frac{1}{8t}\sum_{\mathbf{q}\nu} \frac{|M_{\mathbf{q}\nu}|^2}{\omega_{\mathbf{q}\nu}}$.

We find $\lambda = 1.2$.

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

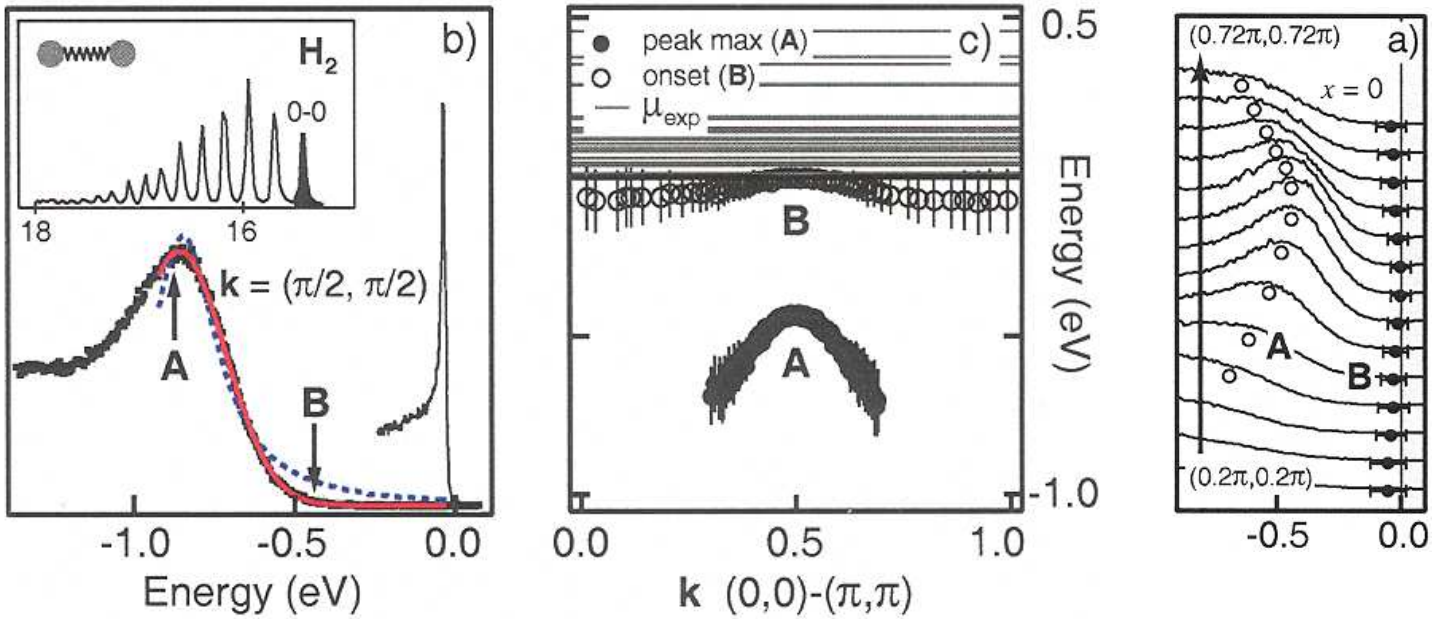


t-J Holstein model: Polarons for $\lambda > 0.4$. Mishchenko and Nagaosa

Phonons sufficient to put undoped cuprates well onto the polaronic side.

Boson side-band. Dispersion

Undoped $CaCuO_2Cl_2$. K.M. Shen *et al.*, PRL **93**, 267002 (2004).



Boson side-band disperses as quasi-particle peak in t-J model without bosons. But quasi-particle now at smaller binding energy. Small dispersion.

Numerical calculation for t-J model with phonons: Phonon side-band follows quasi-particle peak in t-J model without phonons.

(A. S. Mishchenko and N. Nagaosa Phys. Rev. Lett. 93, 036402 (2004))

Adiabatic approximation

$$g(\mathbf{k},z) = \langle E_0|c_{\mathbf{k}}^{\dagger}\frac{1}{z-H+E_0}c_{\mathbf{k}}|E_0\rangle$$

$$= \int dQdQ^{'}\langle E_0|Q\rangle\langle Q|c_{\mathbf{k}}^{\dagger}\frac{1}{z-H+E_0}c_{\mathbf{k}}|Q^{'}\rangle\langle Q^{'}|E_0\rangle$$

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

I. Neglect $\frac{1}{2M}\hat{P}^2$. Phonon satellites smeared out.

$$g(\mathbf{k},z) = \int dQdQ^{'}\langle E_0|Q\rangle\langle Q|c_{\mathbf{k}}^{\dagger}\frac{1}{z-\mathcal{H}(Q)+E_0}c_{\mathbf{k}}|Q^{'}\rangle\langle Q^{'}|E_0\rangle$$

Then there is only a contribution for $Q = Q^{'}$.

$$g(\mathbf{k},z) = \int dQ\langle E_0|Q\rangle\langle Q|c_{\mathbf{k}}^{\dagger}\frac{1}{z-\mathcal{H}(Q)+E_0}c_{\mathbf{k}}|Q\rangle\langle Q|E_0\rangle$$

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

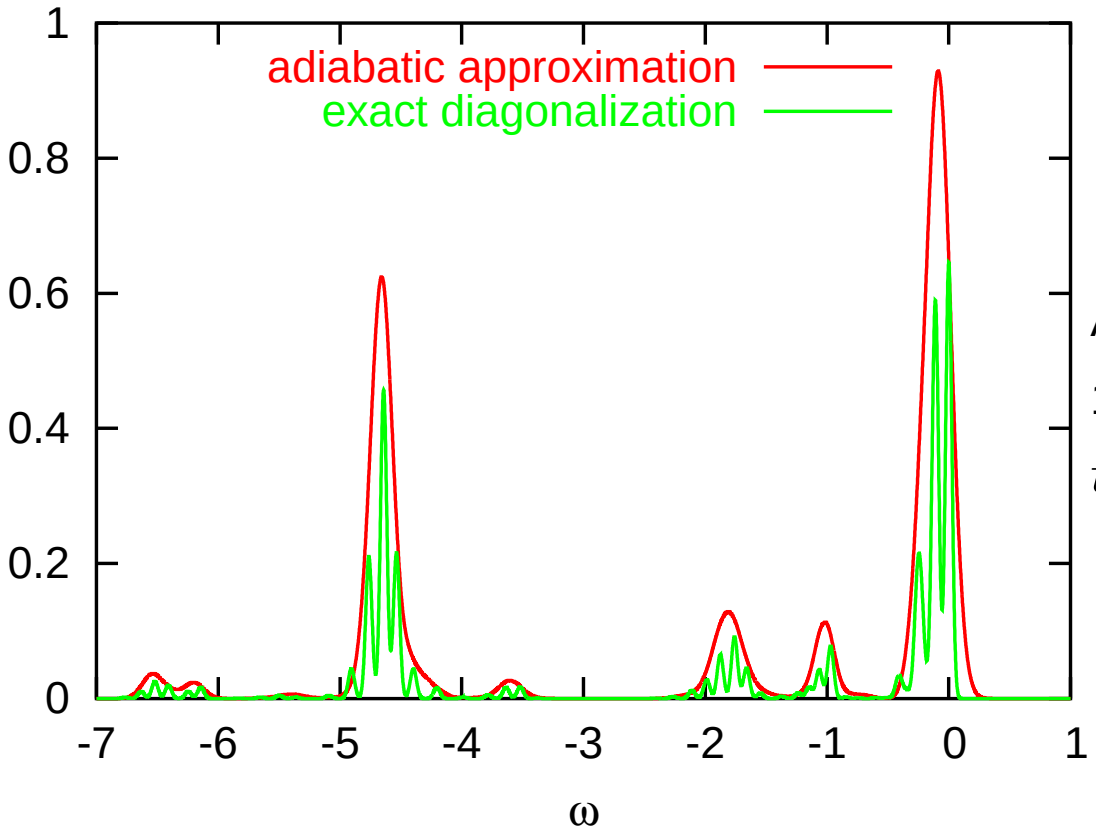
$$g(\mathbf{k},z) \approx \int dQ\phi_0^2(Q)G(\mathbf{k},z,Q).$$

$$G(\mathbf{k},z,Q) = \langle\Phi_0(Q)|c_{\mathbf{k}}^{\dagger}\frac{1}{z-\mathcal{H}(Q)+E_0}c_{\mathbf{k}}|\Phi_0(Q)\rangle.$$

$G(\mathbf{k},z,Q)$ calculated *without* (dynamic) electron-phonon coupling but for distorted lattice (Q treated as c-number). Weighted by $\phi_0^2(Q)$.

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

Accuracy of approximations



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

t=1, J=0.4, ω_{ph}=0.1, g=$\sqrt{0.05}$

Quite accurate. Phonon satellites smeared out.

Undoped system

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

In general: $\phi_0(Q)$ very complicated. Potential energy surface has several minima for $Q_0 \neq 0$. $\phi_0(Q)$ large around Q_0. Knowledge of $G(\mathbf{k}, z, Q = 0)$ not sufficient.

Undoped system: No electron-phonon coupling in *initial* state (for t-J model).

$\phi_0^2(Q)$ centered around $Q = 0$. Spectrum essentially the spectrum without el-ph. coupling ($G(\mathbf{k}, z, Q = 0)$) but broadened due to contributions from (small) $Q \neq 0$.

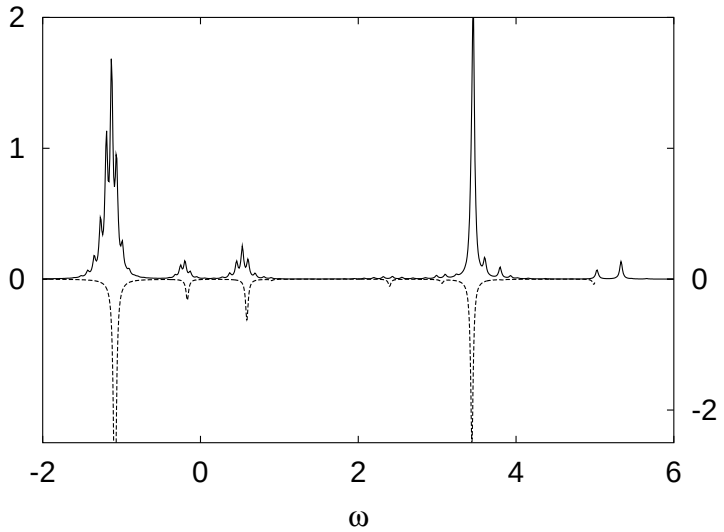
Explains why t-J model with phonons puts phonon sideband at quasi-particle in t-J model without phonons for undoped system.

10-site t-J model with one phonon mode (π,π). Exact diagonalization.

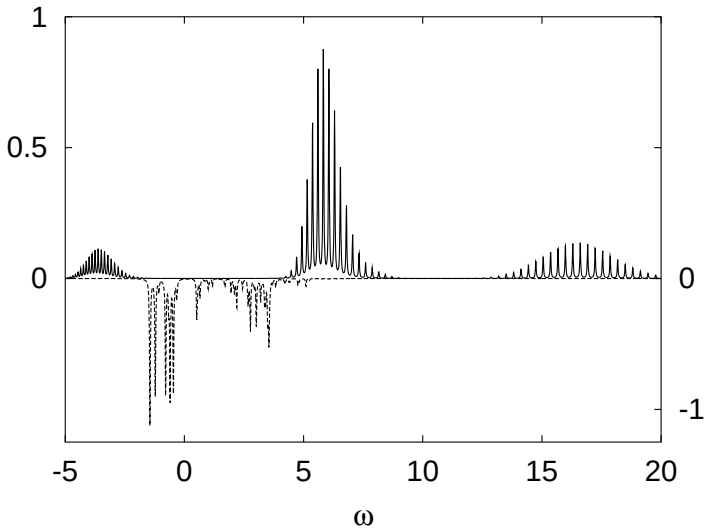
Coupl.

$g > 0$

$g = 0$



Undoped



Doped

$g > 0$ broadened version of $g = 0$ spectrum

$g > 0$ *can* be quite different from $g = 0$ spectrum

Method for calculating spectra for undoped system

When phonons included, Hilbert space very large. In particular if coupling strong.

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

For the undoped system $\phi_0(Q)$ is known and simple.

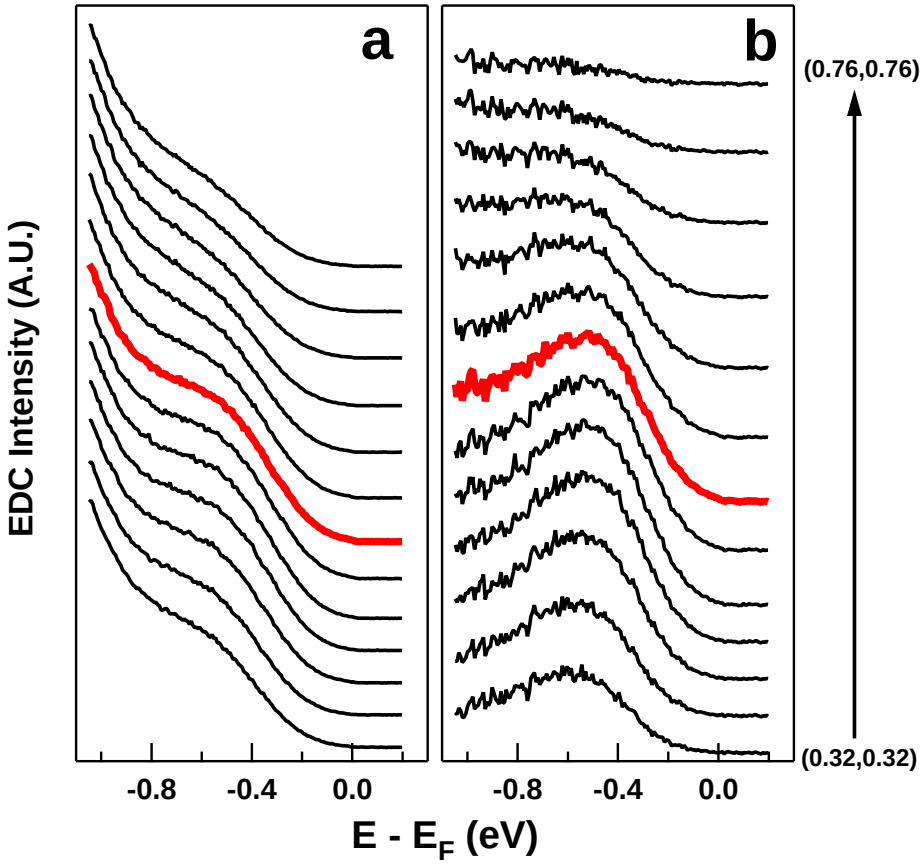
Sample Q using Monte-Carlo. Calculate $G(\mathbf{k}, z, Q)$ for each sampled Q value.

$G(\mathbf{k}, z, Q)$ is the Green's function for a distorted lattice but without (dynamical) electron-phonon coupling.

Hilbert space has the same size as for a system without electron-phonon coupling.

In this approximation the introduction of electron-phonon coupling is not a drastic complication. Possible to consider all 21 modes in La_2CuO_4 with $\mathbf{q}$-dependent coupling constants.

ARPES. $LaCuO_4$



Background subtracted

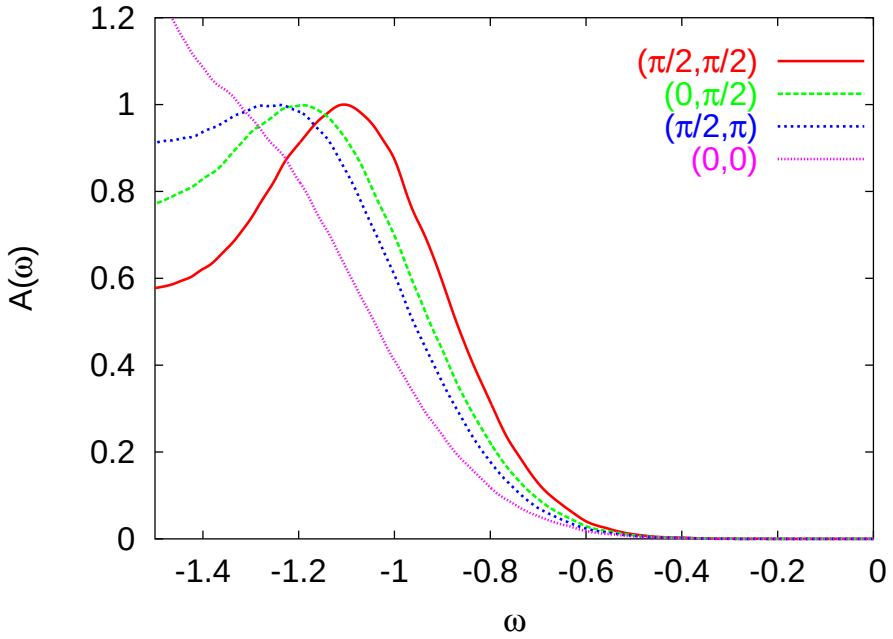
Very broad phonon satellite. No visible quasiparticle peak.

Rösch, Gunnarsson, Zhou,Yoshida,Sasagawa, Fujimori, Hussain, Shen and Uchida, cond-mat/0504660

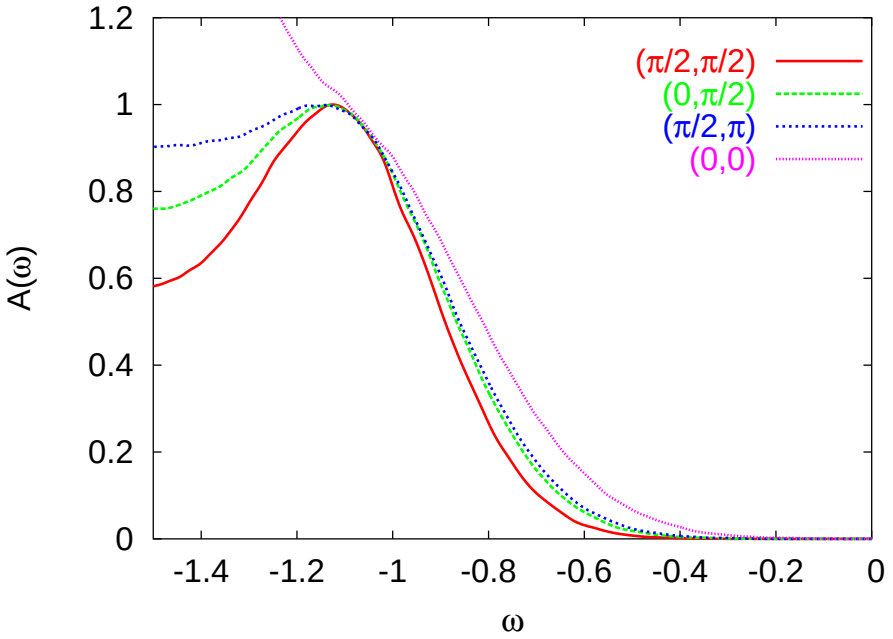
Width of phonon side-band

X. Zhou *et al.*: Width $(\pi/2, \pi/2)$ $(2\times$HWFM$)\sim 0.48$ eV (La_2CuO_4).

K.M. Shen *et al.*: Width $\sim$ binding energy ($Ca_2CuO_2Cl_2$) (PRL **93**, 267002 (2004)).



Peak heights aligned.



Heights and positions aligned.

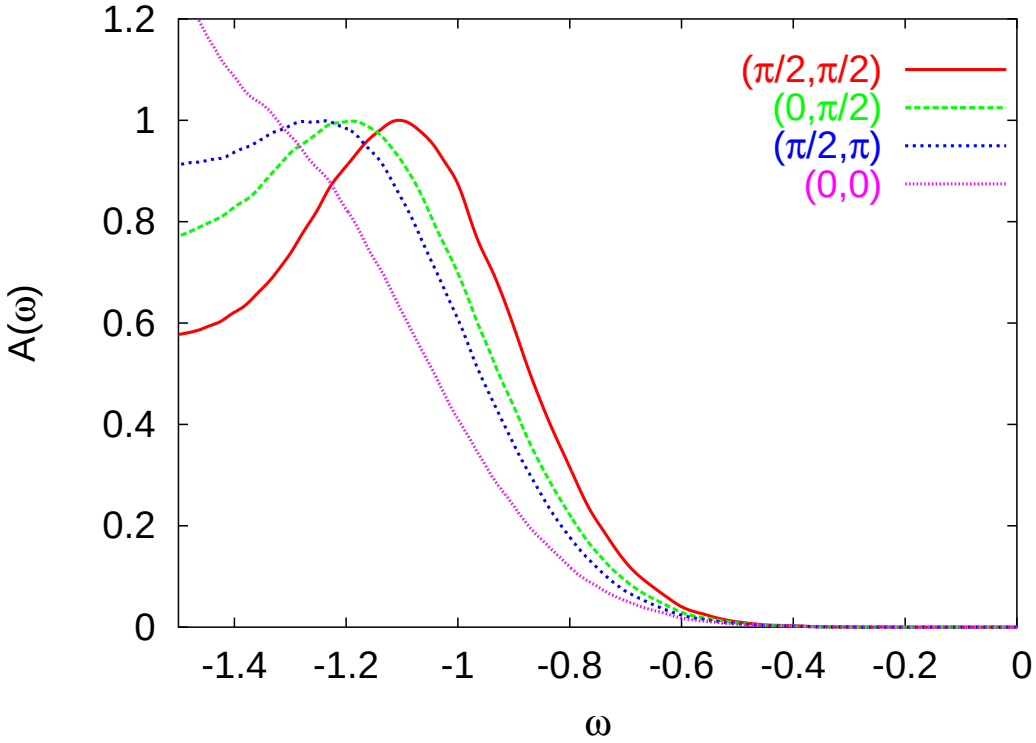
La_2CuO_4. 21 phonon modes. q-dependent coupling constants. 4×4 cluster.

50 000 samples.

Width $(\pi/2, \pi/2)$ $(2\times$HWFM$) \sim 0.5$ eV. Increases with binding energy.

Rösch, Gunnarsson, Zhou,Yoshida,Sasagawa, Fujimori, Hussain, Shen and Uchida, cond-mat/0504660

Tails of phonon side-bands



Coupling for La_2CuO_4.

$\mathbf{q}$-independent coupling.

4×4 lattice.

≈ 5000 samples.

$$\frac{1}{\pi}\mathrm{Im}G(\mathbf{k},\omega) = \sum_n |\langle n, N-1|c_{\mathbf{k}}|0,N\rangle|^2 \delta(\omega - E_0(N) + E_n(N-1))$$

Ordered system without phonons: Momentum conservation $\Rightarrow$ $\mathbf{k}$-dependent lower limit for $E_n(N-1)$ coupling to $c_{\mathbf{k}}|0,N\rangle$, upper limit for spectrum.

Disordered system (phonons approximately included): No momentum conservation $\Rightarrow$ Coupling to lowest state independent of $\mathbf{k}$.

Peak extends up to the same threshold (in this approximation).

Summary

- Apparent el.-ph. coupling in strongly correlated materials
  depends strongly on property studied.
- Sum rule for phonon but not electron self-energy satisfied,
  even when vertex corrections neglected.
- El.-ph. coupling in undoped system strong enough
  to give polaronic behavior.
- Adiabatic approximation explains why phonon sideband follows
  quasiparticle dispersion in absence of el.-ph. coupl. for undoped system.
- Side-band width reasonable. Increases with binding energy.