Polaron formation in cuprates

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1. Polaronic behavior in undoped cuprates.

    a. Is the electron-phonon interaction strong enough?

    b. Can we describe the photoemission line shape?

2. Does the Coulomb interaction enhance or suppress the electron-phonon interaction?

    Large difference between electrons and phonons.

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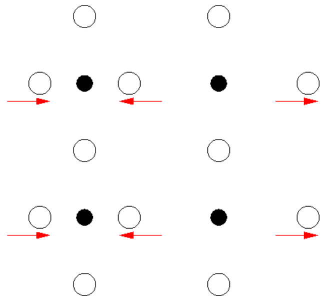
Important effects of electron-phonon coupling

- Photoemission: Kink in nodal direction.
- Photoemission: Polaron formation in undoped cuprates.
- Strong softening, broadening of half-breathing and apical phonons.
- Scanning tunneling microscopy. Isotope effect.

Models

Coulomb interaction important.

Here use Hubbard or t-J models.

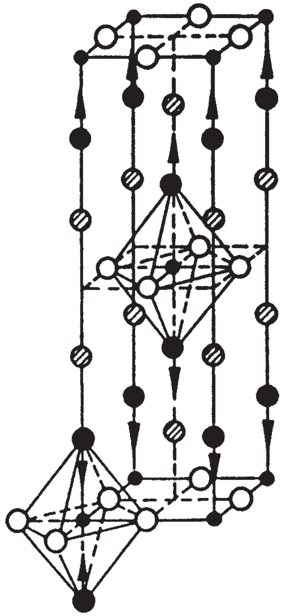


Half-breathing.

Breathing and apical phonons:

Coupling to level energies $>>$ coupling to hopping integrals.

$\Rightarrow g(\mathbf{k},\mathbf{q}) \approx g(\mathbf{q})$.



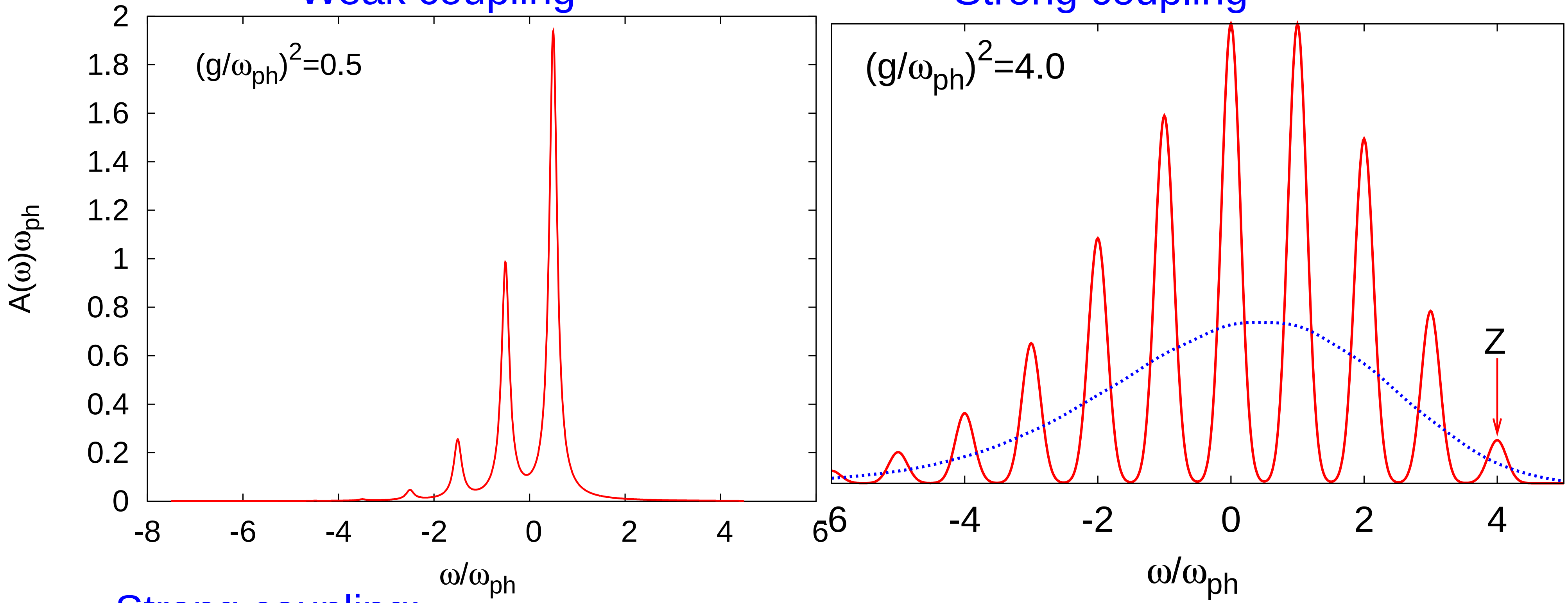
Apical.

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

Photoemission. Polarons

$$\mathbf{H} = \varepsilon_{\mathbf{0}}\mathbf{c}^{\dagger}\mathbf{c} + \mathbf{g}\mathbf{c}^{\dagger}\mathbf{c}(\mathbf{b} + \mathbf{b}^{\dagger}) + \omega_{\mathbf{ph}}\mathbf{b}^{\dagger}\mathbf{b}.$$

Weak coupling — Strong coupling

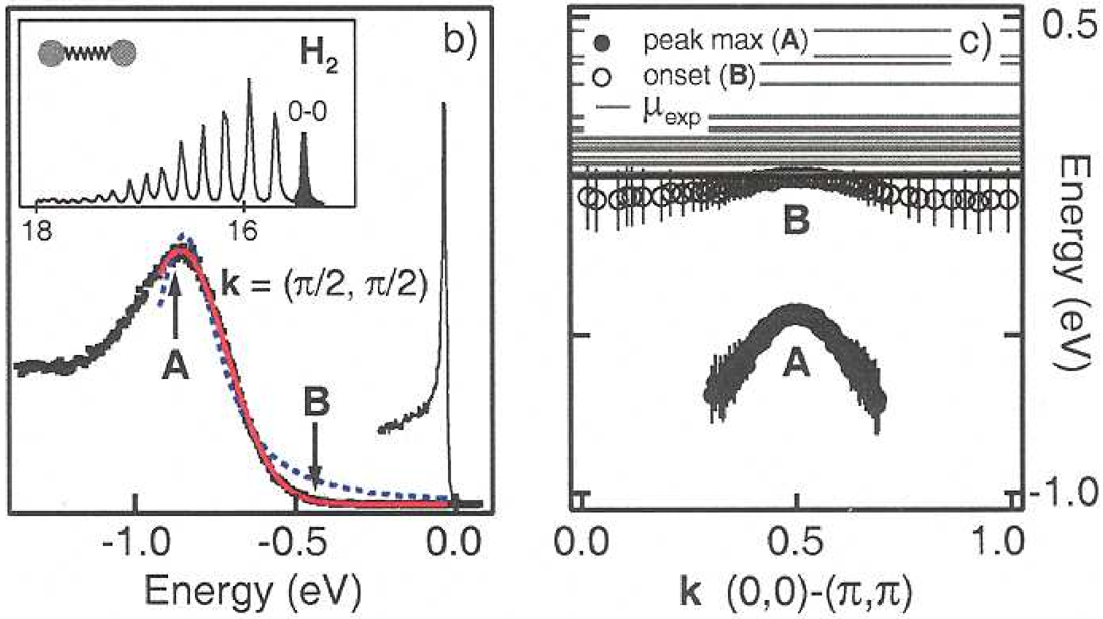


Strong coupling:

Exponentially small quasi-particle weight (here criterion for polarons).

Broad, approximately Gaussian side band of phonon satellites.

Polaronic behavior



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

Spectrum *very* broad (insulator: no electron-hole pair exc.)

Shape Gaussian, not like a quasi-particle.

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

Polarons: Quasi-particle ($\approx$ 0 weight). Broad boson side band.

Strong coupling to bosons. Phonons, spin fluctuations?

Electron-phonon coupl. Undoped system. Shell model

Find the electron-phonon coupling strength to carriers (t-J model).

1. Use a shell model (Pintschovius) to describe electrostatic coupling.

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

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

LDA too effective screening.

2. Add coupling due to modulation of hopping integrals.

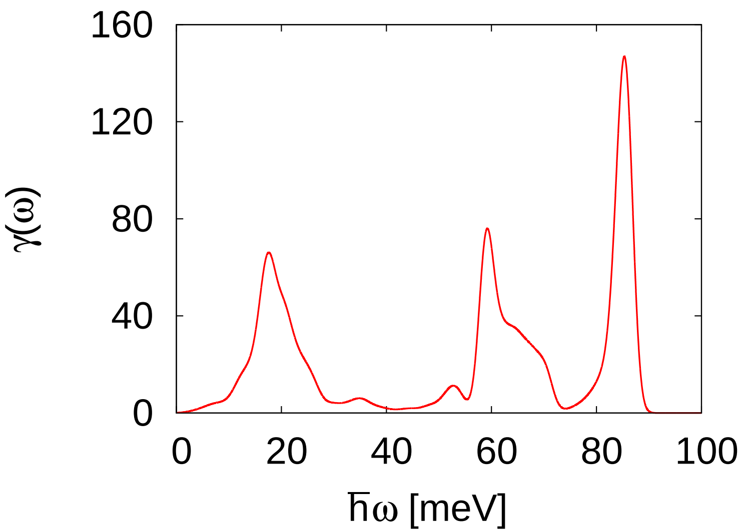
Electron-phonon coupling strength. La_2CuO_4

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

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

Calculations: $\lambda = 1.2$.

(Half-)breathing (80 meV), O_z (60-70 meV), La (Cu) modes (20 meV).



Hubbard-Holstein:

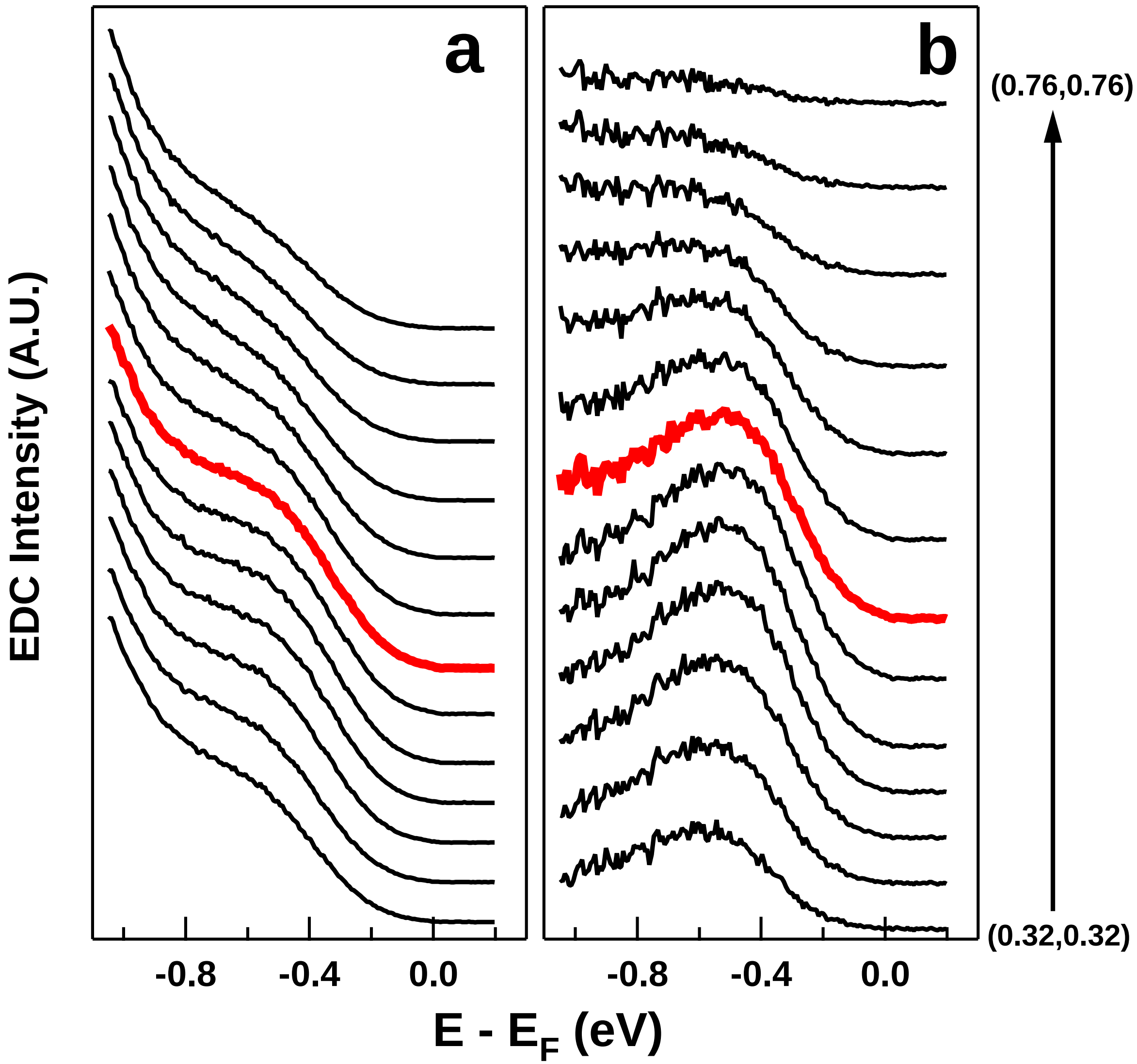
Polarons for $\lambda > 0.55$

Sangiovanni, Gunnarsson, Koch, Castellani, Capone, PRL **97**, 046404 (2006).

Sufficient to put undoped cuprates well into the polaronic regime.

Rösch, Gunnarsson, Zhou, Yoshida, Sasagawa, Fujimori, Hussain, Shen, Uchida, PRL **95**, 227002 (2005).

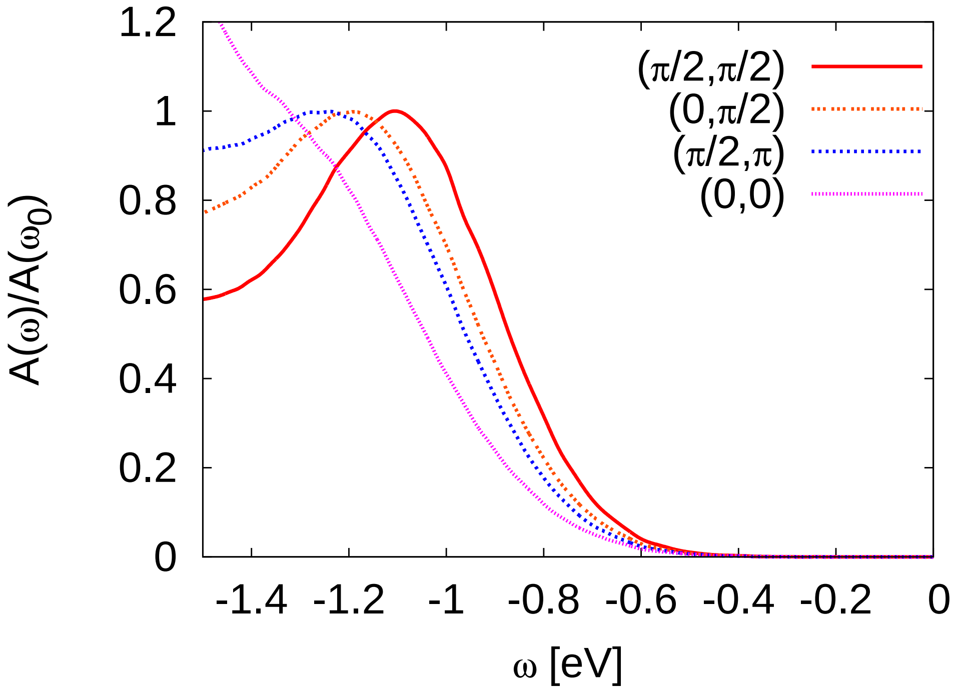
Experimental PES for La_2CuO_4



Broad phonon side band.

Width 0.48 eV.

Width of phonon side-band. La_2CuO_4



Exact diagonalization.

4×4 cluster. t-J model.

Nearest neighbor hopping.

21 modes. q-dependent coupl.

50 000 samples.

Peak heights aligned.

Calc. width $(\pi/2, \pi/2) \sim 0.5$ eV.

Exp.: Width $\sim$ 0.48 eV. Binding energy $\sim$ 0.5 eV.

Reduction of coupling constants by factor 0.8 ($\lambda = 0.75$) $\Rightarrow$

Width 0.4 eV, Bind. energy 0.6 eV, in rather good agreement with exp.

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

Coulomb suppression of electron-phonon inter.?

Strong Coulomb repulsion suppresses charge fluctuations,

in particular in weak doping limit.

$$\mathbf{H_{ep}} = \sum_{\mathbf{n}\mu} \mathbf{g_{n\mu\mu}} \mathbf{c}^\dagger_\mu \mathbf{c}_\mu (\mathbf{b_n} + \mathbf{b^\dagger_n}).$$

Important phonons couple to charge fluctuations.

Suppression of electron-phonon interaction?

Paramagnetic dynamical mean-field theory (P-DMFT):

Very strong suppression.

But: Spin correlations enhance electron-phonon interaction?

Sum rules. t-J-Holstein model

Phonon self-energy

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

(Khaliullin, Horsch)

As $\delta(\mathrm{doping}) \rightarrow 0$, $\Pi \rightarrow 0$. Suppression by Coulomb interaction.

Electron self-energy

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

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

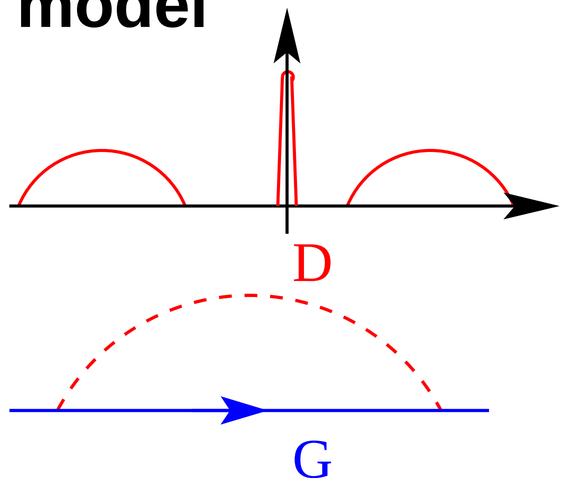
Identical to the lowest order result for noninteracting electrons.

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

Σ describes creation of a hole, which interacts strongly with phonons.

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

Paramagnetic DMFT. Hubbard-Holstein model



P-DMFT: Strong suppression of electron-phonon inter.

Half-filling: Only mechanism for Mott insulator: $Z \rightarrow 0$.

Lowest order self-energy: $\Sigma_{ep} \sim GD$

If Z small, strong suppression of Σ_{ep}, since incoherent weight enters with a large energy denominator.

Electron-phonon interaction strongly suppressed because $Z \rightarrow 0$.

Allowing for antiferromagnetism, insulator possible without $Z \rightarrow 0$.

Less strong suppression of electron-phonon interaction?

Antiferromagnetic DMFT

P-DMFT: $\Sigma_\sigma(\mathbf{k},\omega) \equiv \Sigma(\omega) \Rightarrow \Sigma_{ij\sigma} = \delta_{ij}\Sigma(\omega)$.

AF-DMFT: $\Sigma_{ij\sigma}(\omega) \equiv \delta_{ij} \times \begin{cases} \Sigma_\uparrow(\omega), & \text{if } \sigma \text{ majority spin on site } i, \\ \Sigma_\downarrow(\omega), & \text{if } \sigma \text{ minority spin on site } i. \end{cases}$

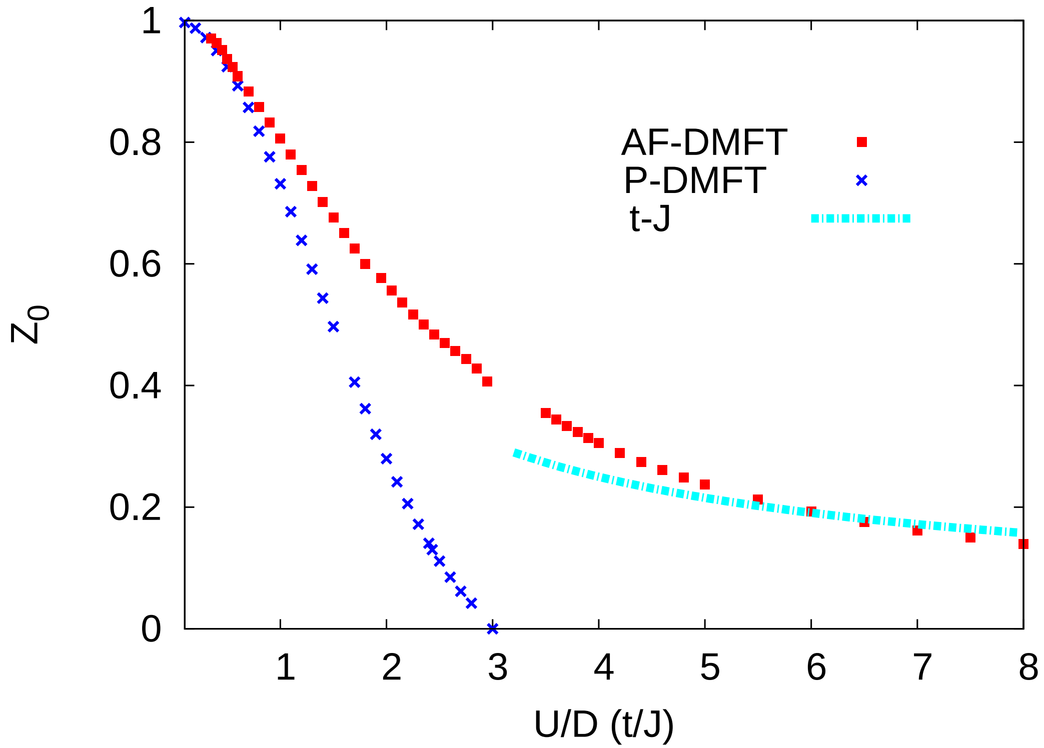
Impurity coupled to self-consistent spin-polarized bath.

Bethe lattice (semi-elliptical DOS).

Impurity model solved using exact diagonalization.

Possible to treat doped systems.

Quasiparticle strength. Undoped system.



$J = \frac{4t^2}{U}$; $\frac{J}{t} = \frac{4t}{U}$

$2d$ system: W=$2D$=$8t$

$\Rightarrow \frac{J}{t} = \frac{W}{2U} = \frac{D}{U}$.

D= Half band width.

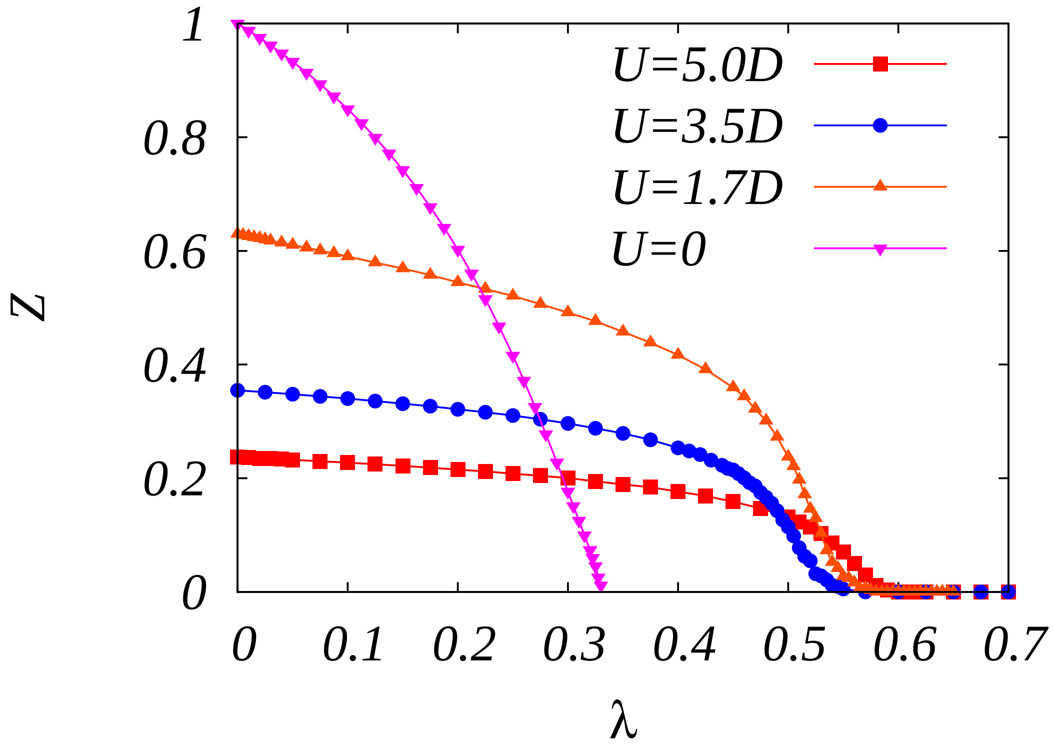
Sangiovanni, Gunnarsson, Koch,

Castellani, Capone, PRL **97**, 046404 (2006).

Reasonable values for Z in AF-DMFT but not in P-DMFT.

$\Rightarrow$ Good description of electron-phonon coupling?

Polaron formation. Dependence on U



Half-filled Holstein-Hubbard model. $2d$ system.

ω_0=$0.025D$; $\lambda = \frac{2g^2}{\omega_0 W}$.

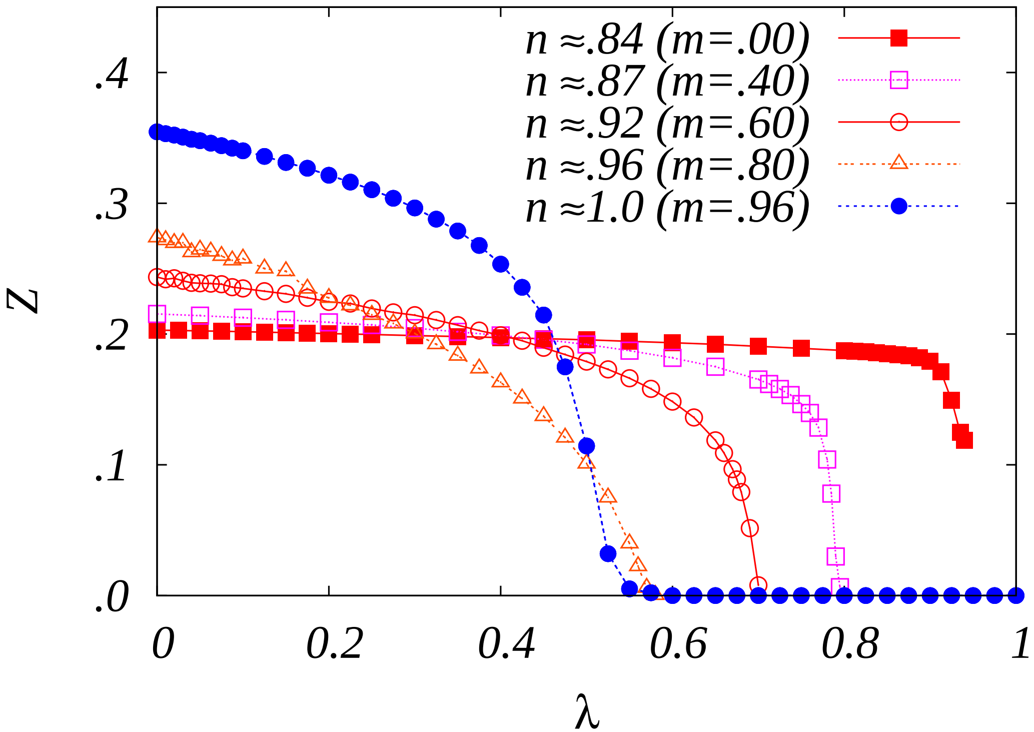
ω_0=$0.1t$=0.04 eV.

Sangiovanni, Gunnarsson, Koch, Castellani, Capone, PRL **97**, 046404 (2006).

U moderately hurts polaron formation, but far less than in P-DMFT.

Crucial to include AF correlations.

Doping dependence



2d Holstein-Hubbard model.

ω_0=$0.025D$; U=$3.5D$; $\frac{J}{t}$=0.29.

Sangiovanni, Gunnarsson, Koch, Castellani, Capone, PRL **97**, 046404 (2006).

AF-DMFT: Incr. doping $\Rightarrow$ Reduced magnetization $\Rightarrow$ Incr. λ_c.

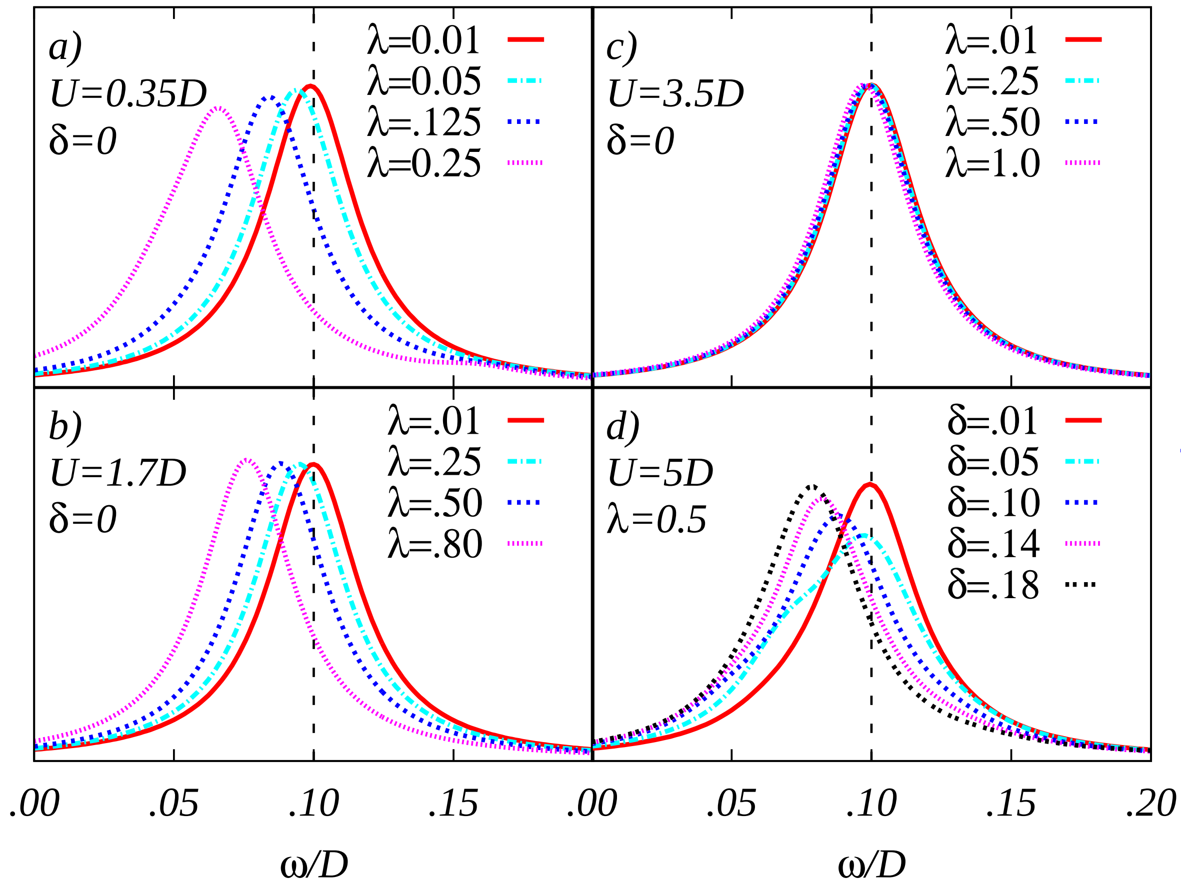
P-DMFT: Increased doping $\Rightarrow$ Reduced (but very large) λ_c.

Exp.: Doping suppresses polaron formation.

AF-P transition at much too large doping due to neglect of AF correlations in P state (use cluster methods, introduce n.n. hopping).

Macridin, Moritz, Jarrel, Maier, PRL **97**, 056402 (2006).

Softening of phonons



a) U small:

Large softening.

b)+c): U large, half-filling: Small softening.

d) Doping increased

$\Rightarrow$ Increased softening.

Phonon soft. strongly suppressed by U. Suppression reduced with δ.

Electron prop. moderately suppressed. Suppression increases with δ.

In agreement with sum rules. Strong property dependence.

Coulomb int. vs. AF corr. (Photoemission)

Effects of Coulomb interaction

Compare correlated system with half-filled Holstein model.

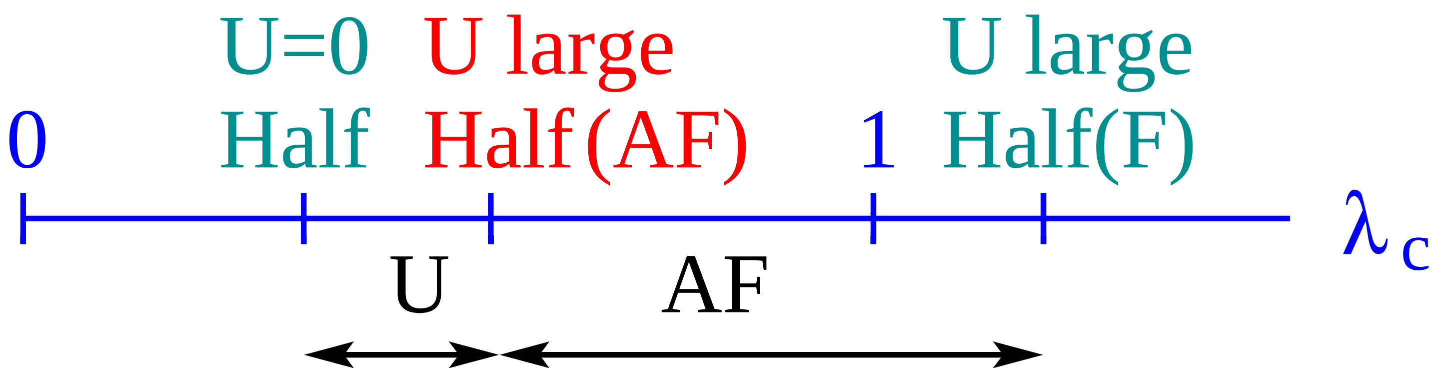
Allows us to turn up U without changing anything else.

Effects of antiferromagnetic correlations

Compare full solution (with antiferromag. correl.) with ferromag. state.

Photoemission for undoped ferromagnetic system $\Rightarrow$ One hole.

Ferromag. state with one hole $\equiv$ Holstein model with one electron.



Total effect of $U \Rightarrow$ suppression.   AF $\Rightarrow$ enhancement of el.-ph. int.

Holstein model. Polaron formation

Half-filled model versus one electron at bottom of band.

Compare states with perfectly itinerant electrons and perfectly localized electrons.

Energy per electron:

System	Itinerant	Localized
One electron	-4t	$-g^2/\omega_{\rm ph}$
Half-filled	-$1.7t$	$-g^2/\omega_{\rm ph}$

Harder to form polaron in one-electron case.

Hopping energy maximum for one electron at bottom of band.

Phonons vs. magnons

Self-consistent Born approx.: Phonons, magnons treated as bosons.

$\lambda = \frac{1}{N^2}\sum_{\mathbf{kq}} \frac{M^2_{\mathbf{kq}}}{8t\omega_{\mathbf{q}}}$. Magnons: $\lambda_M = \frac{t}{2J}$.

$\frac{J}{t} = 0.3 \Rightarrow \lambda_M = 1.67$. La_2CuO_4: $\lambda_{\rm ph} \approx 1.2 < \lambda_M$!

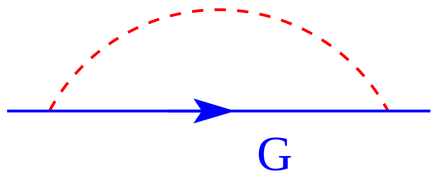
Why not polarons due to magnons?

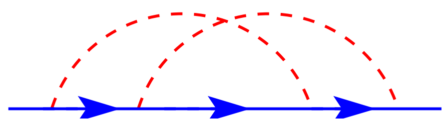
QMC, Exact diag. t-J model: No polarons.

Crossing phonon line diagrams crucial for polarons.

Many classes of crossing magnon line diagrams zero due to symmetry of coupling.

No polarons caused by magnons alone.





Symmetry of magnon coupl. $\Rightarrow$ 0.

Alternative explanation: Spin 1/2 syst. Spin can only be flipped once. Magnons not bosons.

How are coupling constants influenced by U?

So far, studied Hubbard-Holstein model with *fixed* coupling constants.

But where do the coupling constants come from?

Half-breathing phonon

Three-band model: One Cu $3d$ and two O $2p$ orbitals. $\Rightarrow$ One-band model with Zhang-Rice singlet. Coupling *constants* enhanced by U.

Rösch and Gunnarsson, PRB **70**, 224518 (2004).

Apical oxygen modes

Strong electrostatic coupling due to net charge of oxygen ions.

$U = 0$: Efficient screening strongly reduces coupling.

Large U: Screening strongly reduced. Stronger coupling.

Summary

- El.-ph. coupl. strong enough to give polarons for undoped cuprates.
- Reasonable PES line shape for undoped cuprates.

Hubbard-Holstein model. *Fixed* coupling constants.

- Antiferromagnetic correlation crucial for el.-ph. coupling.
- U moderately suppresses el.-ph. coupl. for electronic properties.
- U strongly suppresses el.-ph. coupl. for phonon properties.
- Opposite doping dependencies for electrons and phonons.
- Trends described by sum rules.

Coupling *constants* can be enhanced by U.