Angle resolved photoemission spectroscopy in high temperature superconductors

A. S. Mishchenko

В сотрудничестве:
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Z.-X. Shen, K.M. Shen, X.J. Zhou (Stanford)
T. Devereaux (Ontario)

Stimulating discussions:

G. Sawatzky, O. Gunnarsson, O. Rosch

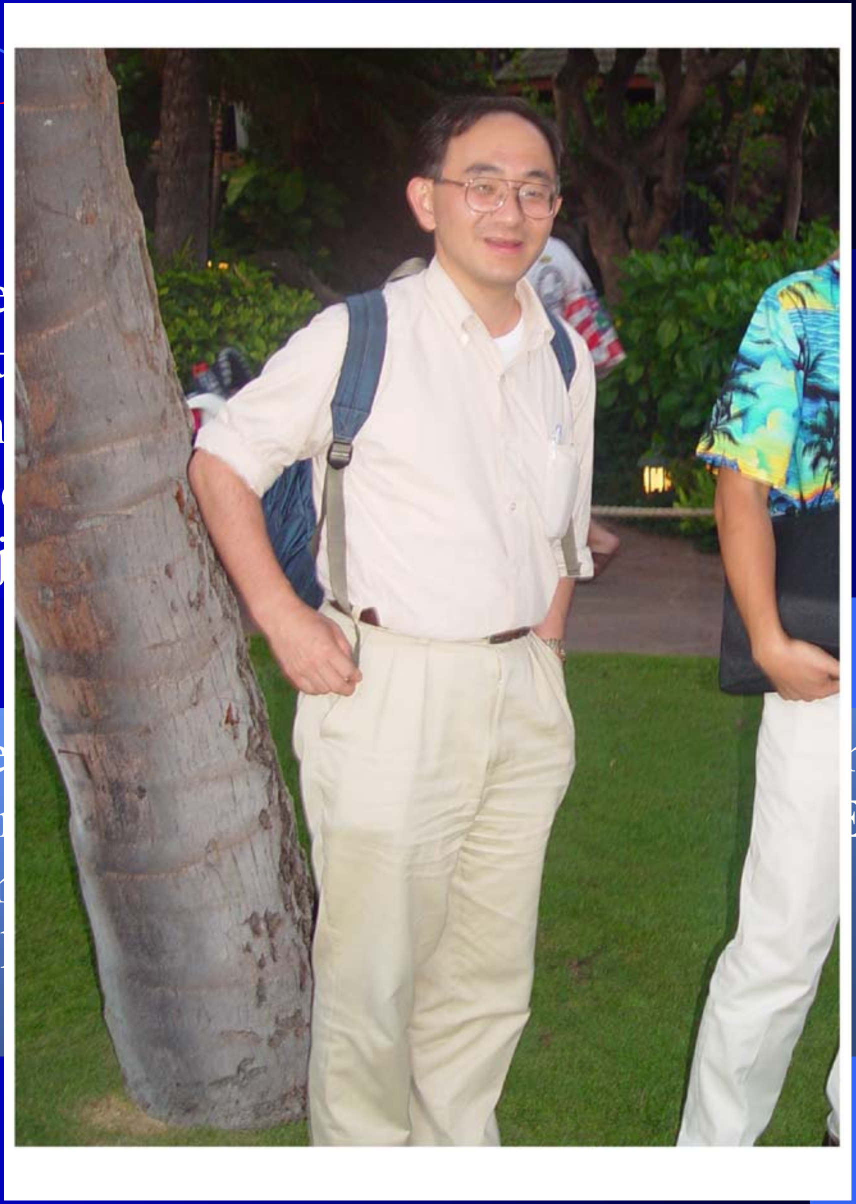
Polaron in a t-J model.

A.S.Mishchenko and N. Nagaosa

Tsukuba, Japan
December 2003

Polaron in t-J model. Theory and ARPES

A.S. Mishchenko and



We present numeric results for ground state
model coupled to optical phonons. The syst
Monte Carlo is employed where the Feynm
function in imaginary time are summed up
variables, while magnetic variables are subj

At electron-phonon coupling constants re
undergoes self-trapping crossover to stro
demonstrate features observed in experim
spectra has momentum dependence whic
t-J model.

Polaron in t-J model. Theory and ARPES

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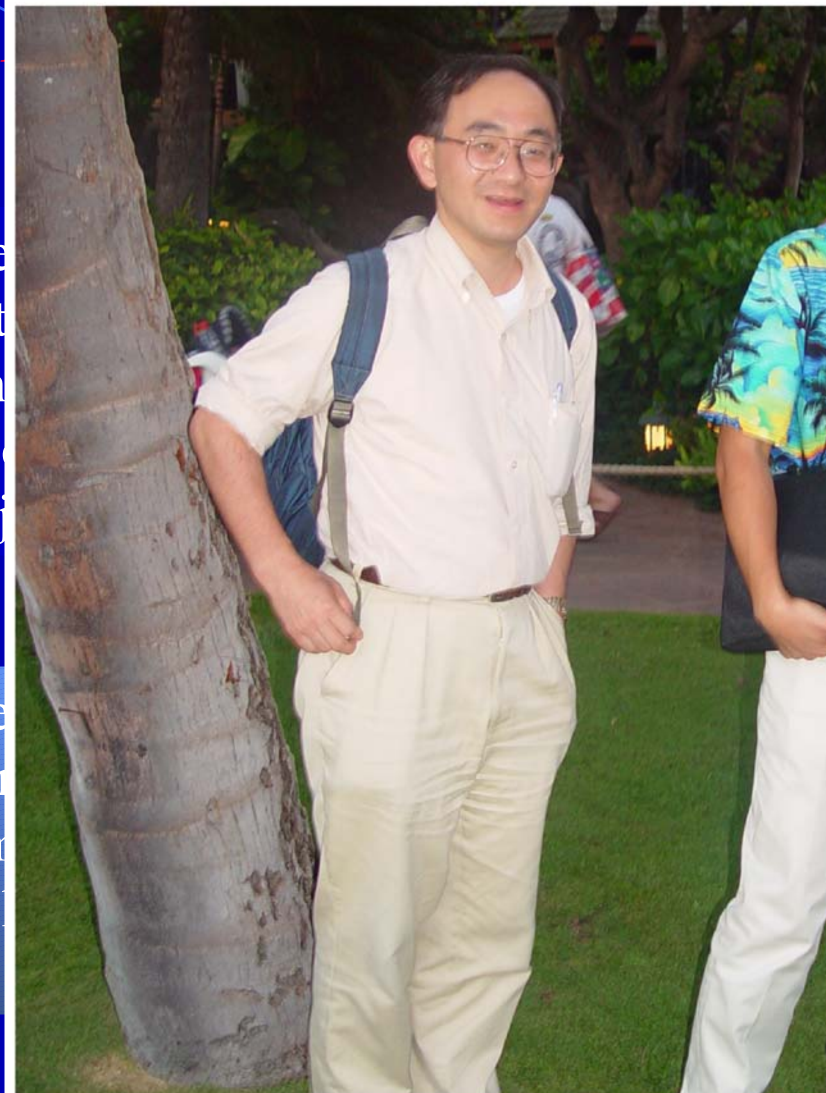
A look to the future



INTRODUCTION

1. Problems of quasiparticle line shape in theory of ARPES. How to introduce electron phonon interaction (EPI) into models of high temperature superconductors.

STRONG COUPLING REGIME OF EPI - UNIVERSALITY

3. Line shapes in tt't"-J models in strong coupling regime of EPI. Comparison with experiment. Universal scaling of the energy and linewidth.

4. Copling constant in $Sr_2CuO_2Cl_2$ and dependence of the EPI coupling constant on doping in $Ca_{2-x}Na_xCuO_2Cl_2$

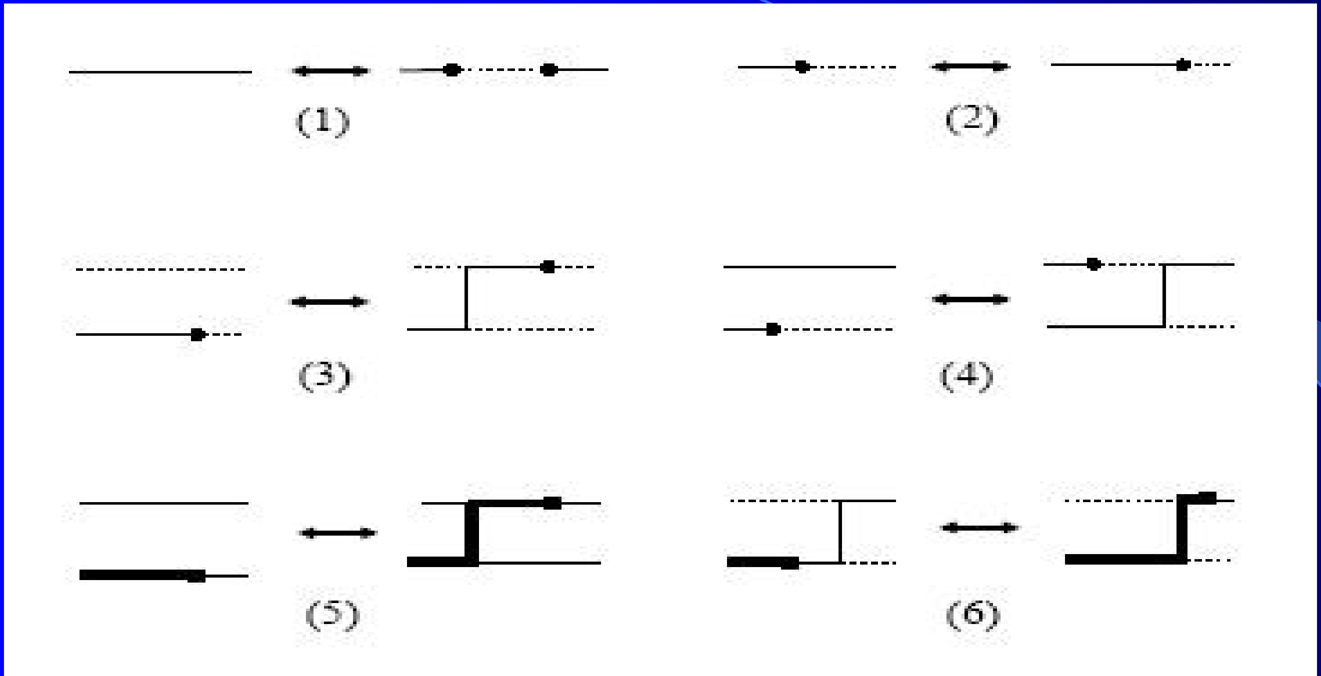
WEAK AND INTERMEDIATE COUPLING REGIME

4. Different pictures which we imagine when hear "a polaron formation". How "polaron formation" is seen with high- and low-resolution ARPES?

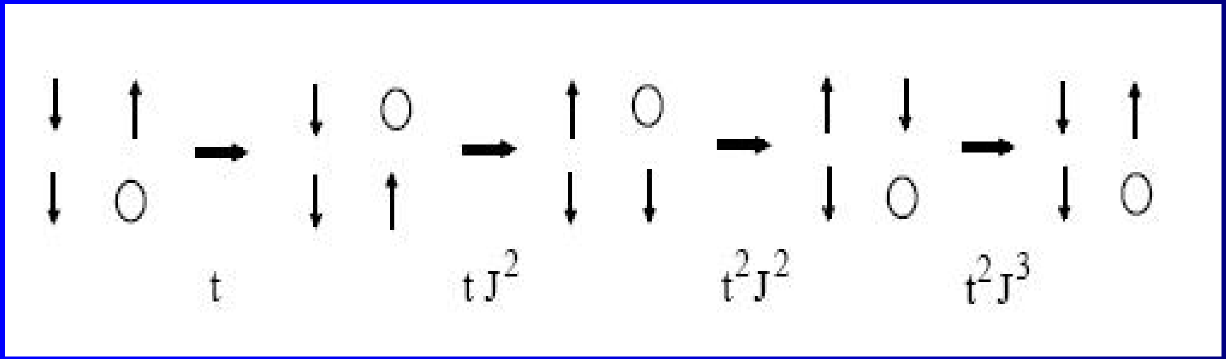
5. Weak and intermediate coupling regime. Nature of the kink in the polaron dispersion. EPI coupling constants in LSCO – doping dependence.

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

Single hole in the t-J model



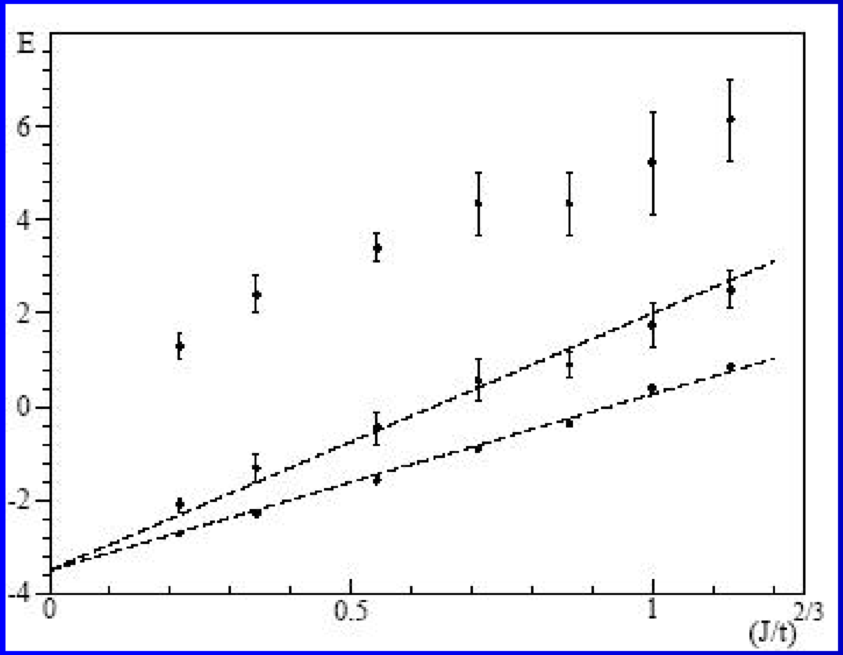
Worm algorithm of DMC

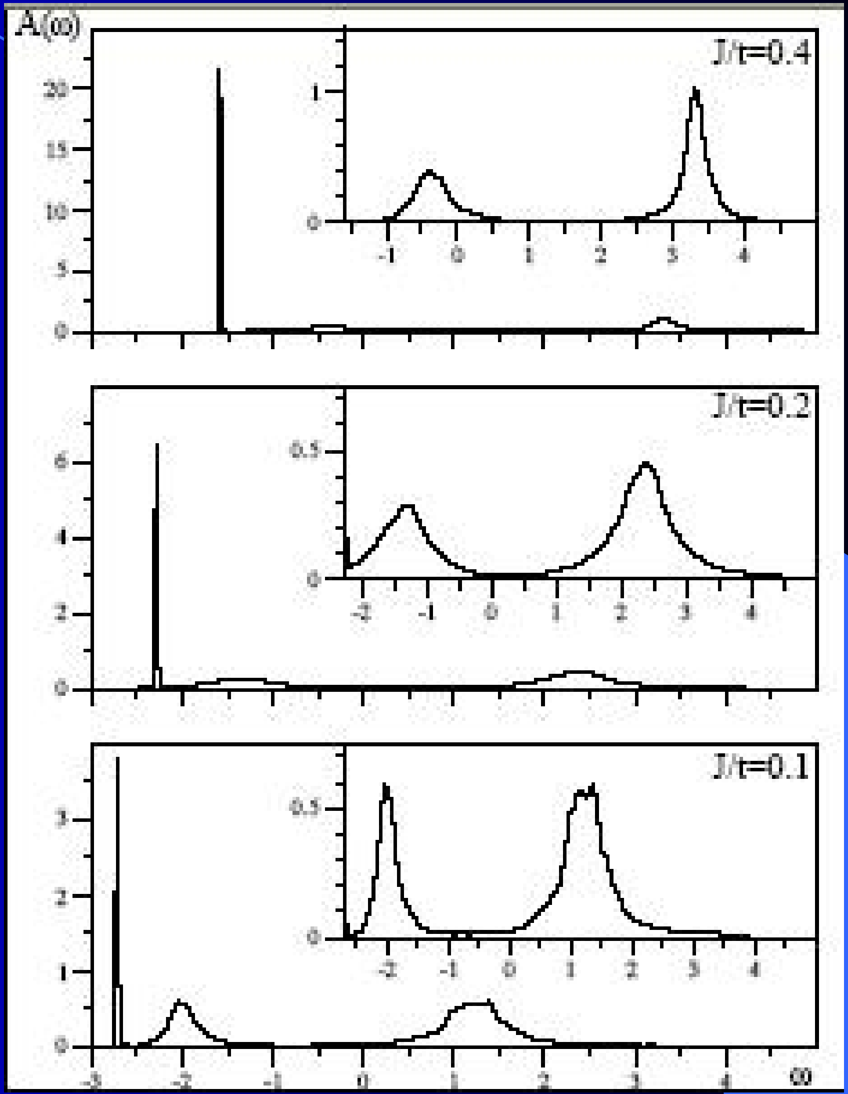


Sign problem

A.S. Mishchenko, B.V. Svistunov, N.V. Prokof'ev, PRB, vol. 64, 033101 (2001)

Single hole in the t-J model





$$E = a + b\,J^{2/3}$$

A.S. Mishchenko, B.V. Svistunov, N.V. Prokof'ev, PRB, vol. 64, 033101 (2001)

Problems of theoretical description of ARPES spectra in *$Sr_2CuO_2Cl_2$ and $Ca_{2-x}Na_xCuO_2Cl_2$*

Theoretical results for undoped insulators:

1. Lehman spectral function at all momenta has a **sharp** quasiprticle peak
2. Sharp quasiparticle peak has dispersion with the banwidth of the order of exchange constant J.

Experimental results:

1. ARPES data at all momenta demonstrate a very **broad** quasiparticle peak in the low energy part with incoherent continuum at high energies.
2. The dispersion of broad quasiparticle peak coincides with prediction of extended t-J model (t-t'-t''-J model).

Complete success of theory in explanation of dispersion and Complete failure of theory in explanation of linewidth.

Main problem is the LINE SHAPE

Spin-wave approximation in momentum representation for single hole in t-t'-t"-J model interacting with phonons

Hole with dispersion ε(k) in magnon and phonon bathes

$$H^{(0)}_{tt't''-J} = \Sigma_k \varepsilon(k)\, h_k^+ h_k + \Sigma_k \upsilon(k)\, \alpha_k^+ \alpha_k + \Sigma_k \omega_{ph}\, b_k^+ b_k$$

Scattering on magnons: $H_{h-m} = N^{-1} \Sigma_{k,q} M_{k,q} [h_k^+ h_{k-q} \alpha_q + h.c.]$

Scattering on phonons: $H_{h-ph} = N^{-1} \Sigma_{k,q} \gamma [h_k^+ h_{k-q} b_q + h.c.]$

Dimensionless EPI constants: $\lambda=2g$, $\lambda=\gamma^2/4t\omega_{ph}$, $g=\gamma^2/8t\omega_{ph}$

ARPES experiment measures the Lehman spectral function

$$L_{\mathbf{k}}(\omega) = \Sigma_f \, \delta[\omega - E_f(\mathbf{k})] \, \langle f | h_{\mathbf{k}}^{+} | vac \rangle$$

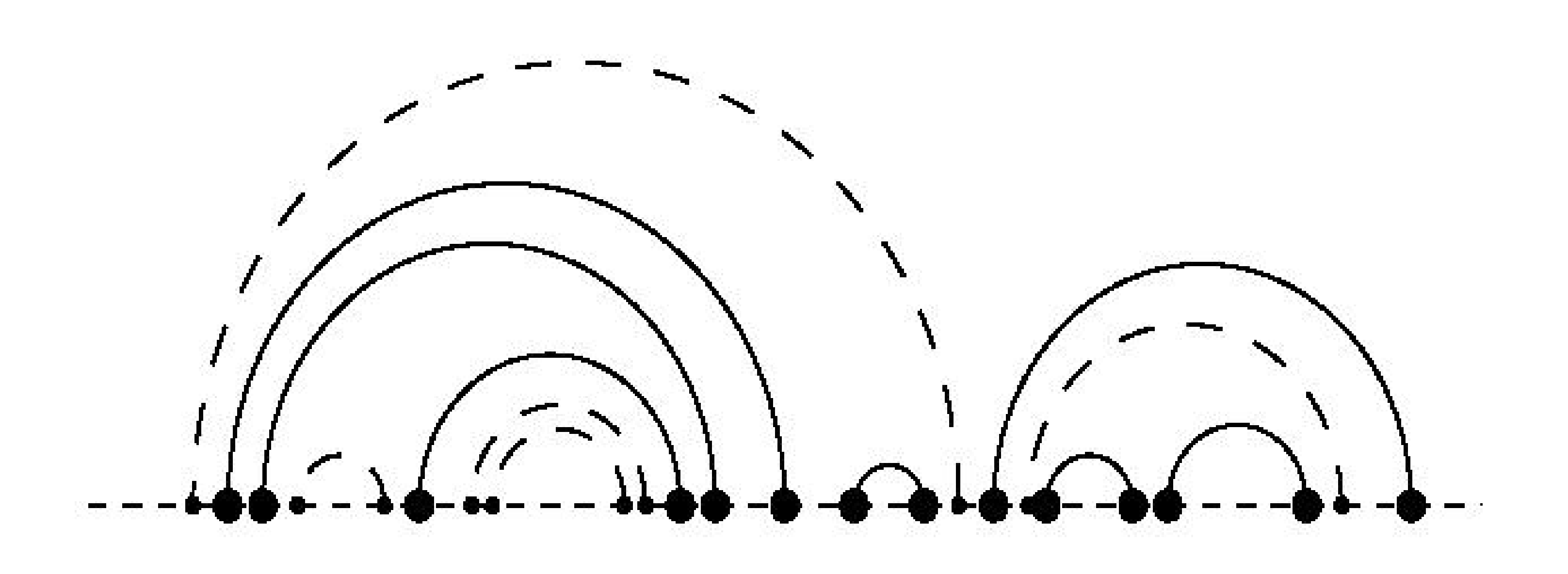
One needs to calculate hole Green function

$$G(\mathbf{k},\tau) = \langle vac | \, h_{\mathbf{k}}(\tau) \, h_{\mathbf{k}}^{+}(0) | vac \rangle$$

and obtain Lehman function $L_{\mathbf{k}}(\omega)$ by analityc continuation to real frequencies

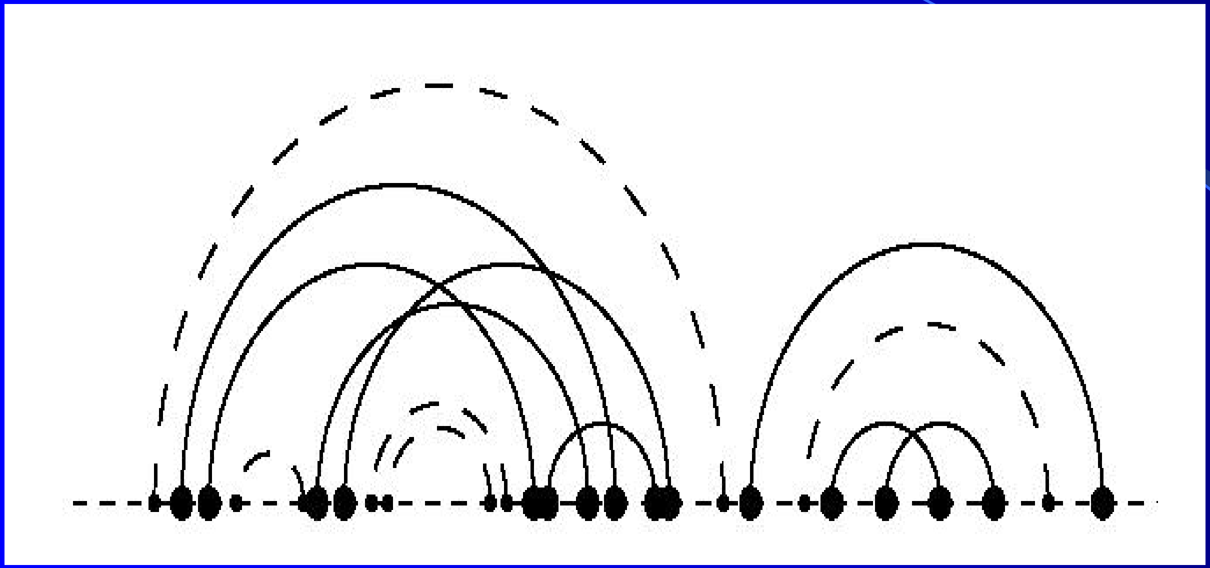
$$L_{\mathbf{k}}(\omega) = - \pi \, Im \, G(\mathbf{k},\omega)$$

Phonon-phonon and magnon-magnon NCA (SCBA)



Most important limitation of SCBA is phonon-phonon non-crossing approximation. Magnon-magnon non-crossing approximation is not important since the interaction with magnons is weak: spin ½ can not flip more than one time in magnon cloud around the hole. On the other hand, phonon-phonon vertex corrections are crucial.

Feynman expansion which is sufficient for problem of one hole in t-J model coupled to phonons.



1. Intercrossing of phonon propagators is taken into account.
2. Magnon-magnon vertex corrections are neglected because coupling of the hole to magnons is weak.

This expansion can be summed by numerically exact Diagrammatic Monte Carlo method where all Feynman graphs are generated by Monte Carlo and summed up without systematic errors.

1. A.S.Mishchenko, N.V.Prokof'ev, A.Sakamoto, and B.V.Svistunov, Phys.Rev. B, vol.62, 6317 (2000).
2. A.S.Mishchenko and N.Nagaosa, Phys.Rev.Lett., vol.86, 4624 (2001).
3. E.A.Burovski, A.S.Mishchenko, N.V.Prokof'ev and B.V.Svistunov, Phys.Rev.Lett., vol.87, 186402 (2001) .
4. A.S.Mishchenko, N.Nagaosa, N.V.Prokof'ev, A.Sakamoto, and B.V.Svistunov, Phys.Rev.Lett., vol.91, 236401 (2003).

Demonstration of the importance of phonon-phonon vertex corrections

Ordinary 2D Holstein model

Near neighbour hopping of hole

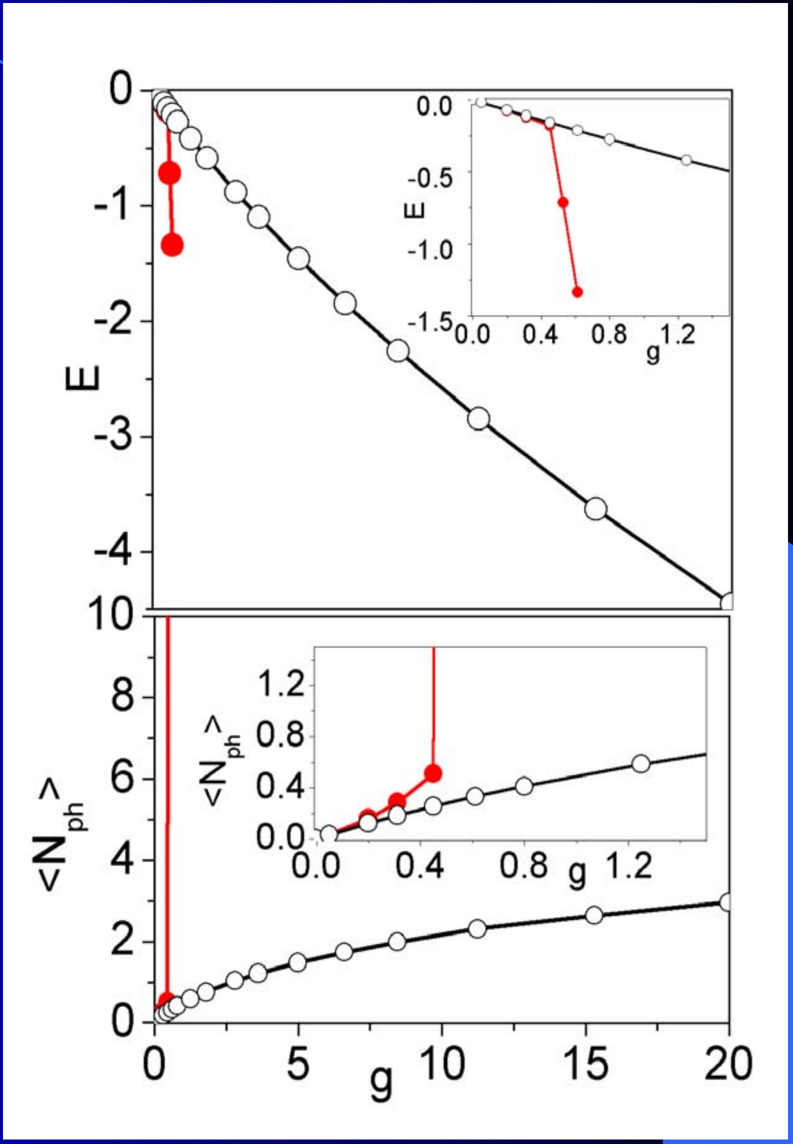
$$H^{(0)}_{t\text{-}J} = \Sigma_k \, \varepsilon_\kappa \, h^+_k h_k \; ; \quad \varepsilon_k = 2t \, \Sigma_{i=x,y} \cos(k_i)$$

Scattering of the hole by phonons

$$H_{e\text{-}ph} = \Omega \, \Sigma \, b^+_k b_k + N^{-1} \gamma \, \Sigma_{k,q} \, [\, h^+_k h_{k-q} b_q + h.c.]$$

For polaron problem DMC method is able to sum up Feynman graphs exactly:
(a) The whole sequence
(b) In non-crossing approximation

$t=1$, $\Omega=0.1$
Dimensionless constant
$g=\gamma^2/(8t\Omega)$

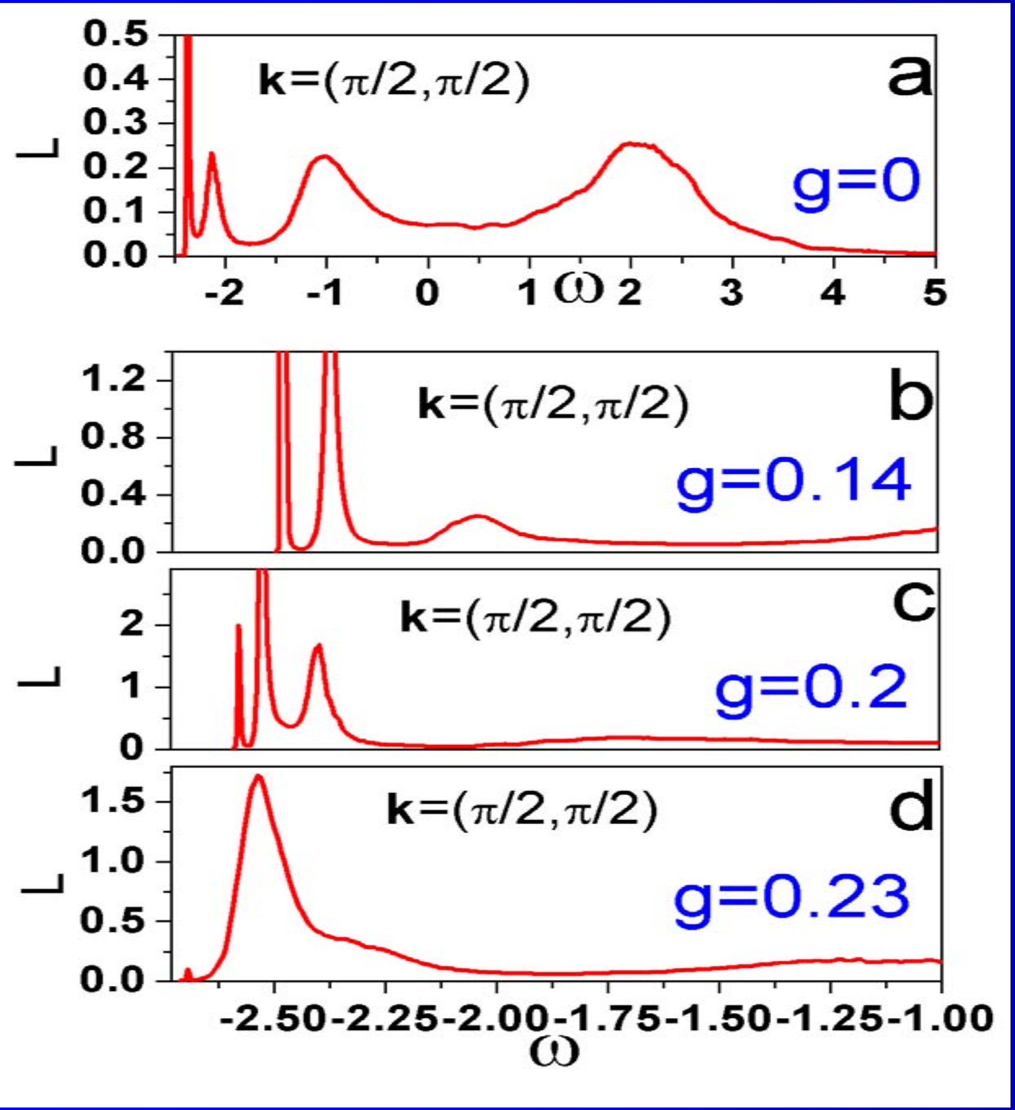


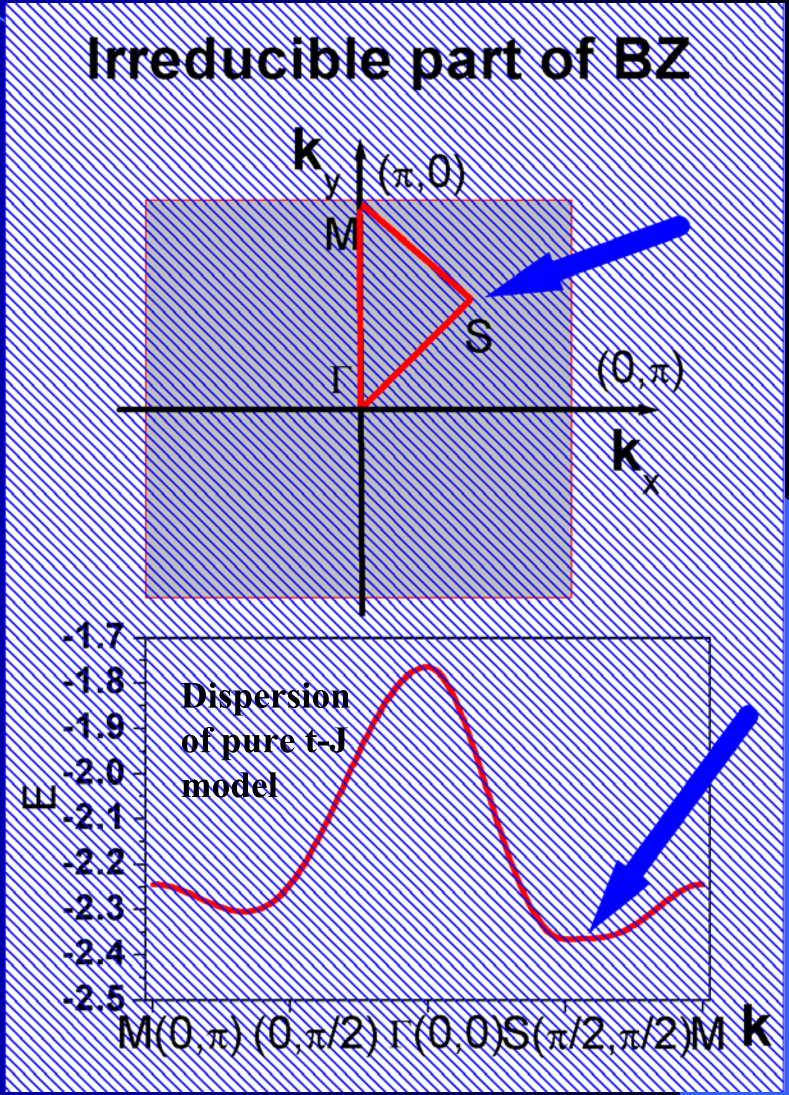
Transition into strong coupling regime:

(a) Occurs at g=0.5 in exact summation

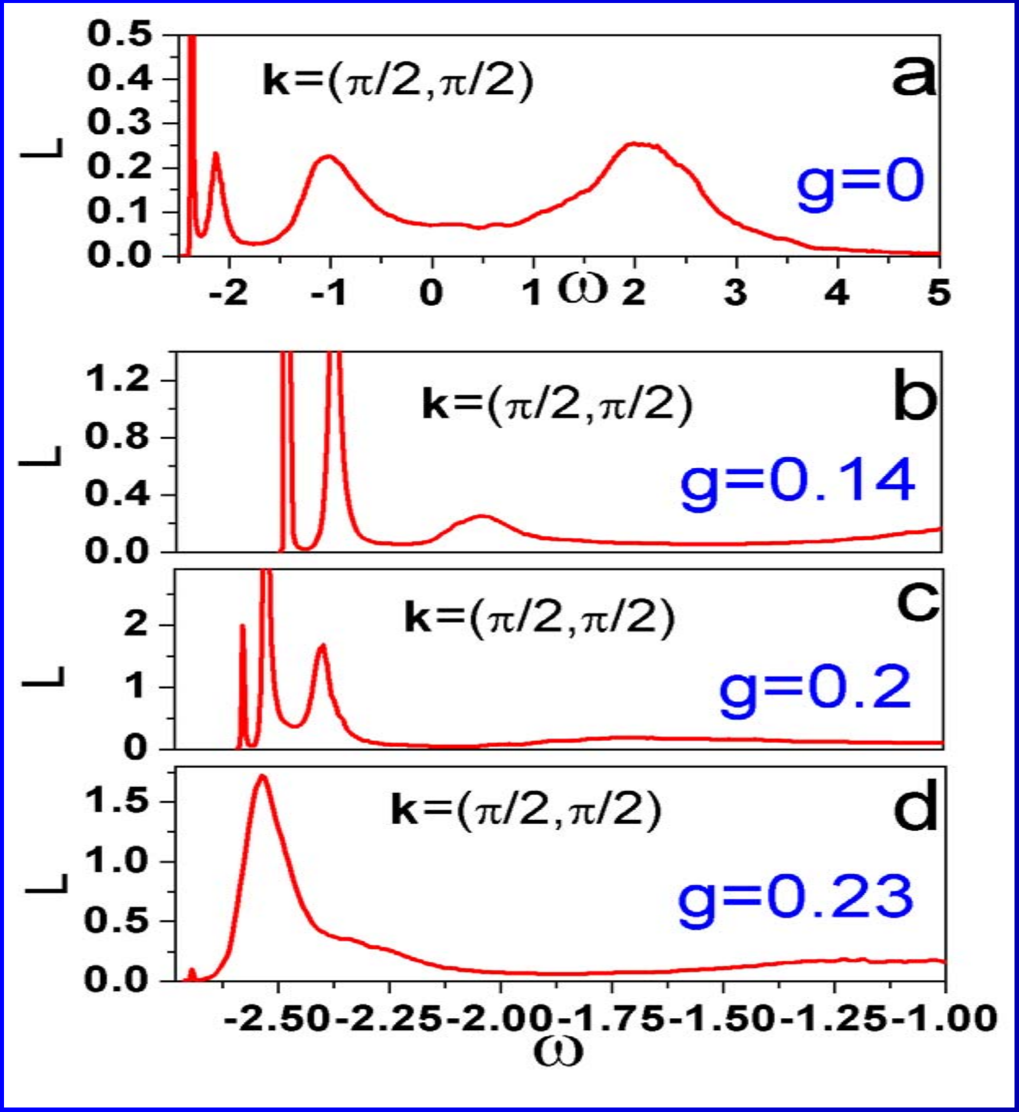
(b) Newer occurs in NCA (g<60)

Dependence of ARPES spectrum in ground state S on the interaction constant g





Dependence of ARPES spectrum in ground state S on the interaction constant g



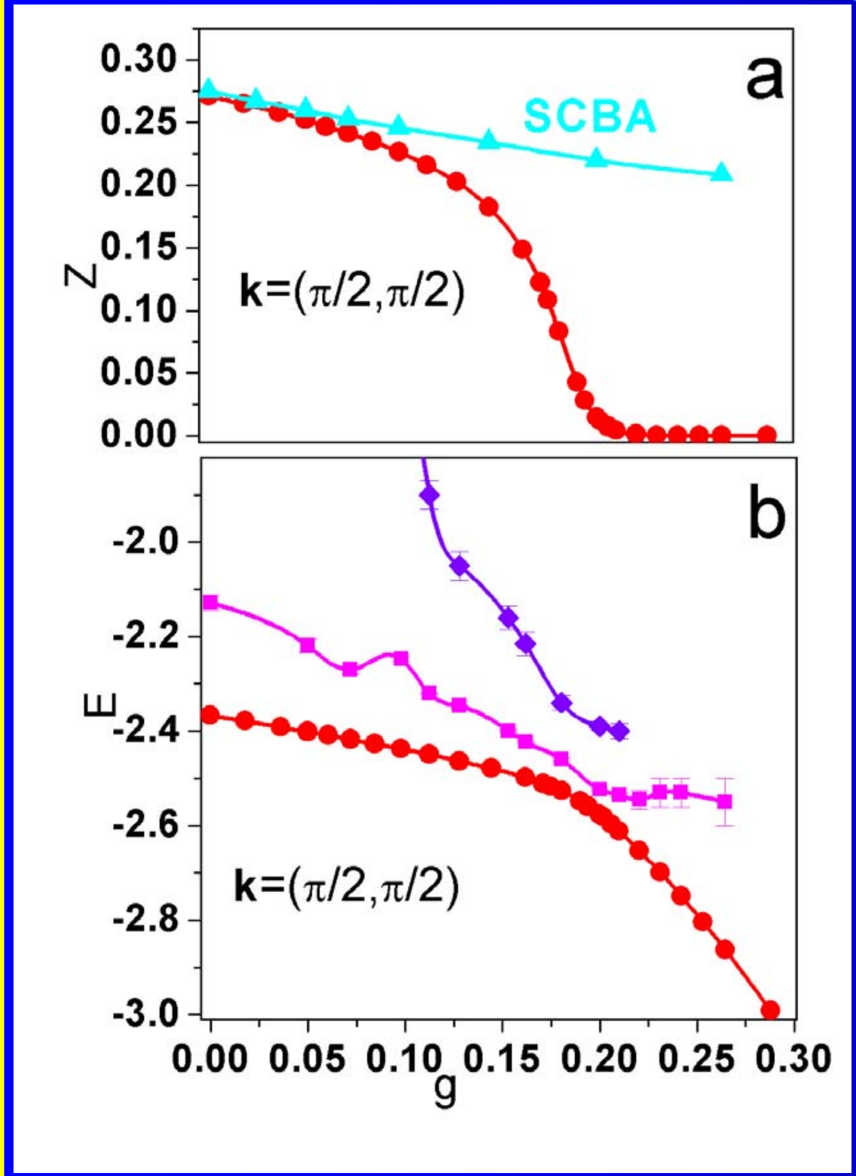
There are three low energy peaks at g=0

These three peaks are observed up to g=0.21

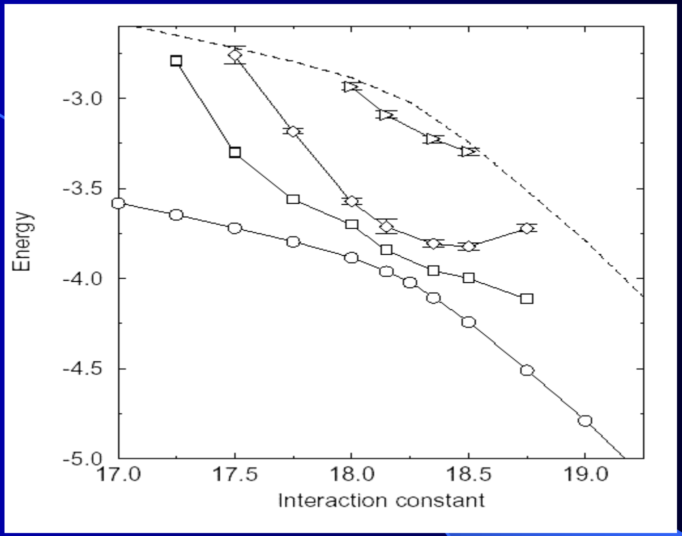
At larger couplings there is one broad peak with large weight and low energy peak with small weight

Dependence of peaks on interaction constants

t-J model



Rashba-Pekar exciton

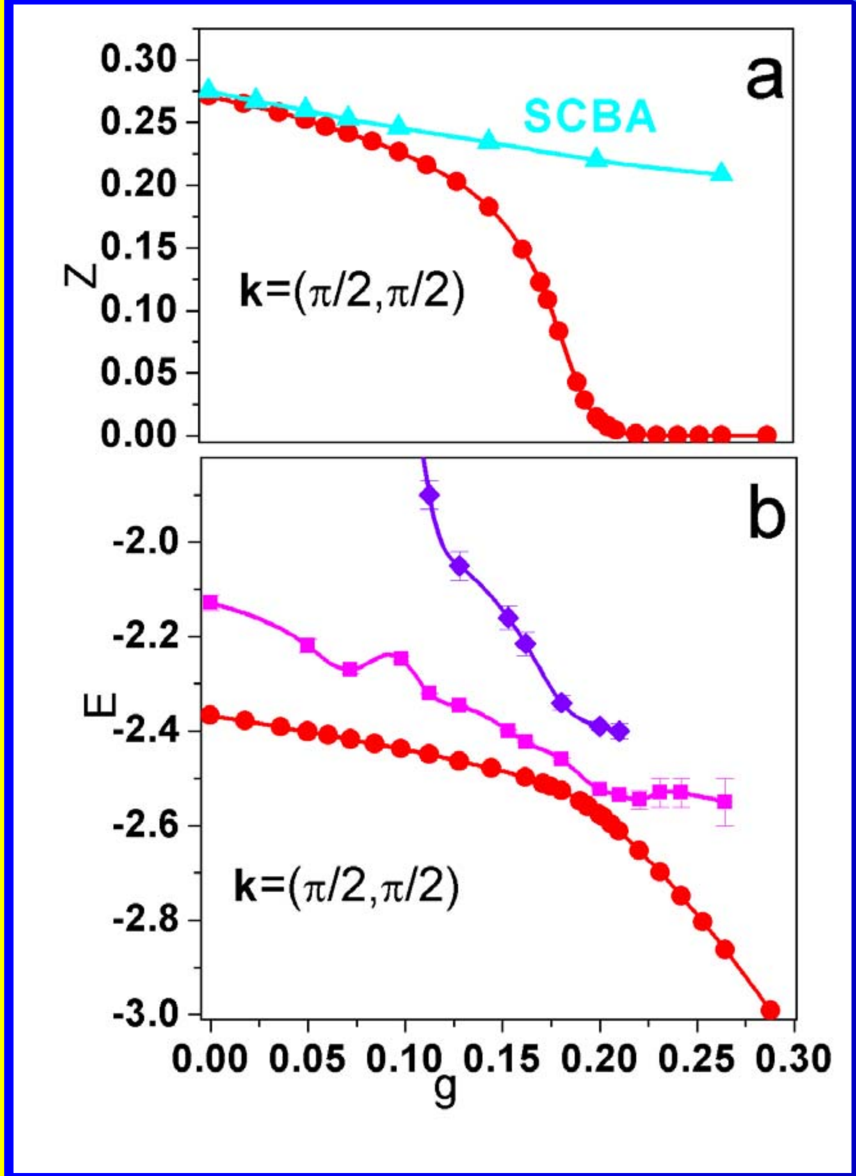


Self-trapping of Rashba-Pekar exciton.
A.S.Mishchenko, N.Nagaosa, N.V.Prokof'ev, A.Sakamoto and B.V.Svistunov, Phys.Rev.B, vol.66, 020301(R) (2002).

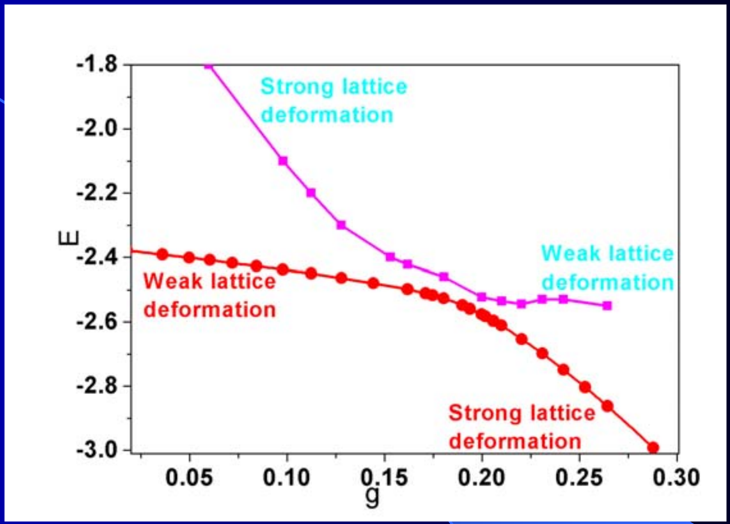
Dependence of the peak energies and ground state Z-factor on g resembles picture inherent in self-trapping phenomenon: the states cross and hybridize at g=0.2 and Z-factor of ground state rapidly decreases.

Dependence of peaks on interaction constants

t-J model



Standard picture of self-trapping



General features of the self-trapping

Small g: Ground state is weakly coupled while excited state is strongly coupled to lattice.

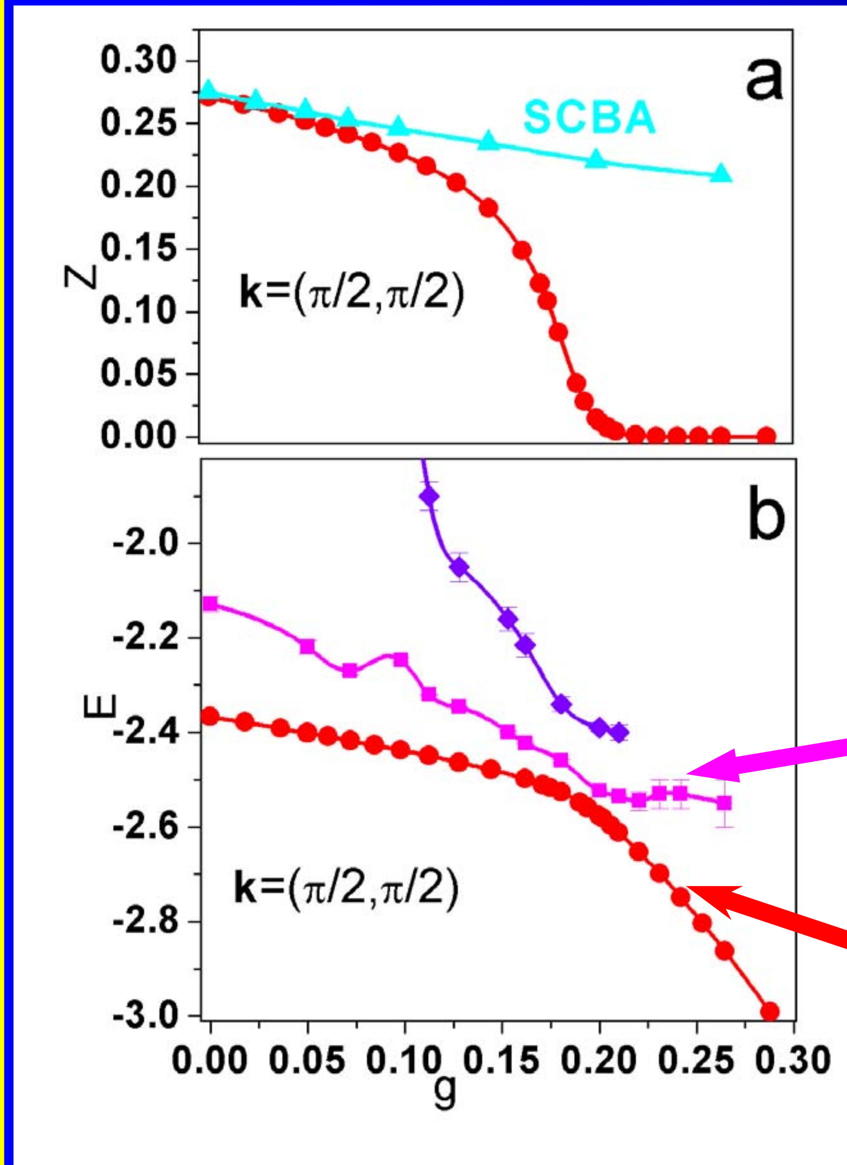
Critical g: Crossing and hybridization occurs

Large g: States exchange. Lowest state is trapped while excited state is weakly coupled to lattice

Yutaka Toyozawa

Dependence of peaks on interaction constants

t-J model



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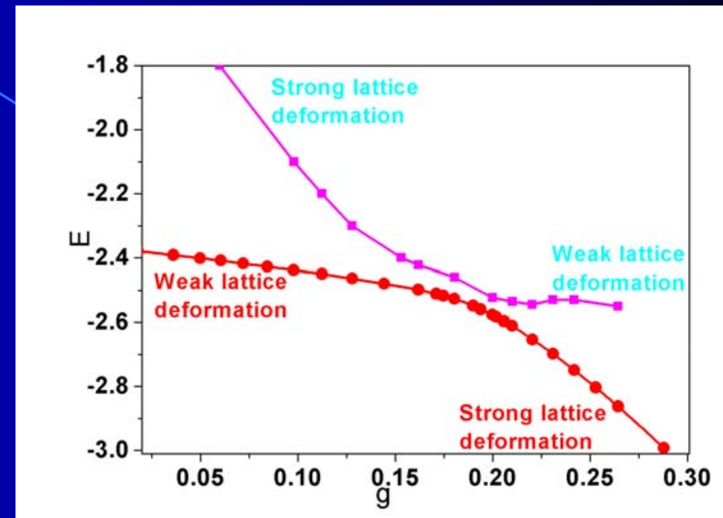
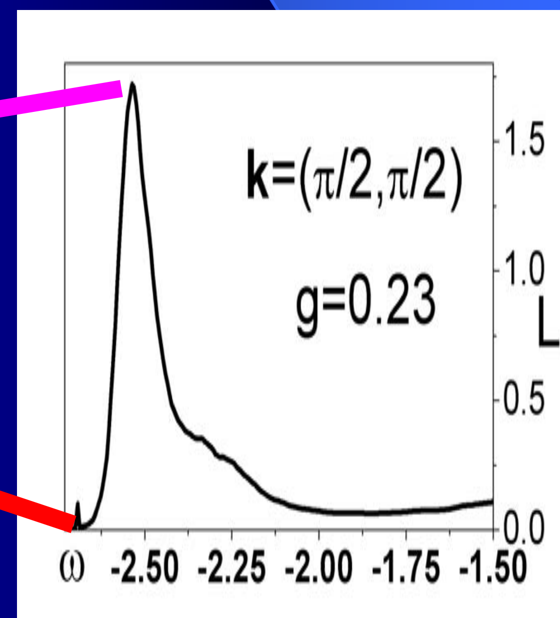


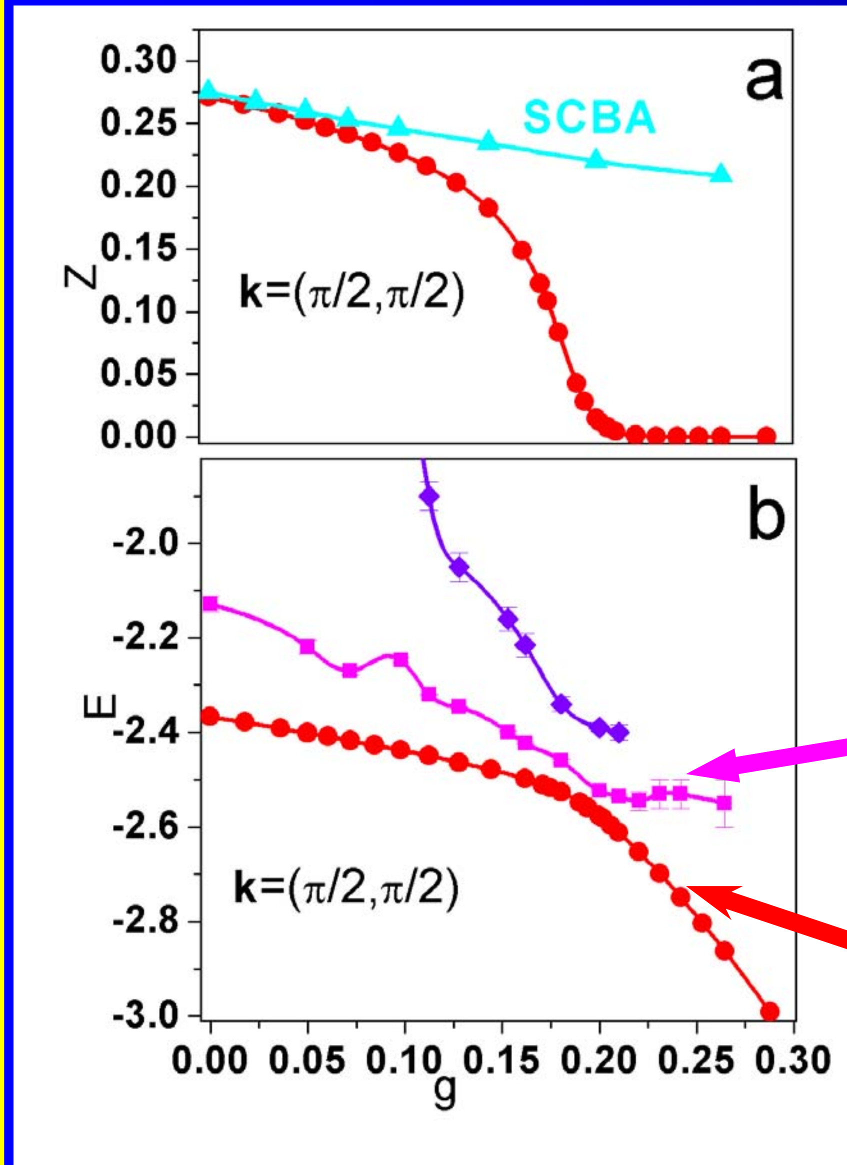
Weak lattice deformation

Strong lattice deformation



Dependence of peaks on interaction constants

t-J model



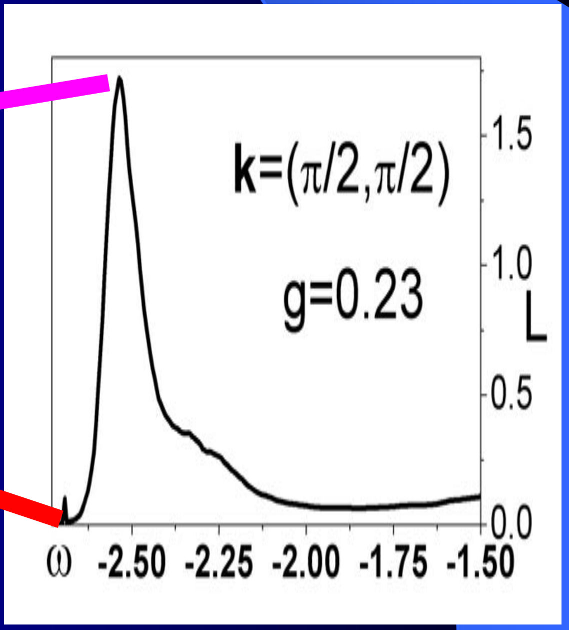
Guess for strong coupling regime:

"Invisible" ground state is momentum independent since it is a small polaron.

Broad peak has strong momentum dependence since this state is weakly coupled to lattice.

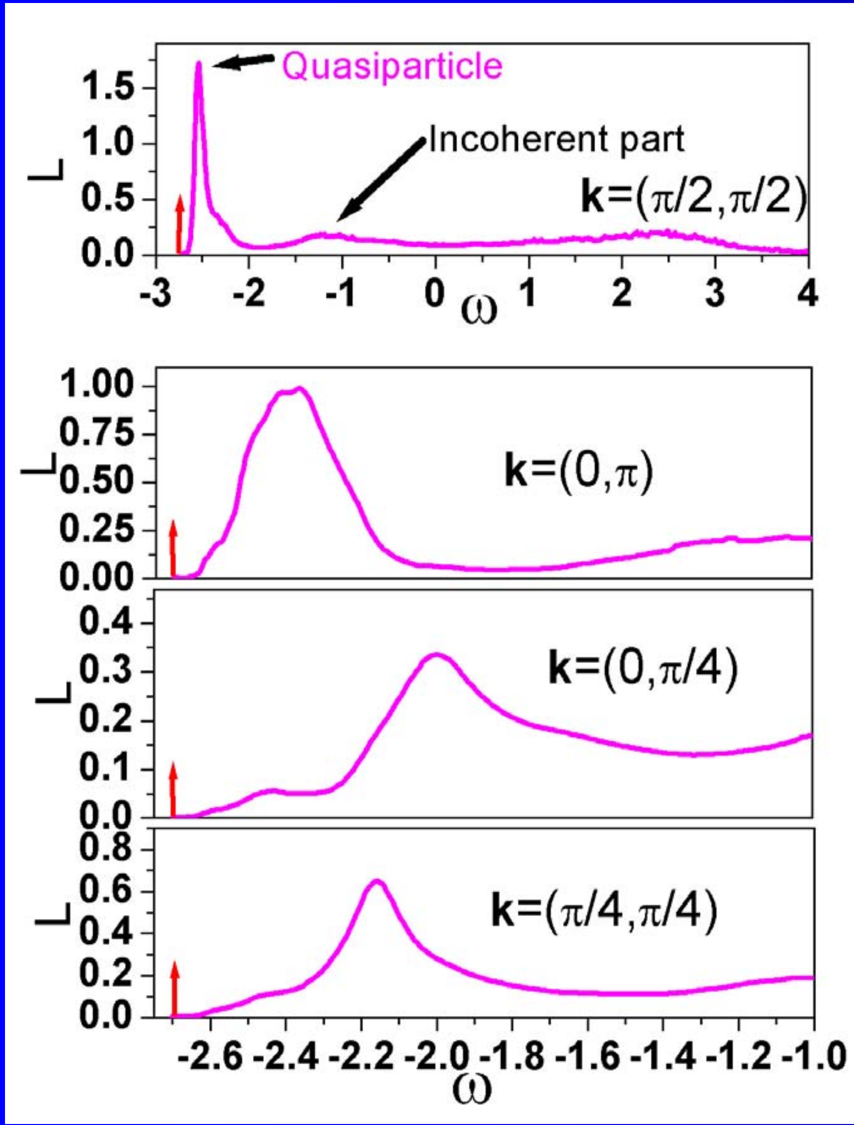
Weak lattice deformation

Strong lattice deformation



Dispersion of the broad peak in strong coupling regime

g=0.23



Guess is confirmed!!!!!

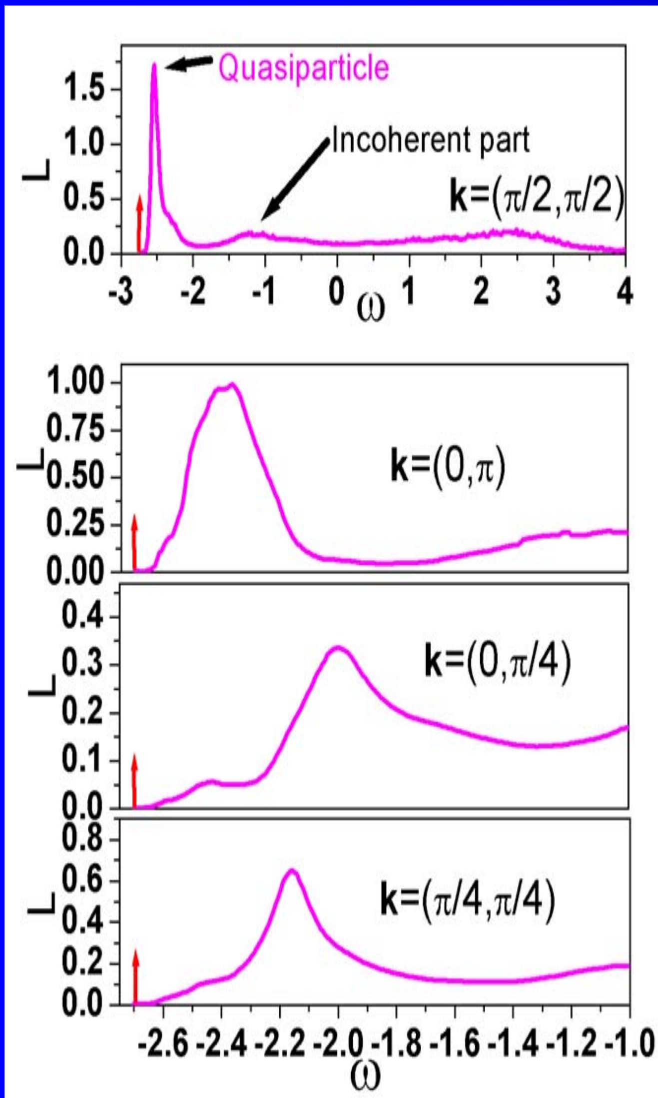
Ground state peak with small weight has no dispersion

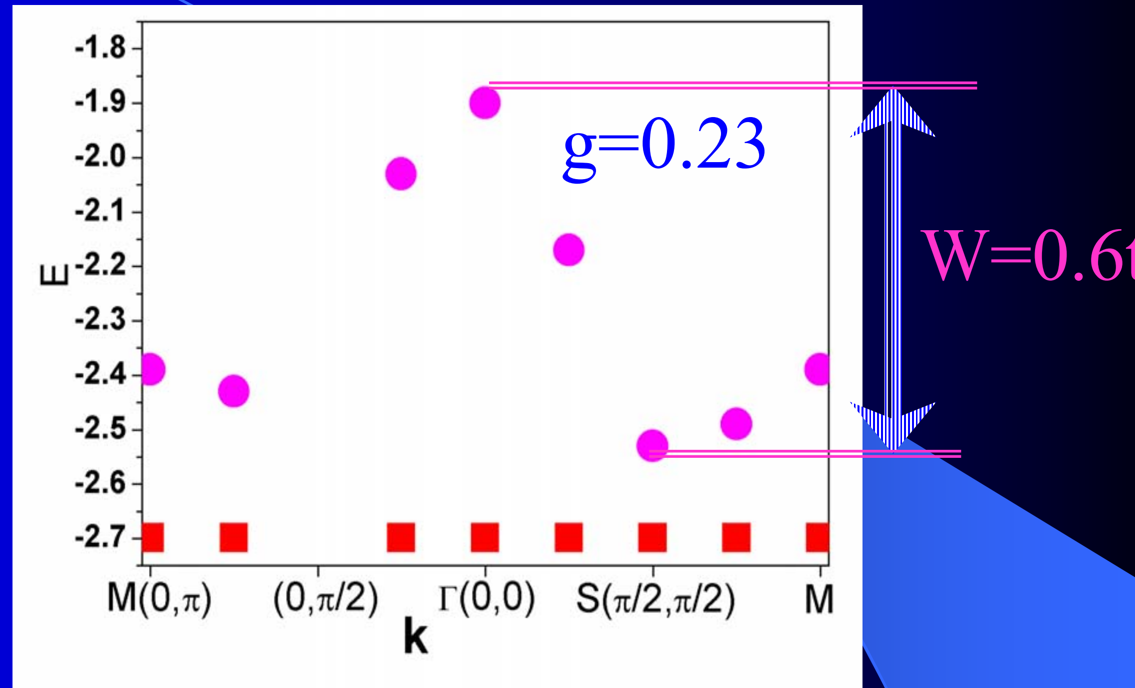
Broad peak with large weight demonstrates considerable dispersion.

<u>Surprise</u>: the bandwidth of broad peak dispersion is the same as it is in pure t-J model

Dispersion of the broad peak in strong coupling regime

g=0.23





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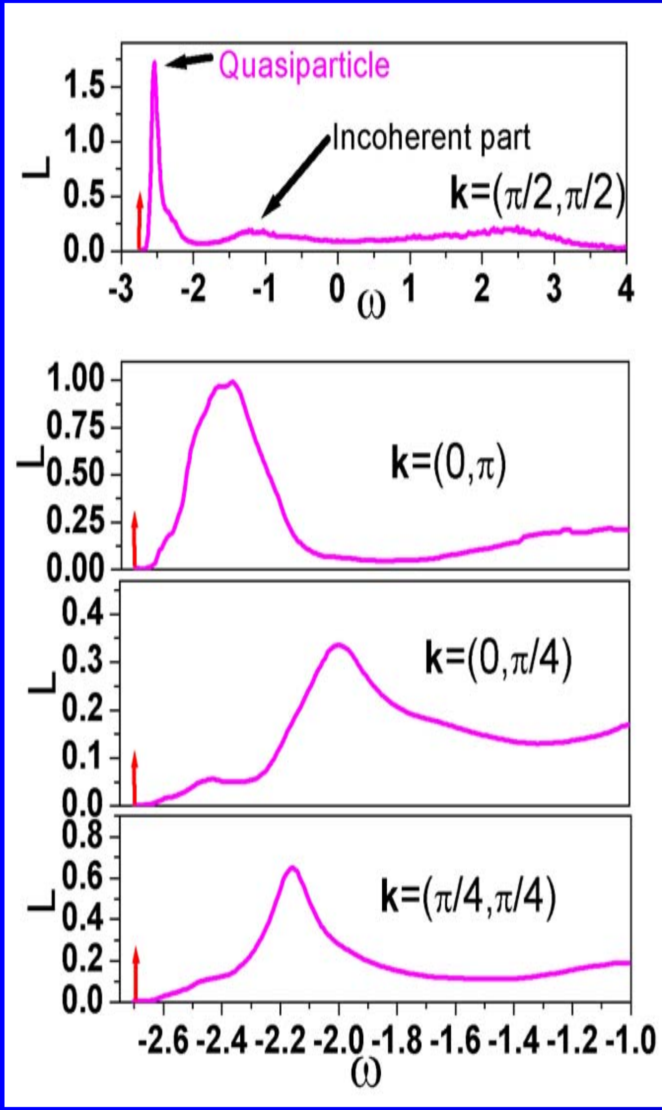
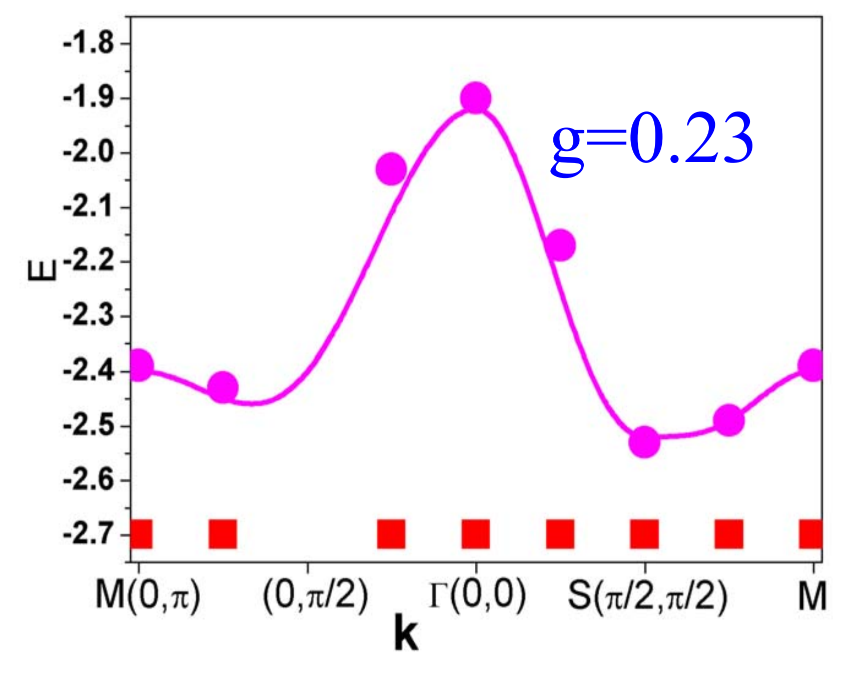
Dispersion of the broad peak in strong coupling regime

g=0.23

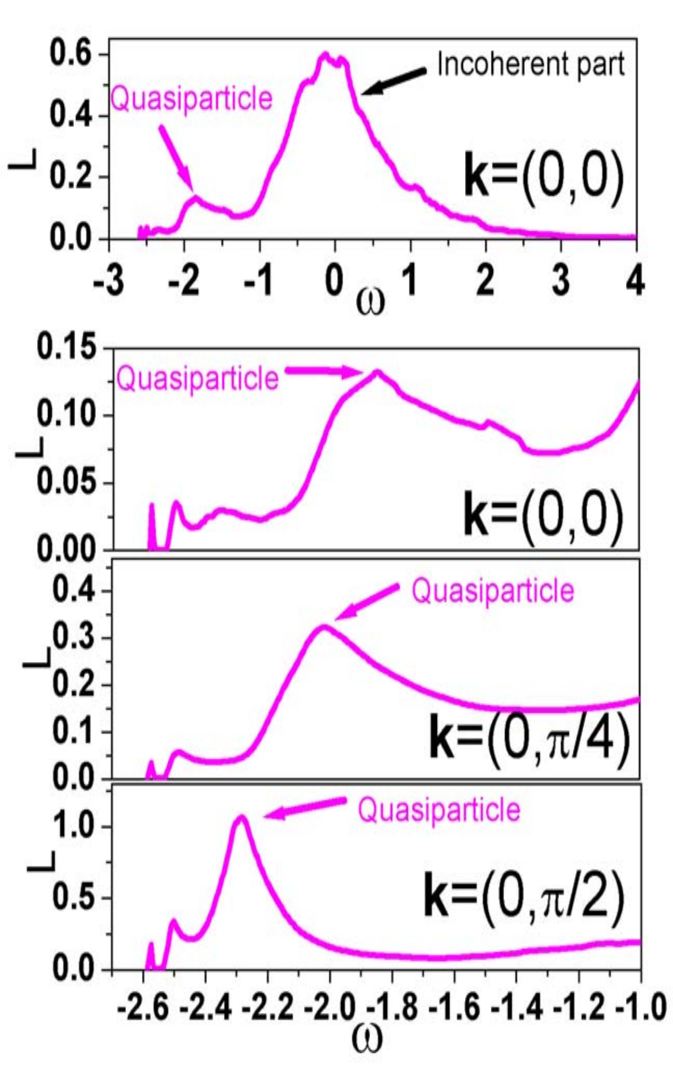


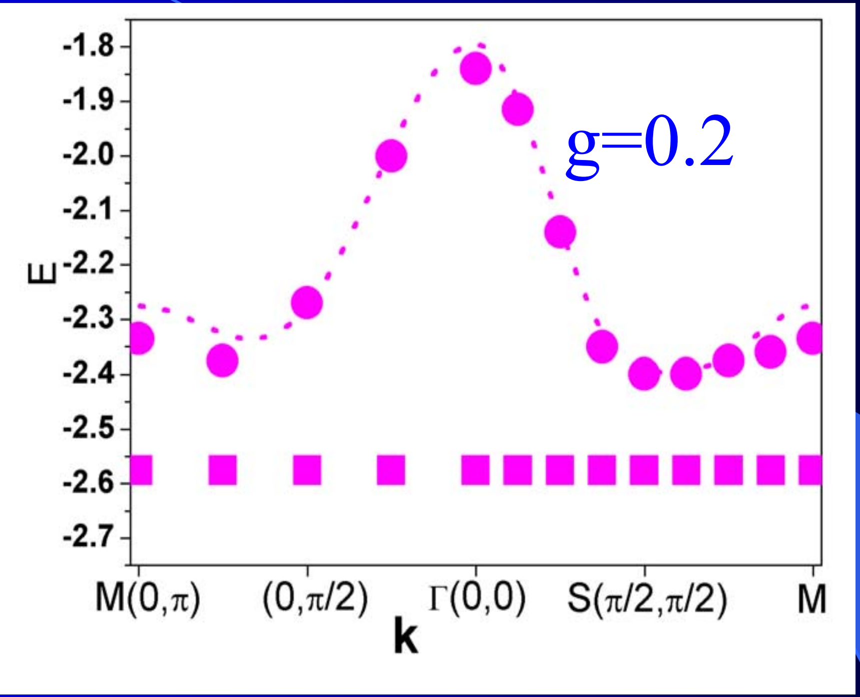


Great surprise: the dispersion of broad peak is *exactly* the same as that of pure t-J model.

Dispersion of the broad peak in strong coupling regime

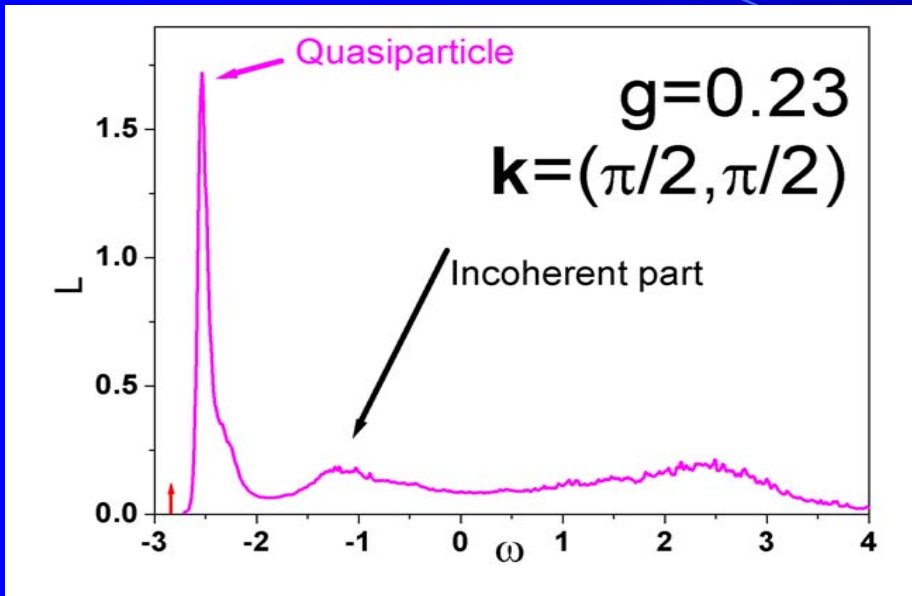
g=0.2

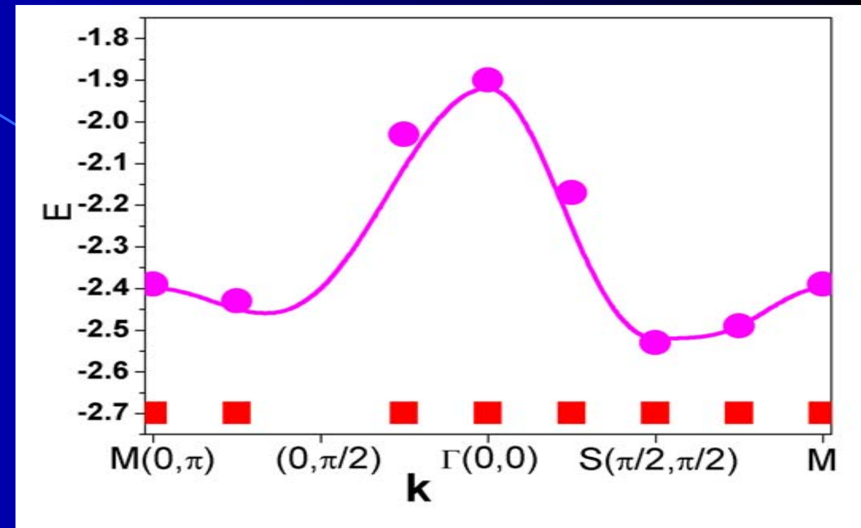


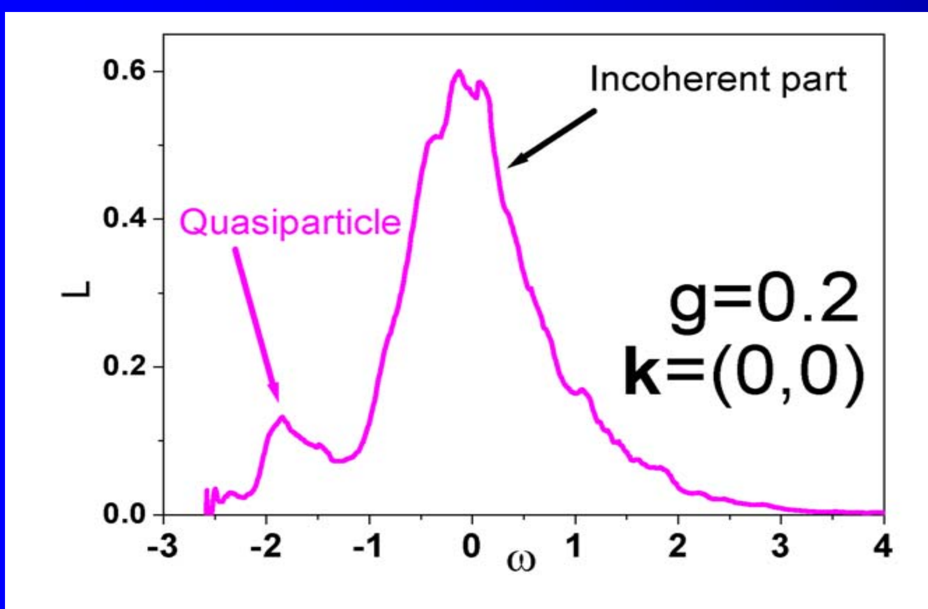


Similar dispersion of broad peak in strong coupling regime and that of pure t-J model is the general feature of strong coupling regime

Theoretical predictions are consistent with experiment



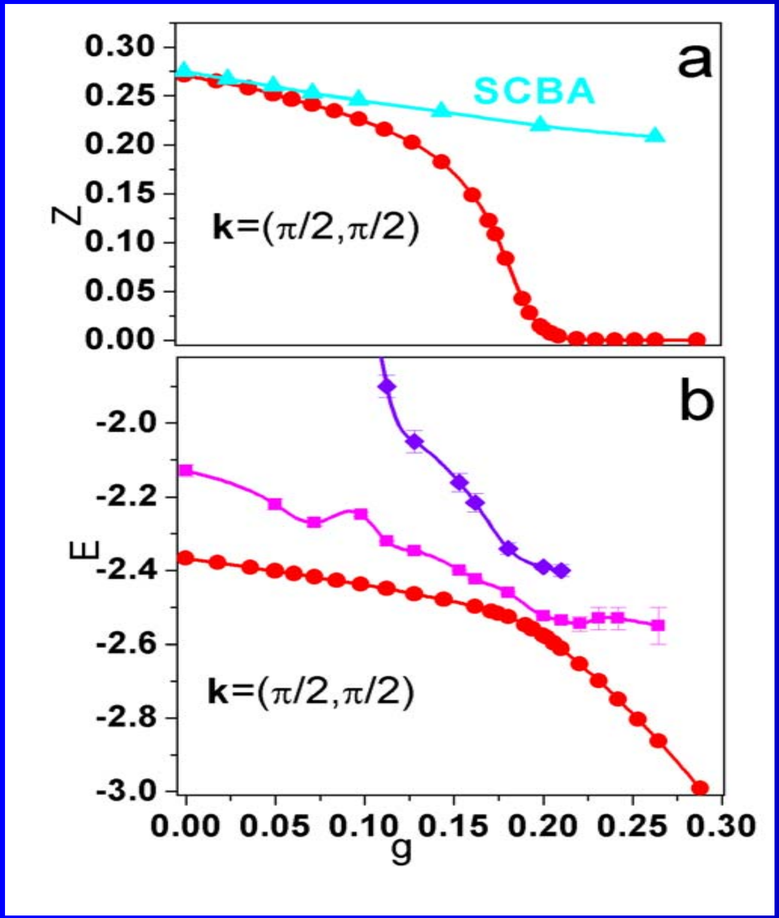




1. Broad quasiparticle has dispersion like in pure t-J model.
2. Weights of broad peaks are the same as in pure t-J model .
3. Nondispersive peak of ground state has small weight and can not be seen in ARPES.

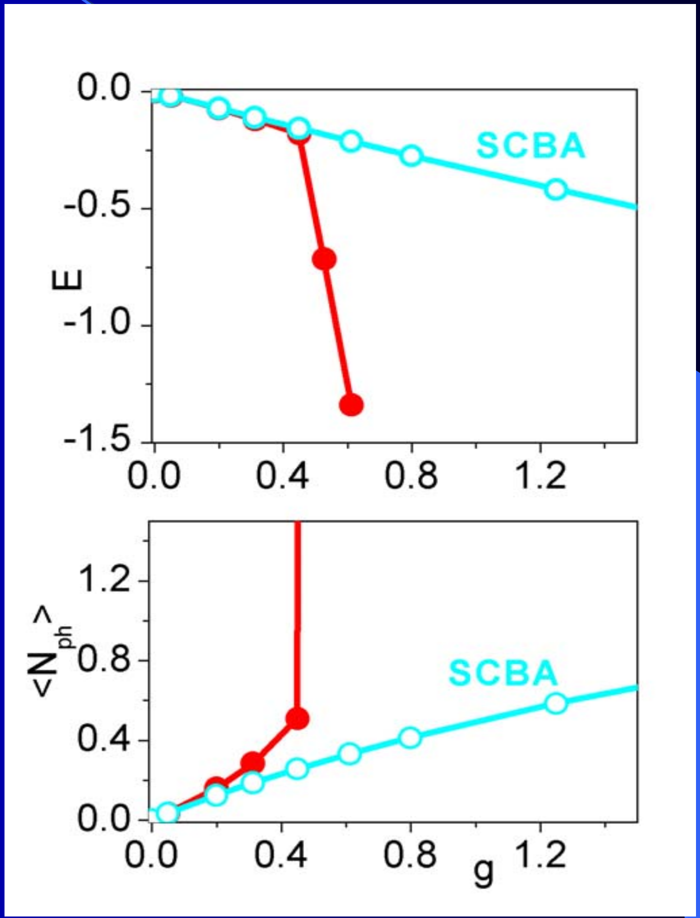
Interaction with spins enhances e-ph coupling: polaron in t-J model undergoes crossover to strong coupling regime at smaller couplings than free polaron with the same parameters.

Polaron in t-J model



Critical coupling: g=0.2

Free polaron



Critical coupling: g=0.5

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Hole with dispersion ε(k) in magnon and phonon bathes

$$H^{(0)}_{tt't''-J} = \Sigma_k \varepsilon(k)\, h_k^+ h_k + \Sigma_k \upsilon(k)\, \alpha_k^+ \alpha_k + \Sigma_k \omega_{ph}\, b_k^+ b_k$$

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Scattering on phonons: $H_{h-ph} = N^{-1} \Sigma_{k,q} \gamma [h_k^+ h_{k-q} b_q + h.c.]$

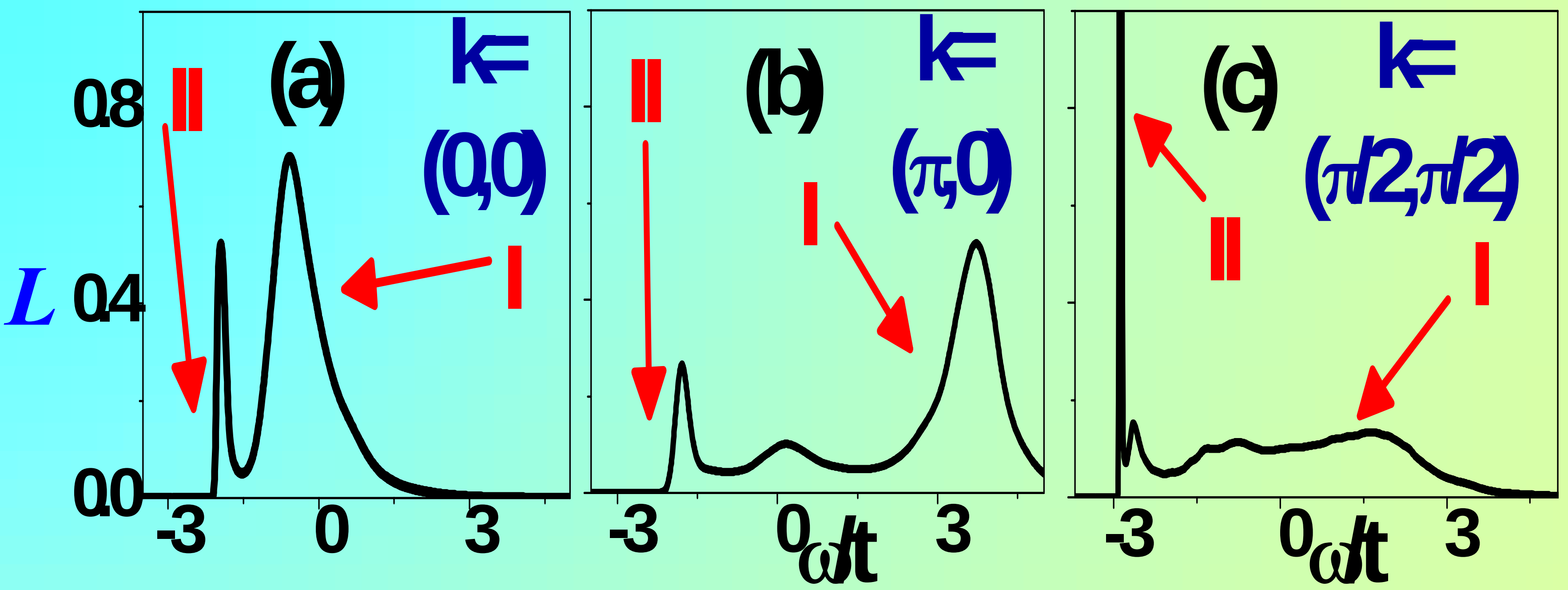
Dimensionless EPI constants:

$$\lambda=\gamma^2/4t\omega_{ph}$$

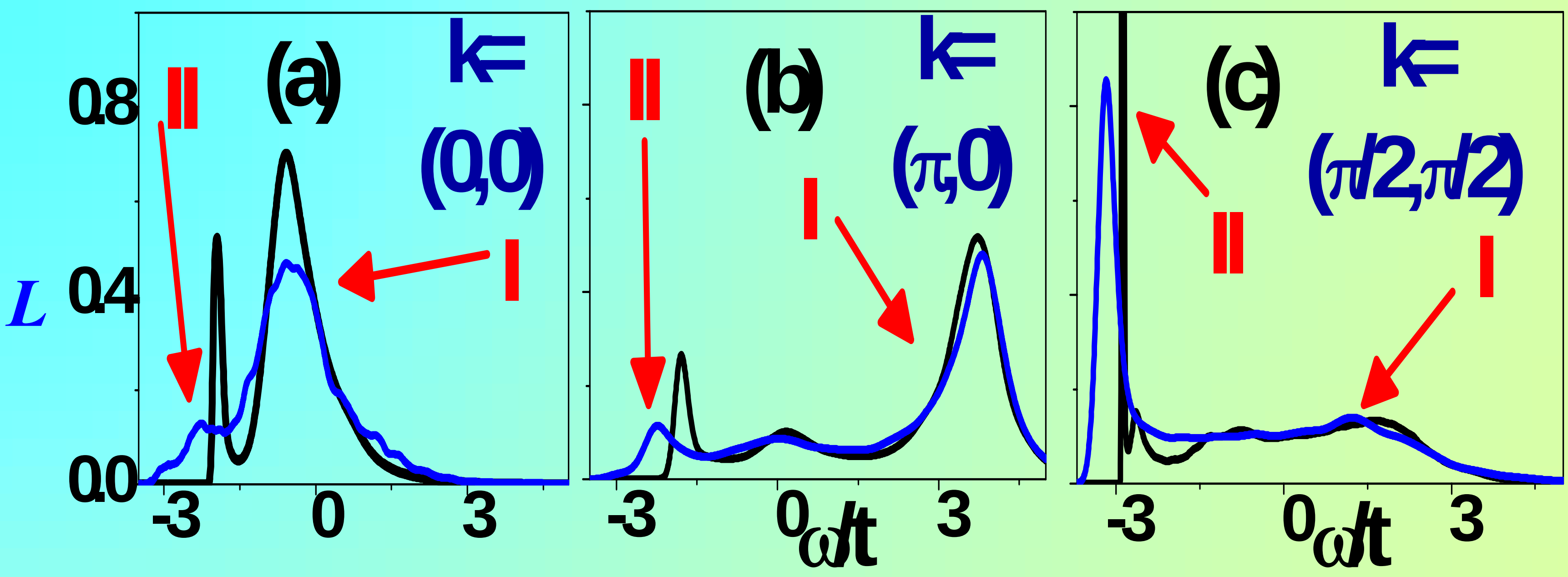
$$\lambda=2g$$

$$g=\gamma^2/8t\omega_{ph}$$

Lehman function of tt’t’’-J model without electron-phonon interaction

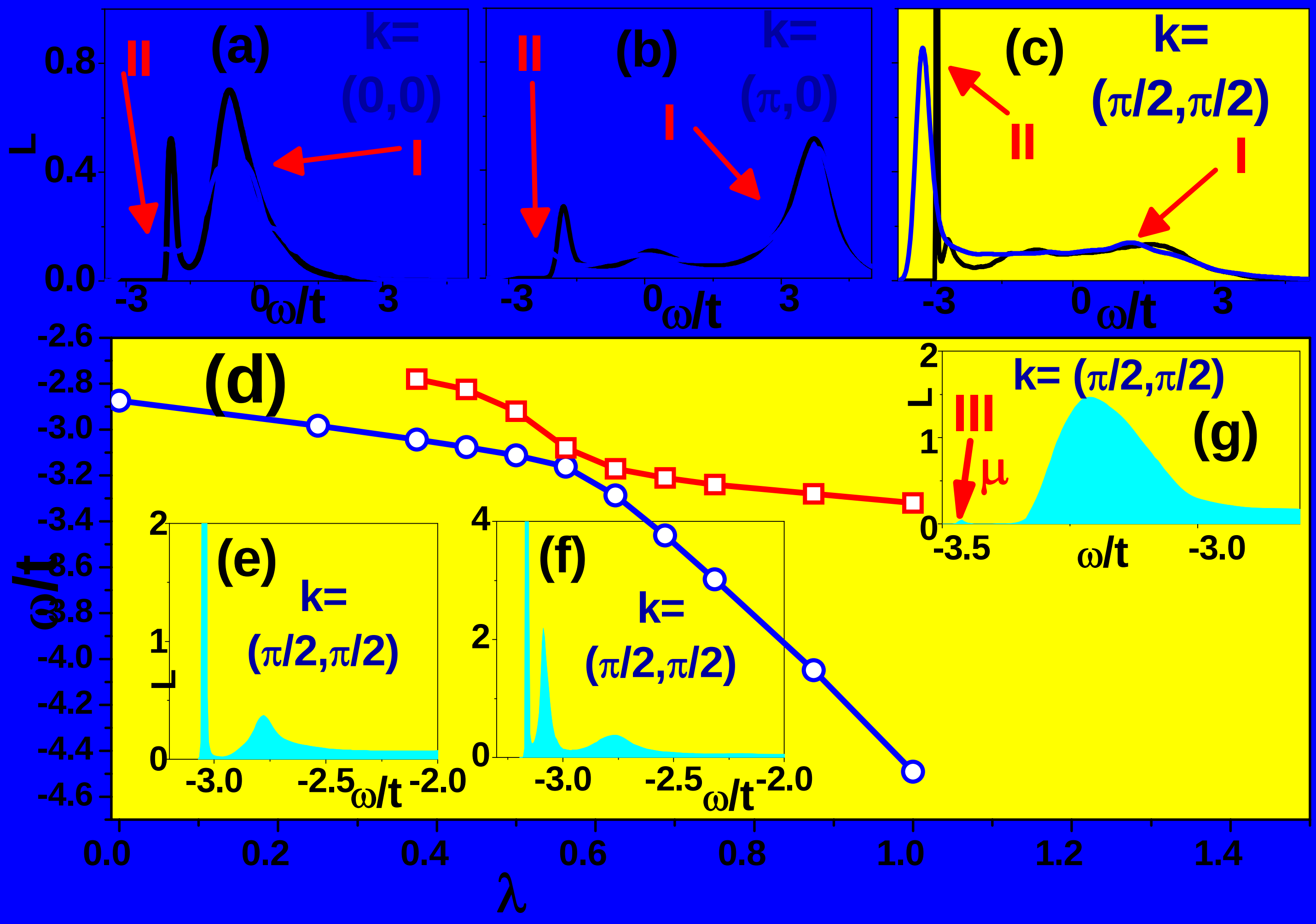


Lehman function of tt't''-J model with strong EPI: λ=0.7

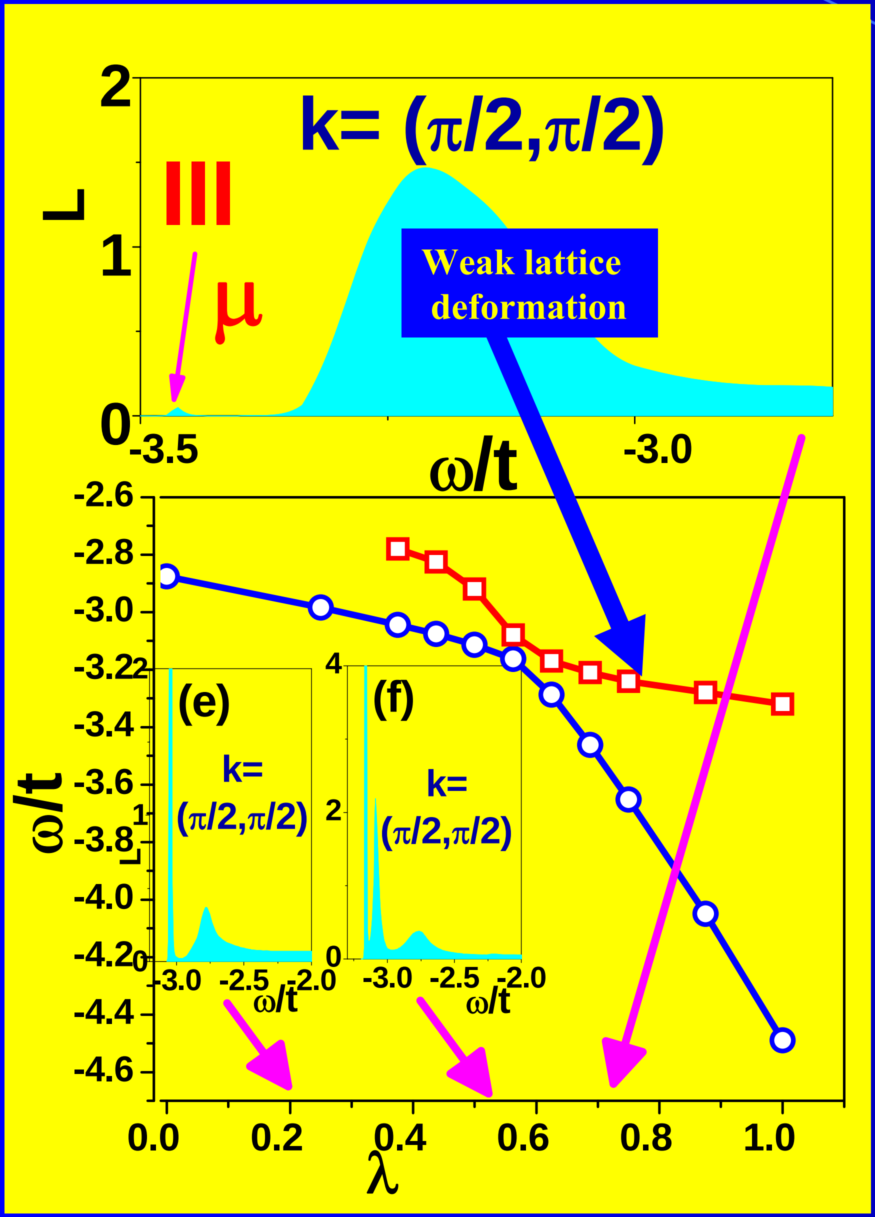


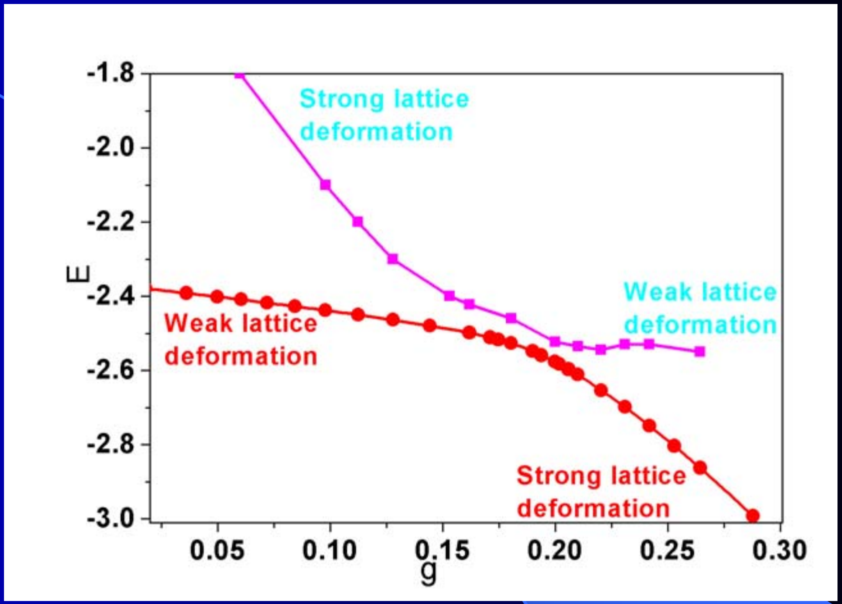
Only low energy part, related to t-J model scale, is altered.

Evolution of the low energy part of the spectrum



Self-trapping in the tt't"-J model





General features of the self-trapping

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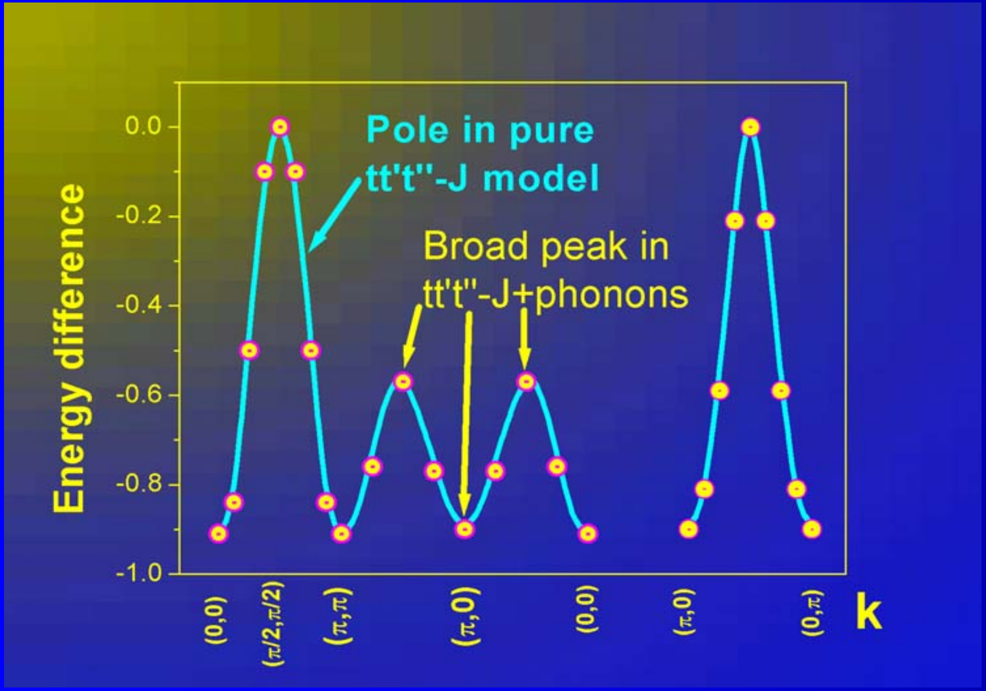
Critical λ: crossing and hybridization occurs

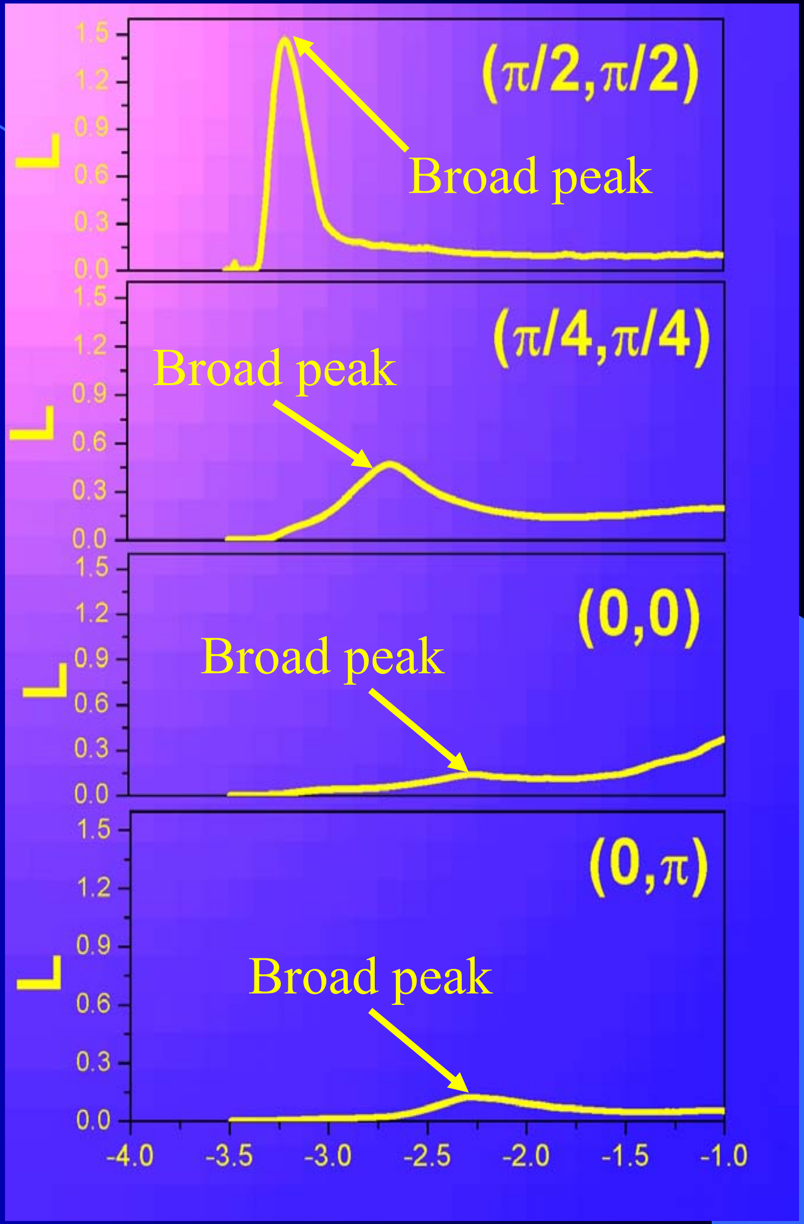
Large λ: States exchange. Lowest state is trapped while excited state is weakly coupled to lattice

Hole in tt’t”-J model strongly interacting with phonons

Broad peak **exactly** reproduces dispersion of tt’t”-J model (shifted by constant energy)

Hence, dispersion of broad peak reproduces experimental one





Hole in tt’t”-J model strongly interacting with phonons

t=1, J=0.4, t’=-0.34, t”=0.23

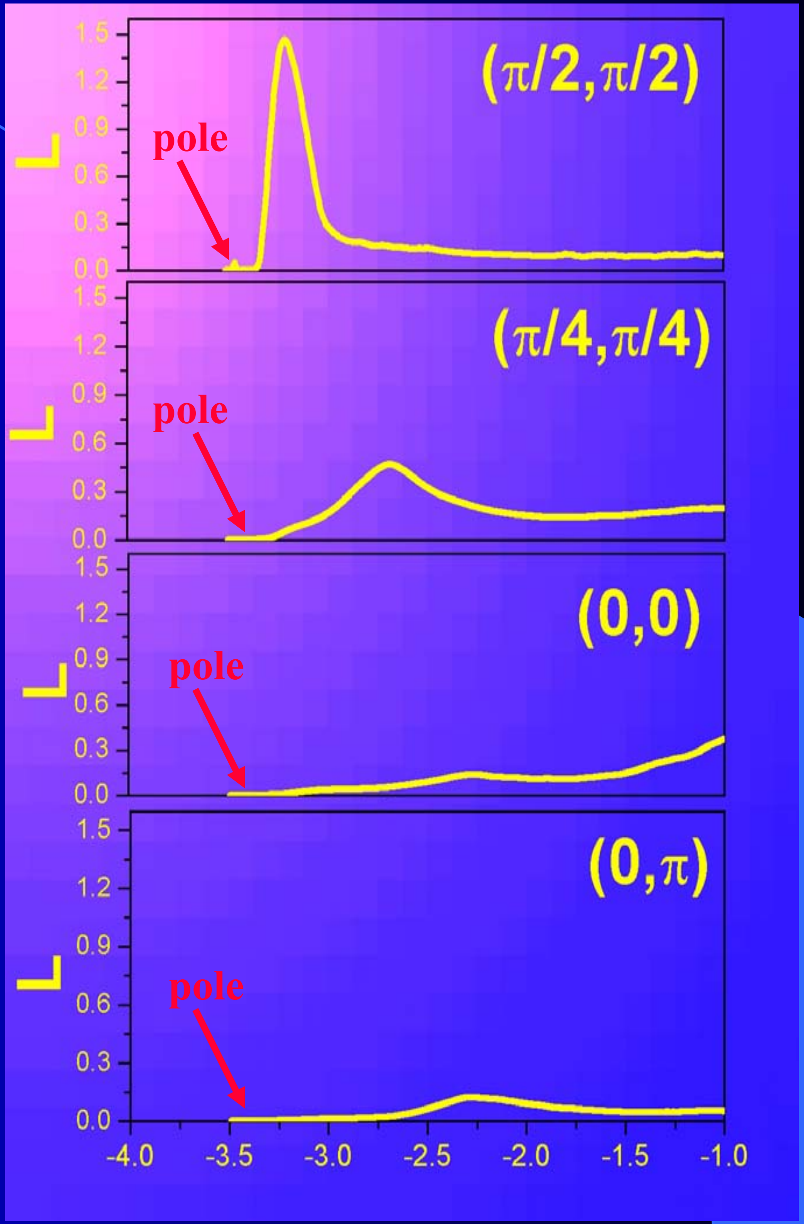
Interaction: λ=0.7

Ω_{ph}=0.2

Polaron pole with negligibly small Z-factor has no dispersion.

Though, the chemical potential is pinned by it.

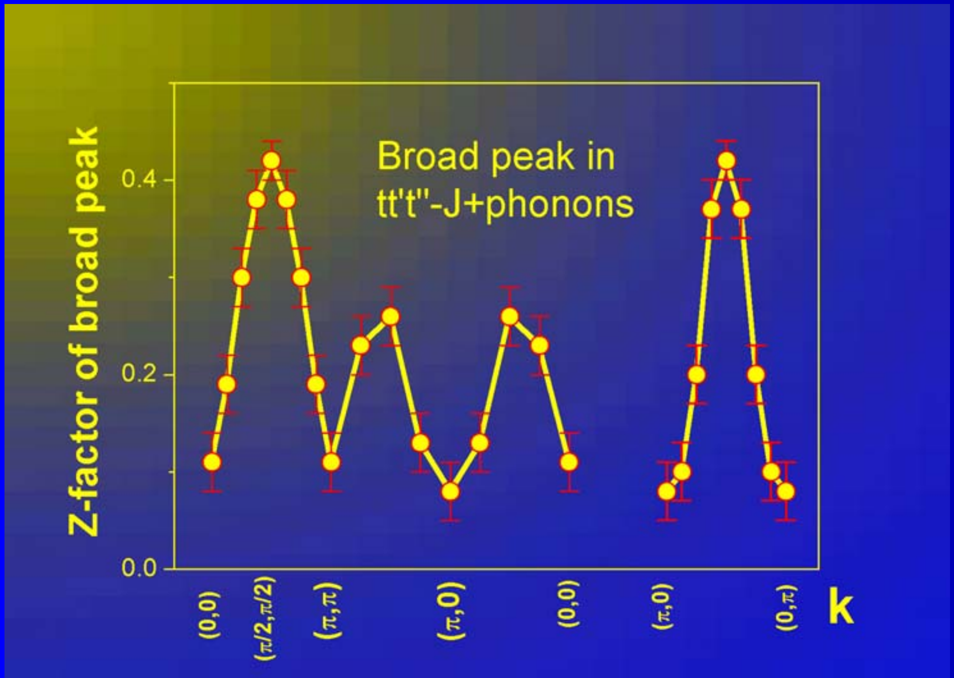
Confirmed by K.M.Shen et.al., PRL (2004)

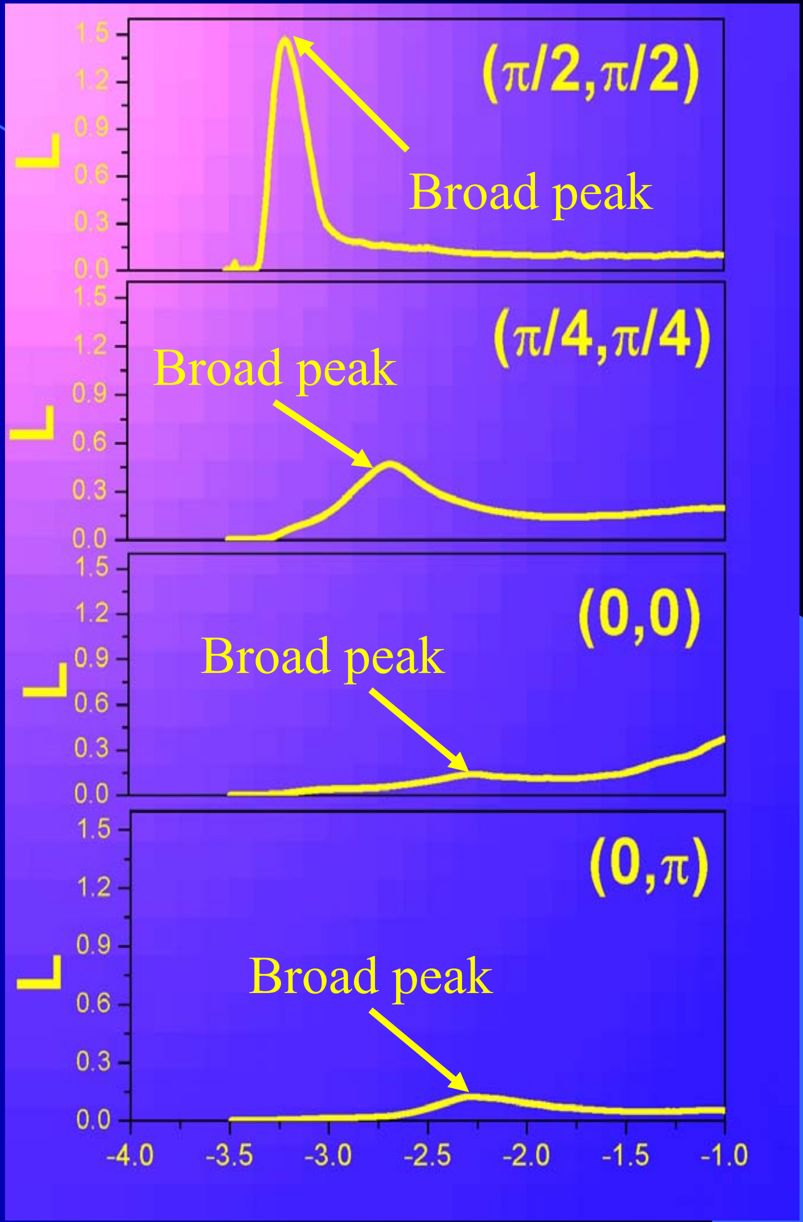


Hole in tt’t”-J model strongly interacting with phonons

In accordance with experimental observations (B.O.Wells et.al. PRL, Vol. 74, p. 964 (1995)) $Sr_2CuO_2Cl_2$

weight of broad peak decreases when momentum approaches points (0,0) and (π,0)

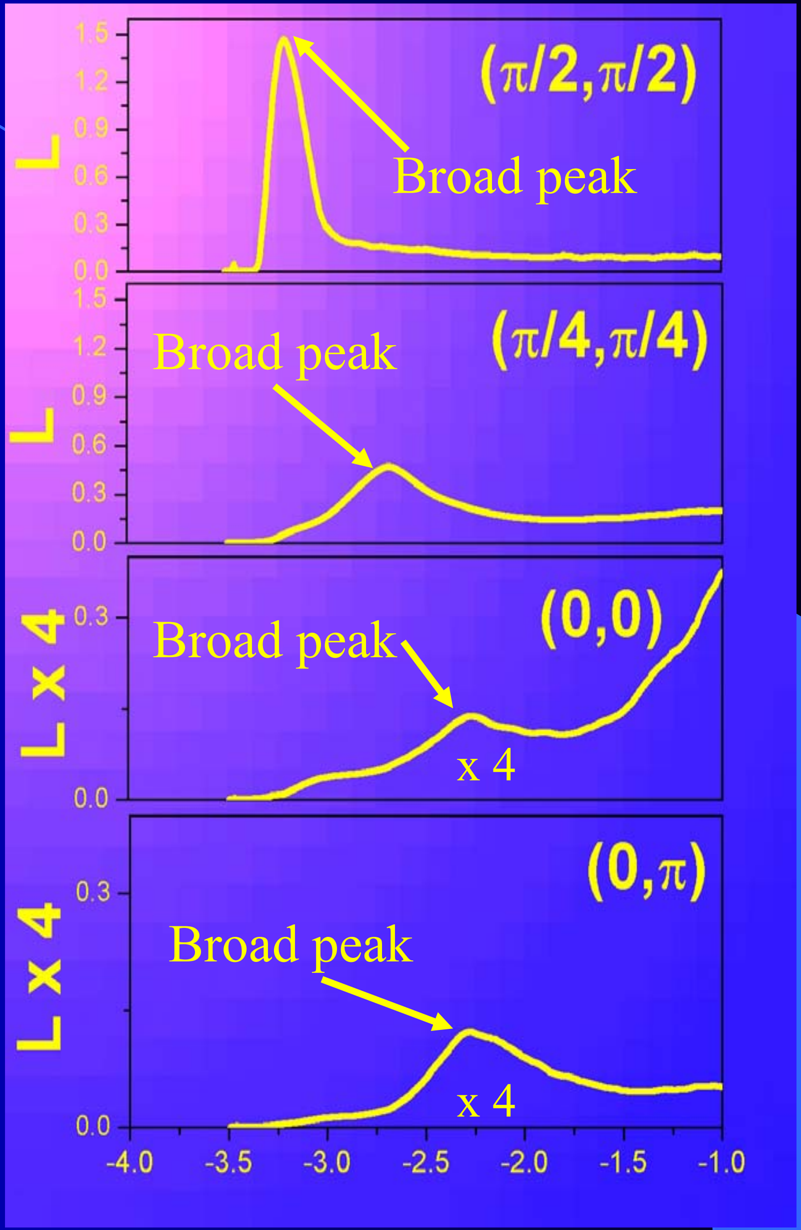




Hole in tt’t”-J model strongly interacting with phonons

In accordance with experimental observations (B.O.Wells et.al. PRL, Vol. 74, p. 964 (1995)) $Sr_2CuO_2Cl_2$

width of broad peak considerably increases when momentum approaches points (0,0) and (π,0)

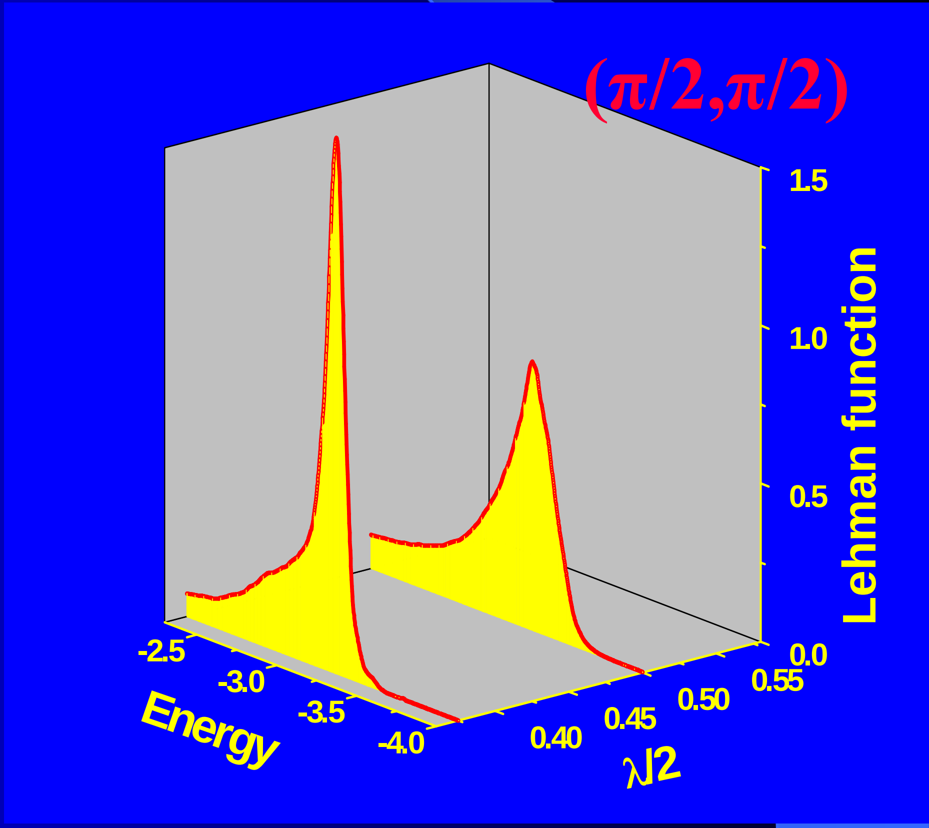


UNIVERSALITY

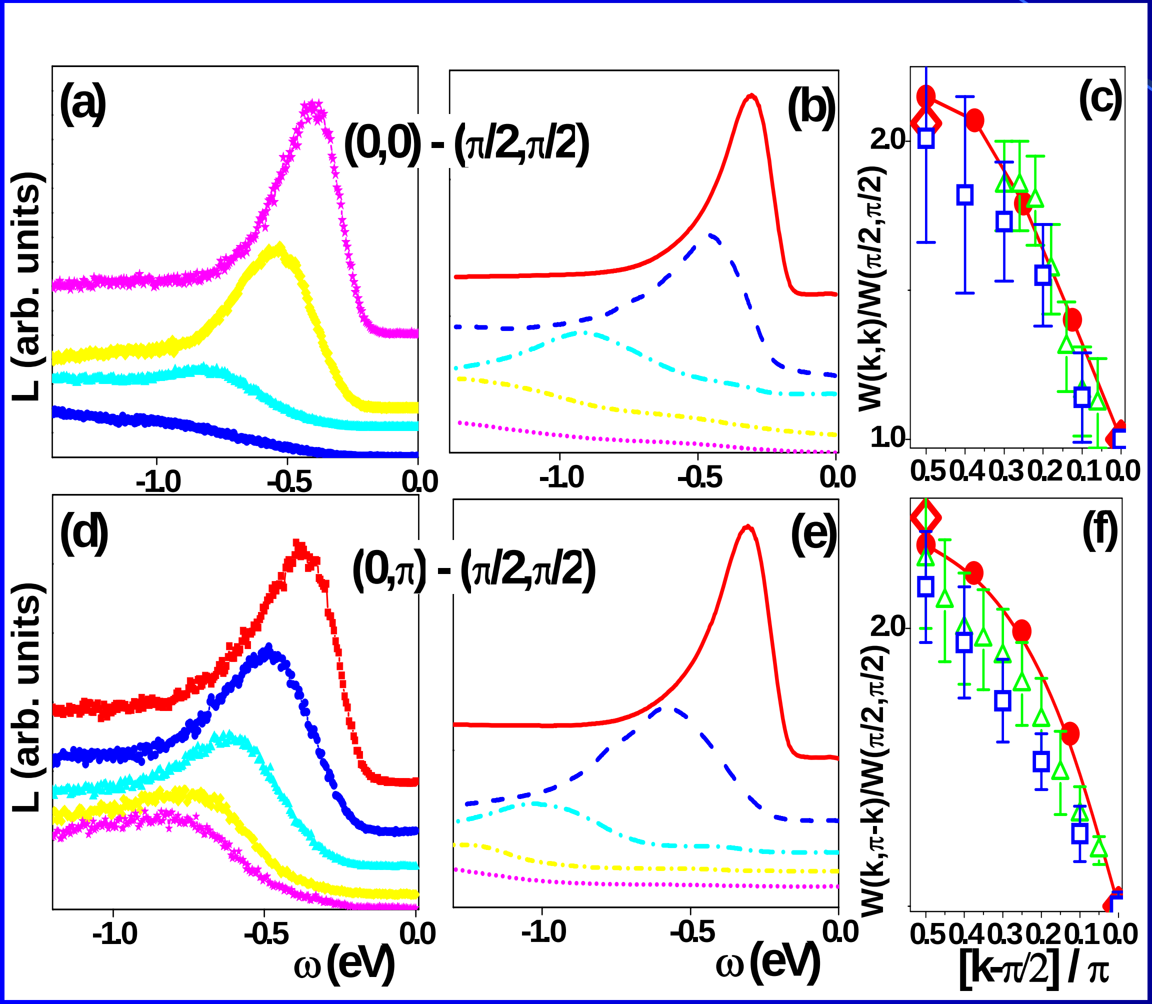
Linewdidth ratio W(x,x)/W(π/2,π/2)
exactly reproduces experiment

Linewidth at (π/2,π/2) depends on the coupling constant g in theory

Linewidth at (π/2,π/2) depends on the compound in experiment



Linewidth ratio W(x,x)/W(π/2,π/2) exactly reproduces experiment

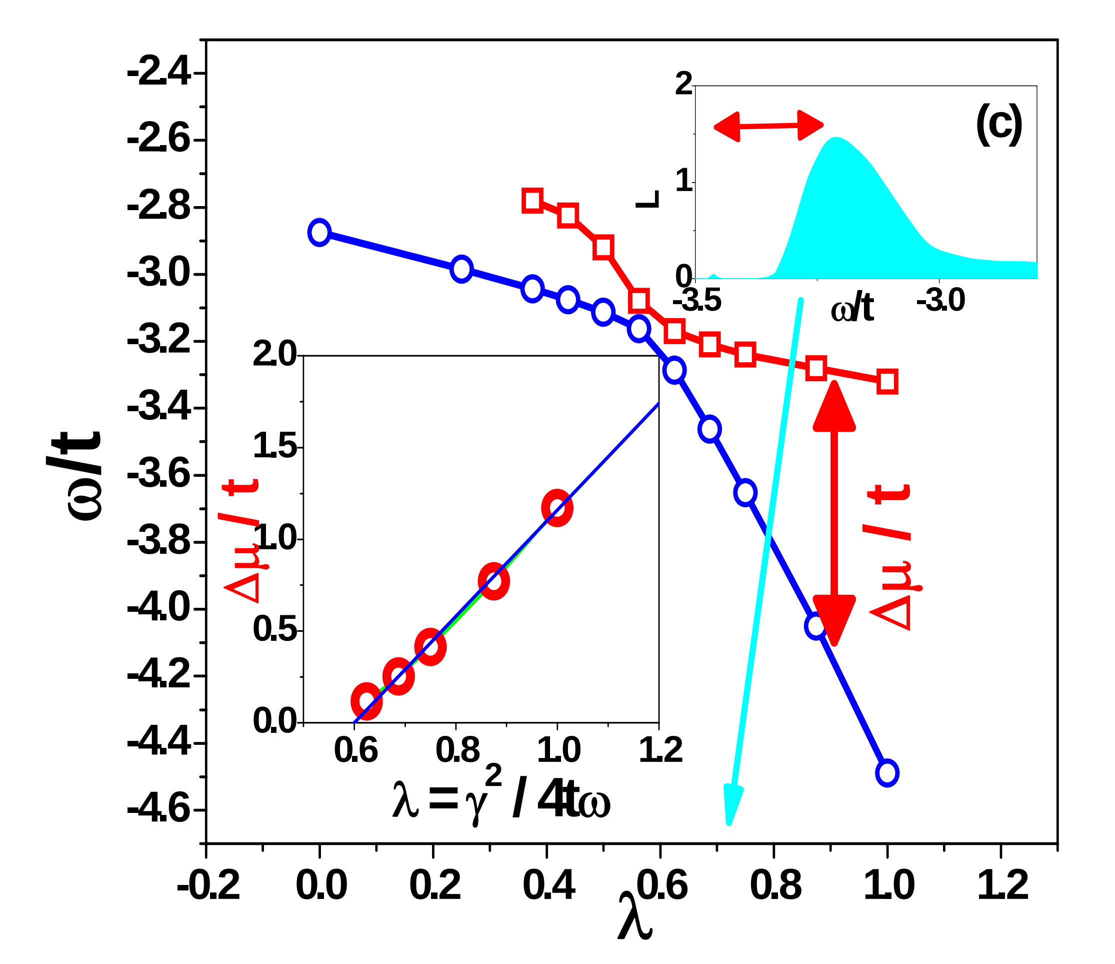


The ratio
W(x,x) / W(π/2,π/2)
is universal
in theory
for any g in
strong coupling regime
(g=0.35,0.5)
and universal
in experiment
for different
compounds
$(Sr,Ca)_2CuO_2Cl_2$

Scaling of the distance of Franc-Condon shake off peak from polaron pole (or μ)

$\Delta\mu/t = 2.9\,(\lambda - \lambda_c)$

$\lambda_c = 0.58$



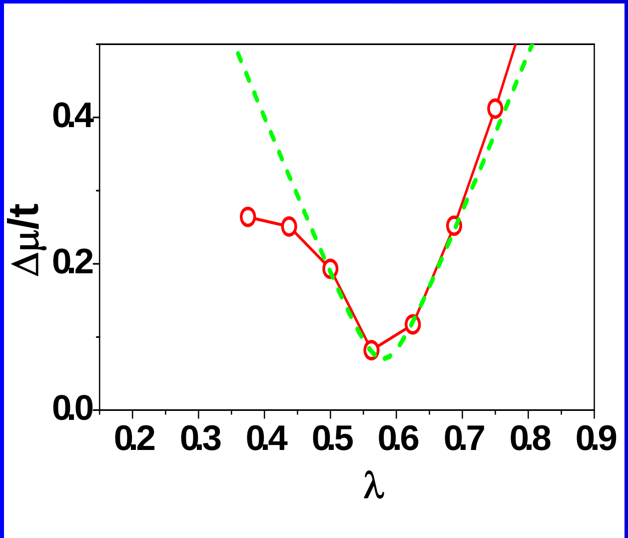
Doping dependence of the coupling strength in $Ca_{2-x}Na_xCuO_2Cl_2$

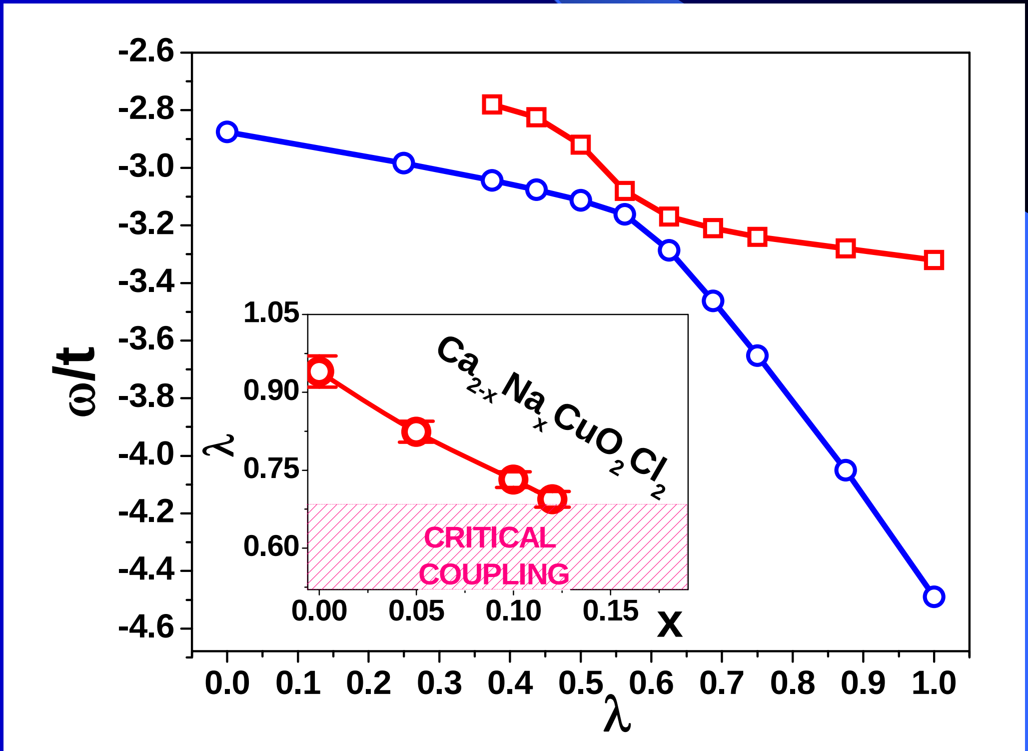
Close to $\lambda_c = 0.58$ energy difference can be fitted as hybridization law

Theoretical results Compared with experiment K.M.Shen et.al PRL(2004)

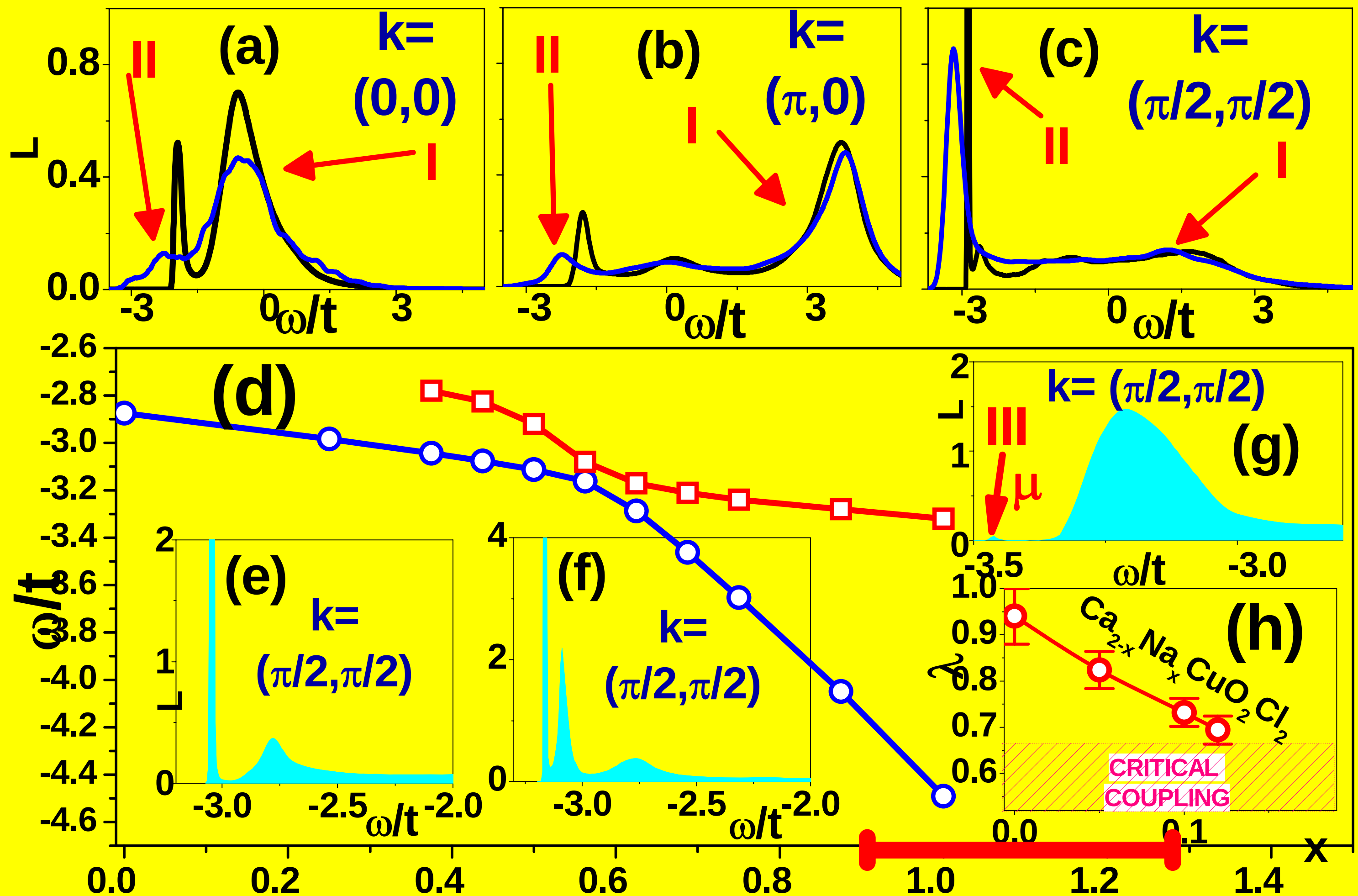
$$\Delta\mu/t = [a(\lambda-\lambda_c)^2+v^2]^{1/2}$$

For α=4.8, ν=0.07





Summary for compounds in strong-coupling regime



Undoped

compounds: LSCO, SCOC, CCOC

Polaron physics in tt'tʺ-J model in weak and intermediate regime

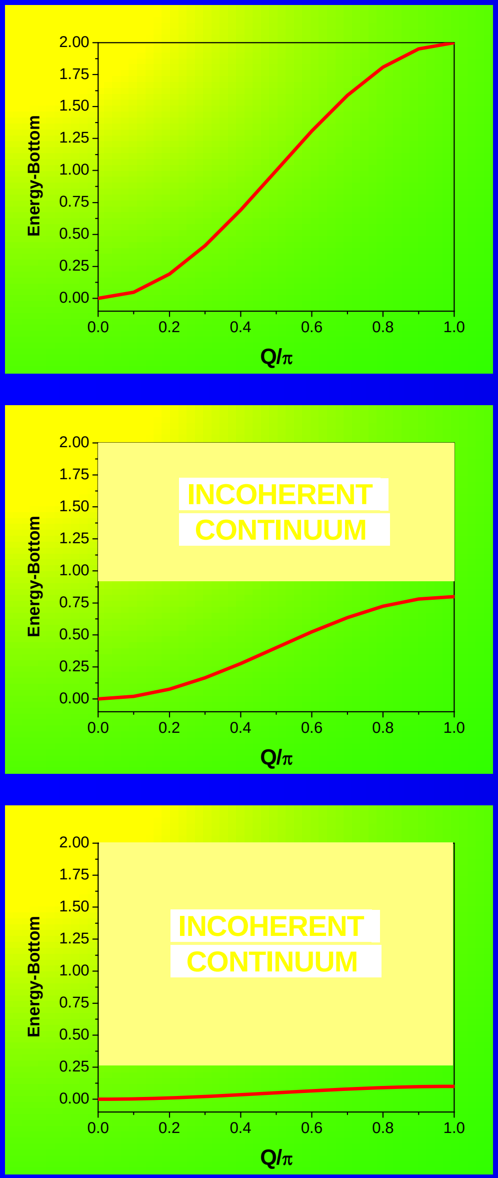
1. Different pictures which we imagine when hear "a polaron formation".

2. How "polaron formation" is seen with high and low resolution in ARPES.

3. What we see when phonon branch is crossed by quasiparticle with high and low resolution.

4. Dependence of λ on the doping in LSCO

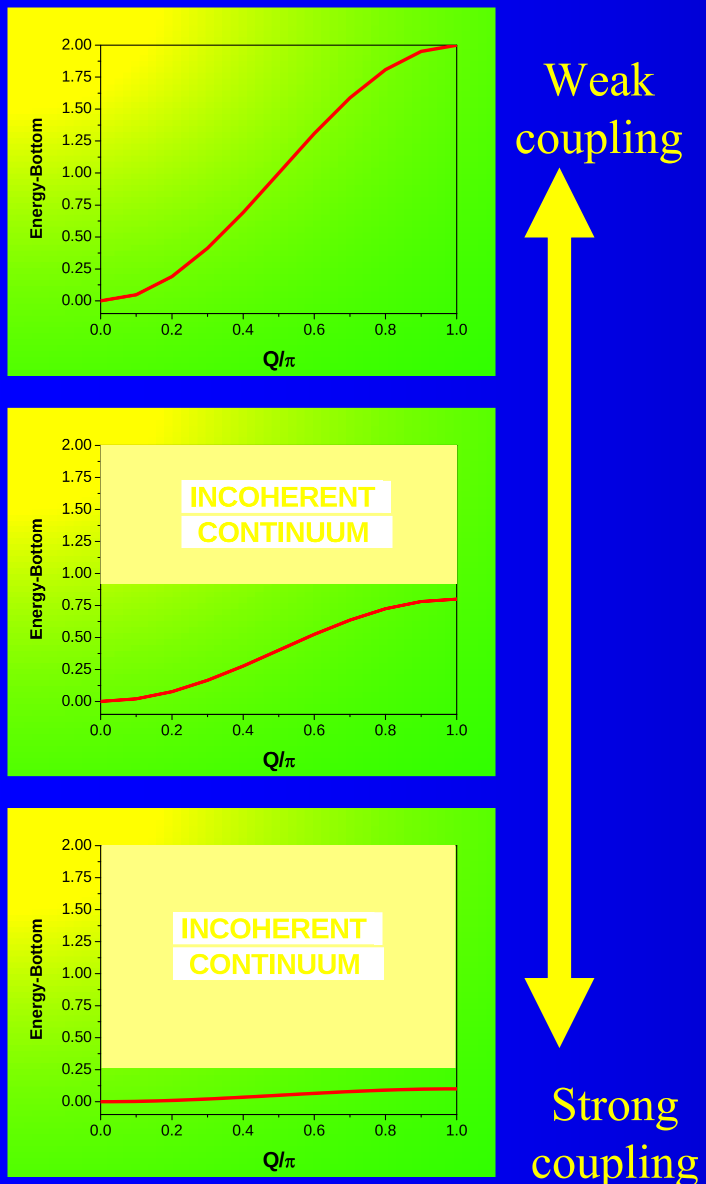
Traditional images of narrow polaron band formation

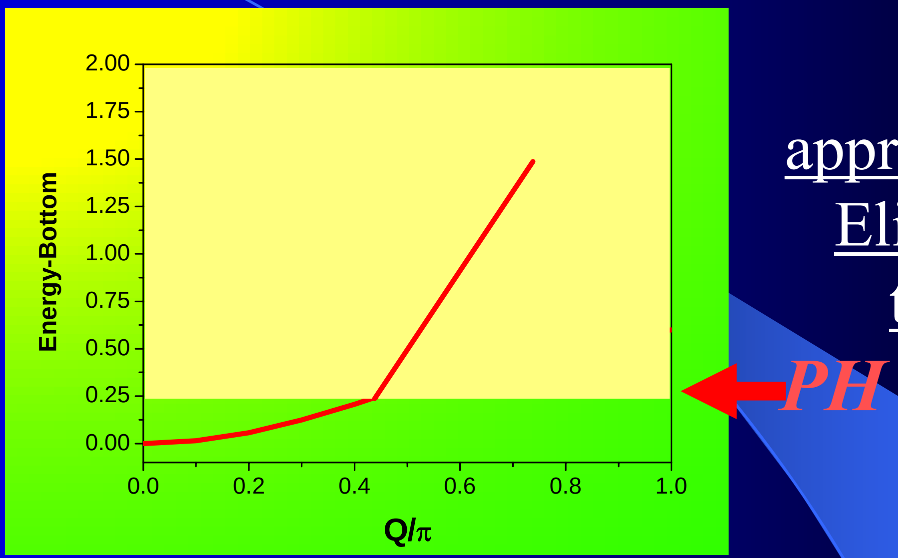


Weak coupling

Strong coupling

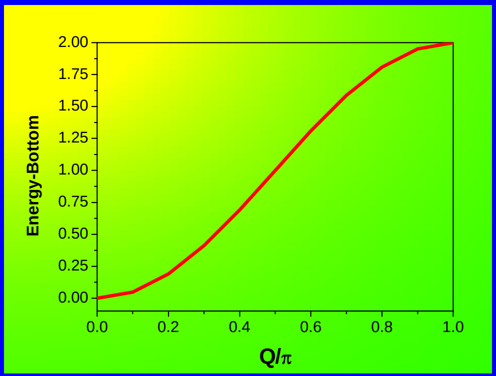
Traditional images of narrow polaron band formation

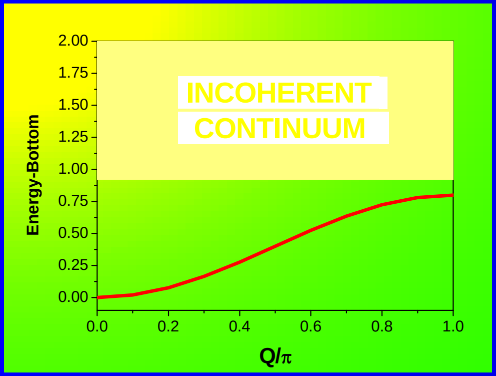


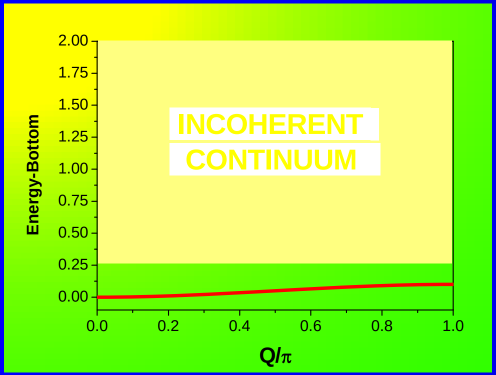


One pole approximation Eliashberg theory

Traditional images of narrow polaron band formation

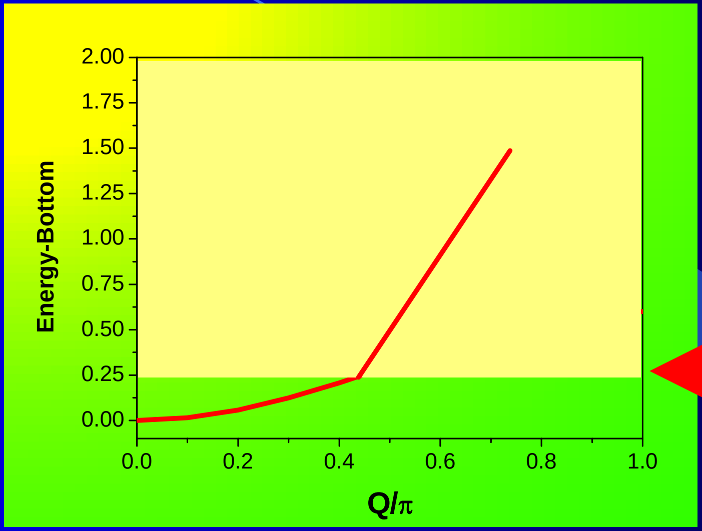






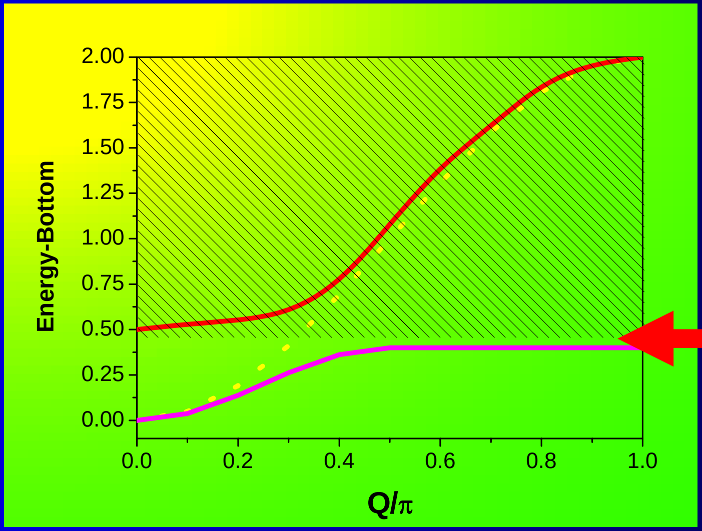
Weak coupling

Strong coupling



PH

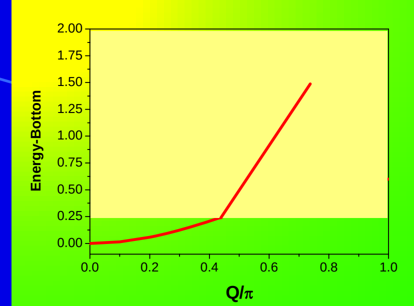
<u>One pole approximation Eliashberg theory</u>

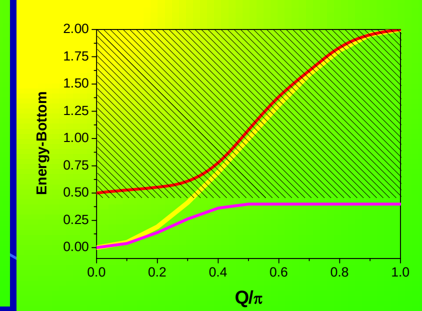


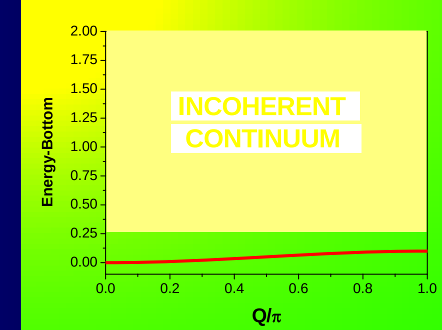
PH

TWO poles Engelsberg-Schrieffer approximation

E-ph interaction dependence spectral function in the top and the bottom of the band



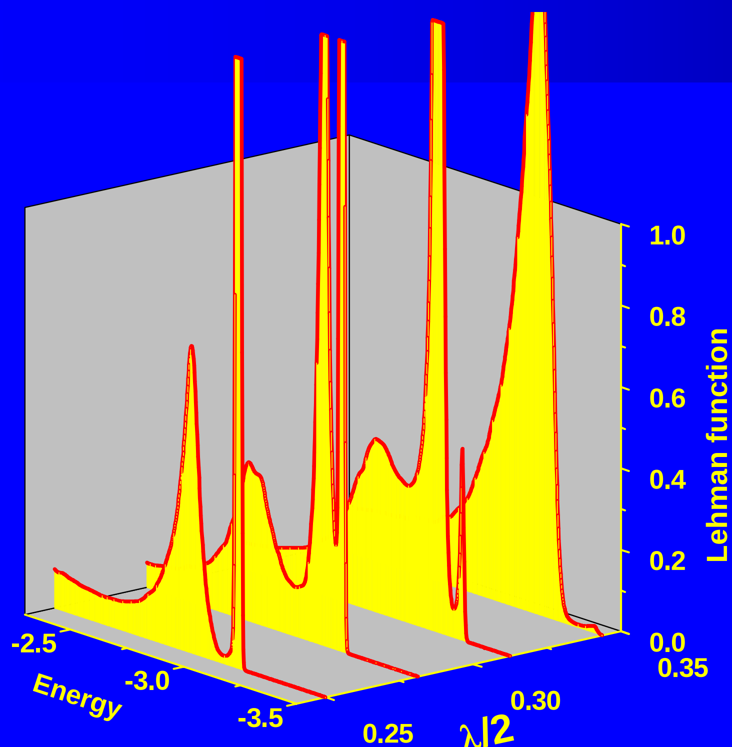




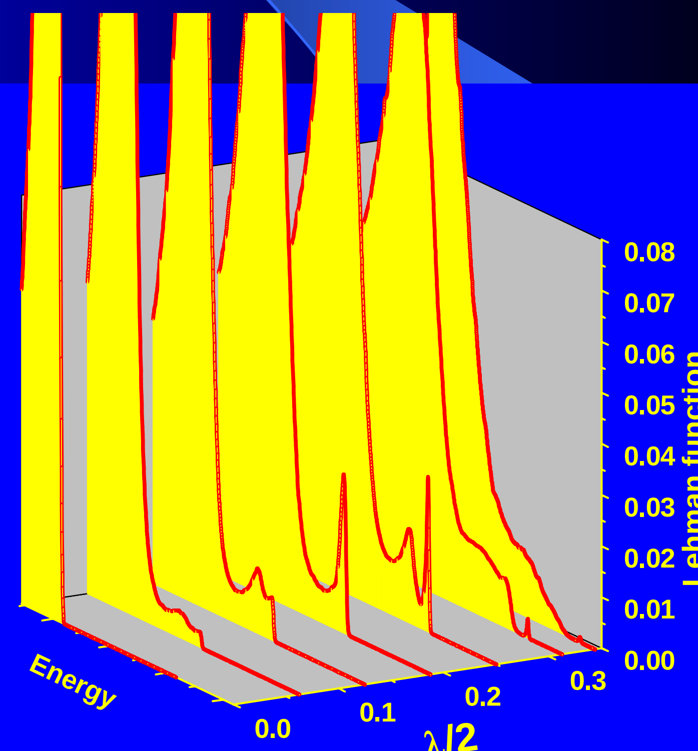
$\lambda<0.6$

$\lambda>0.6$

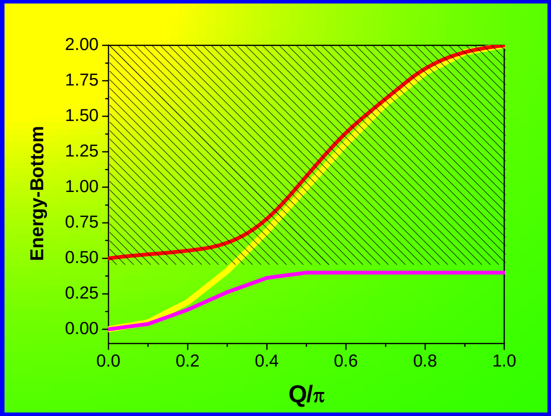
Band bottom (π/2,π/2)



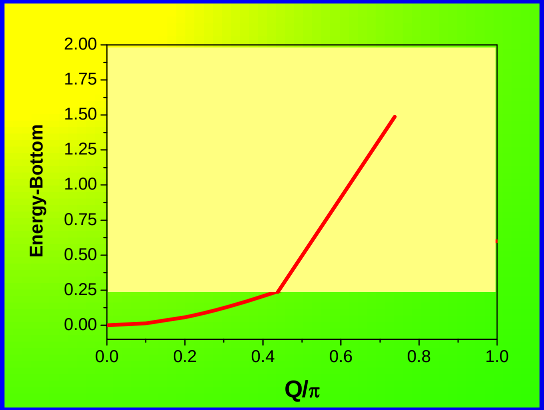
Band top (0,π)



What happens when phonon branch crossing occurs

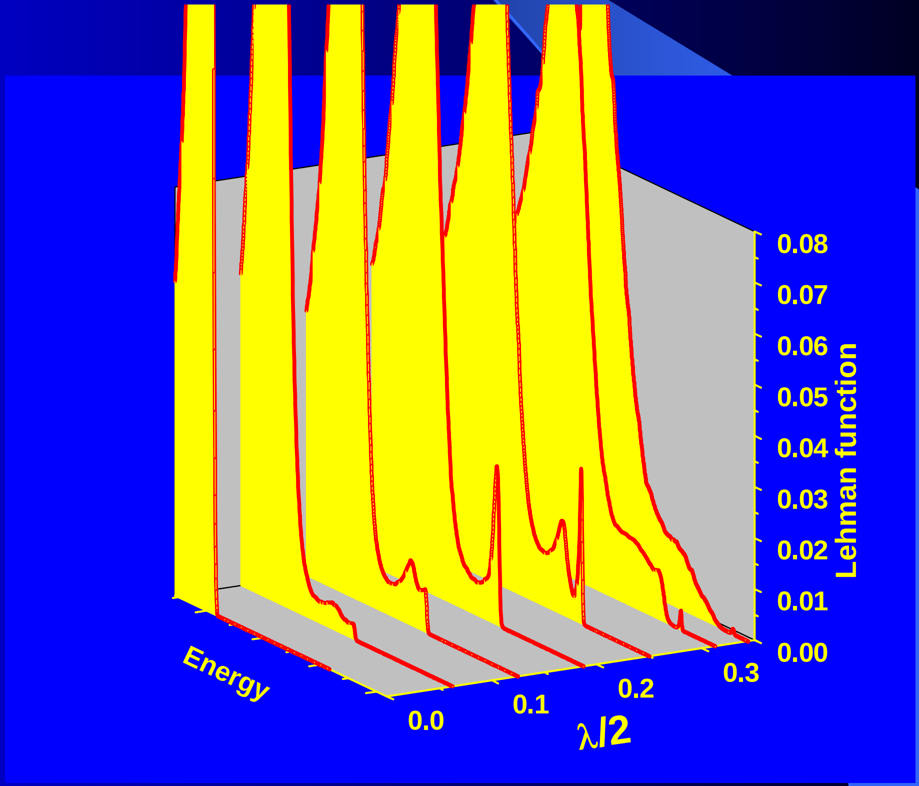


OR?

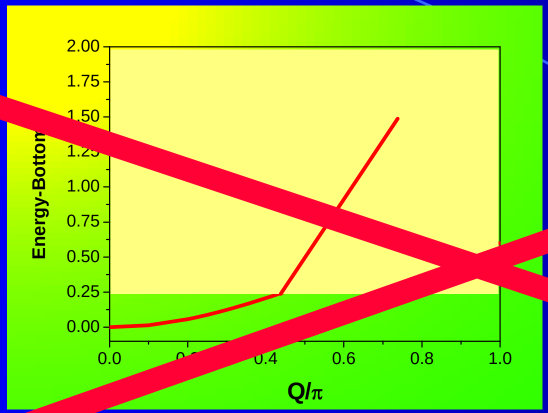


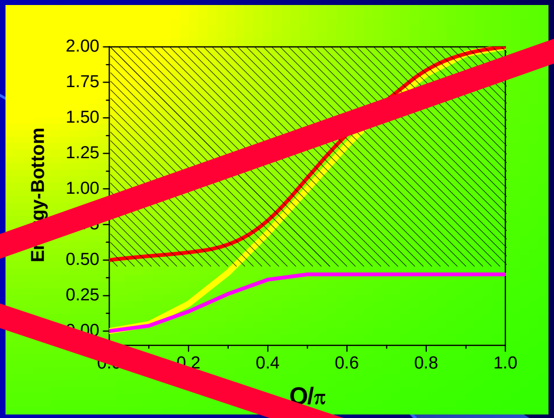
$\lambda<0.6$

Band top $(0,\pi)$

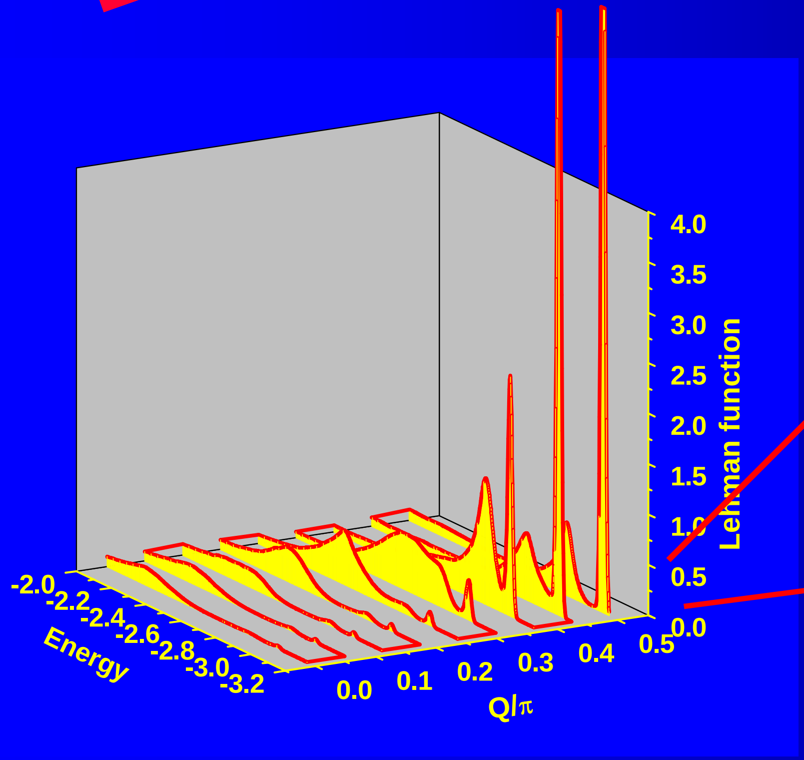


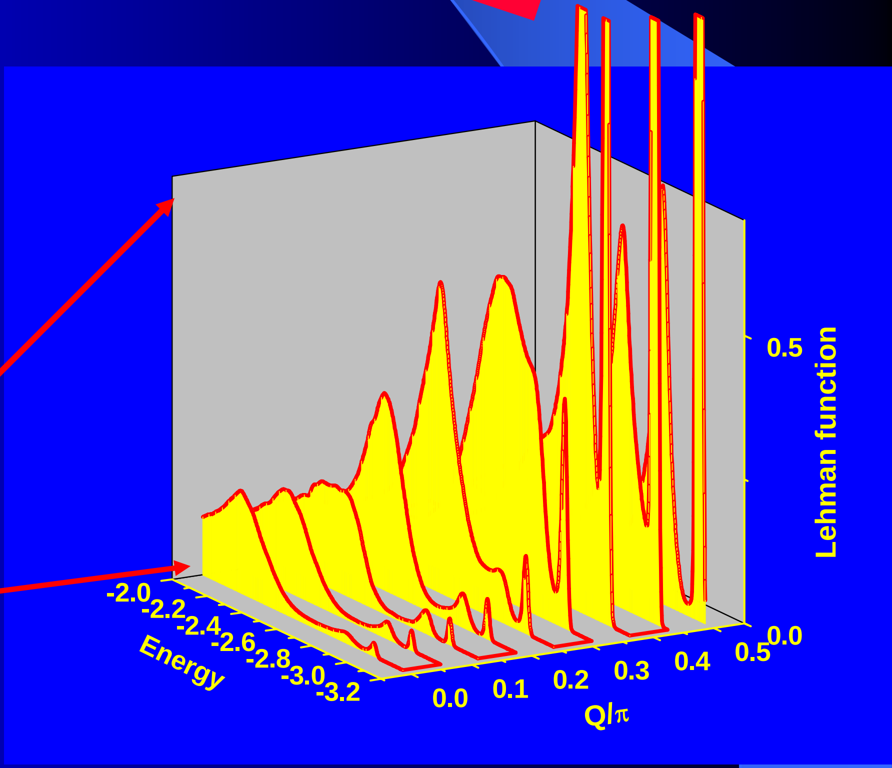
Spectra: (0, π) --- (π/2,π/2) at λ=0.5



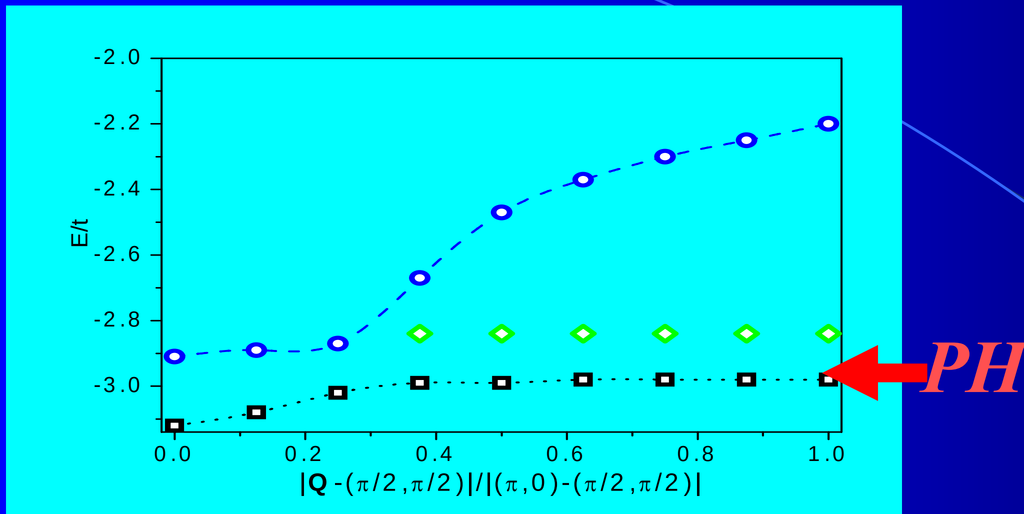


Both incorrect

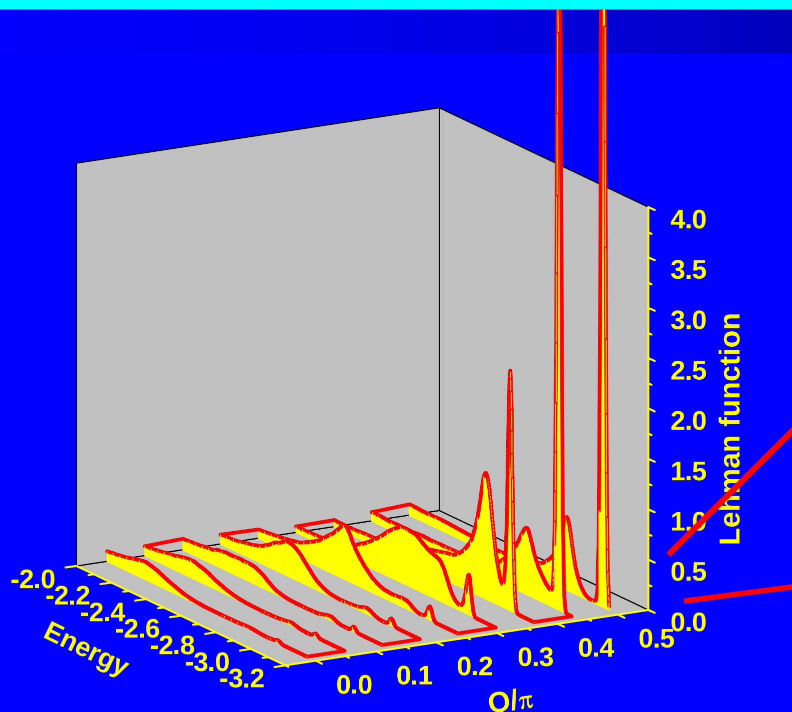


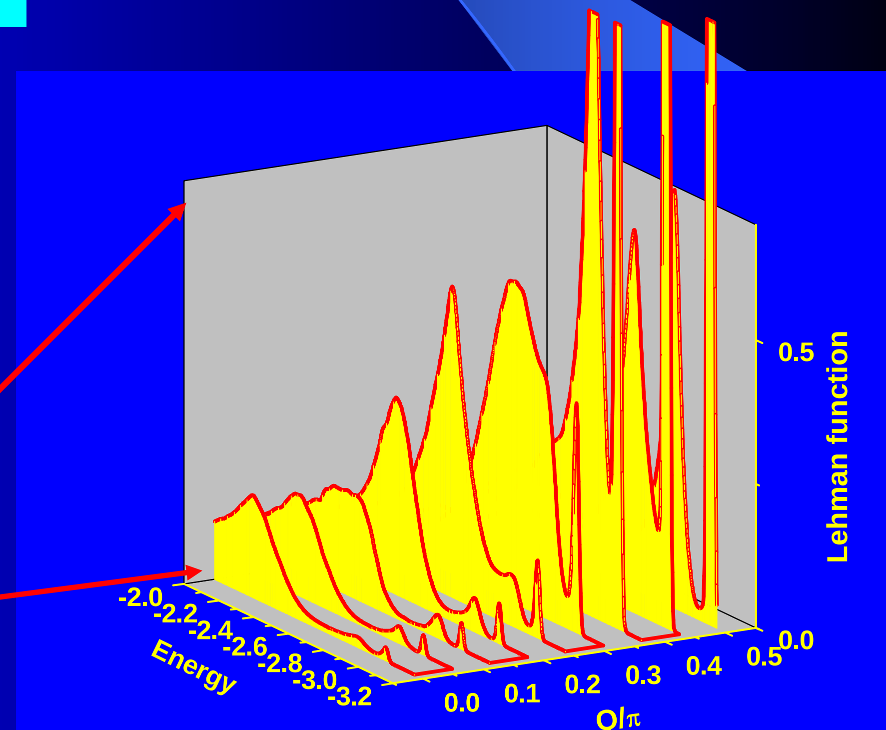


Spectra: (0, π) --- (π/2,π/2) at λ=0.5

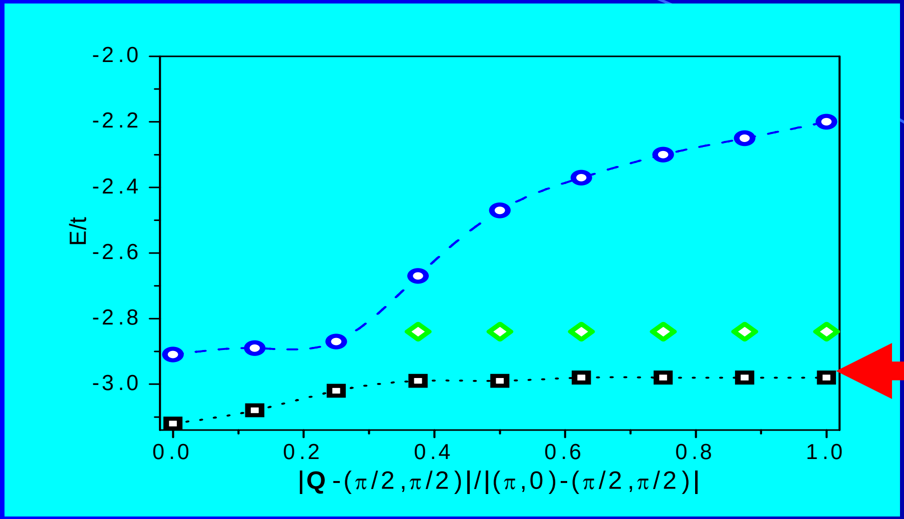


Picture is more reach with high resolution



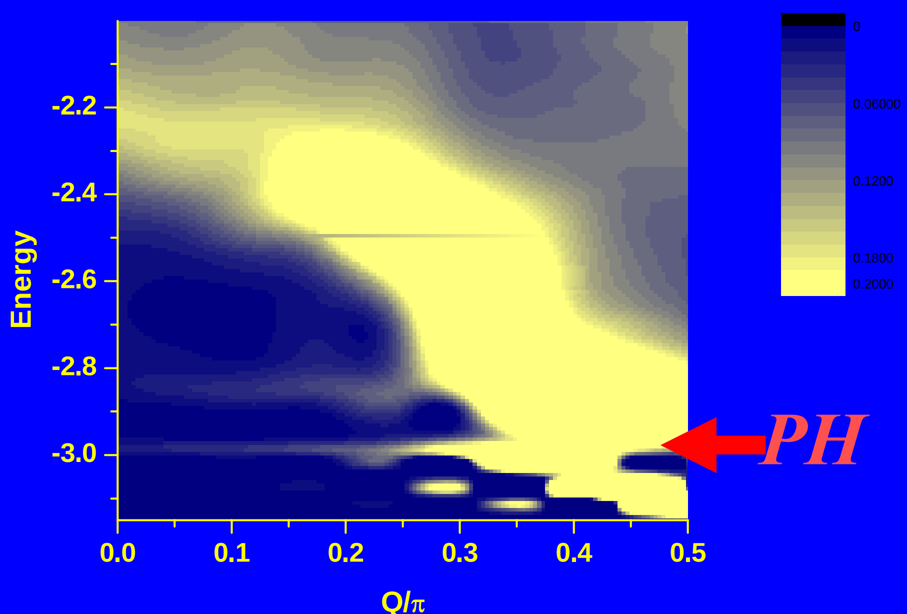


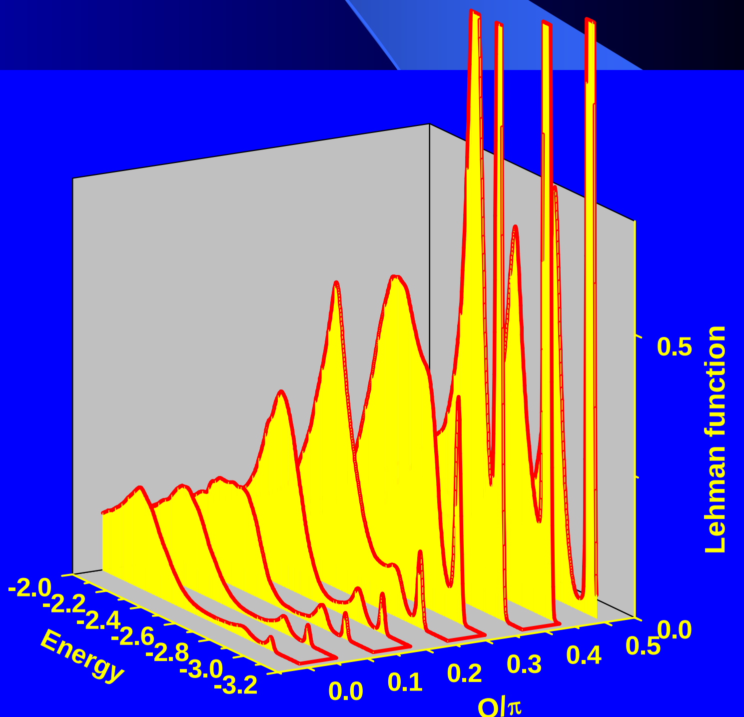
Spectra: (0, π) --- (π/2,π/2) at λ=0.5



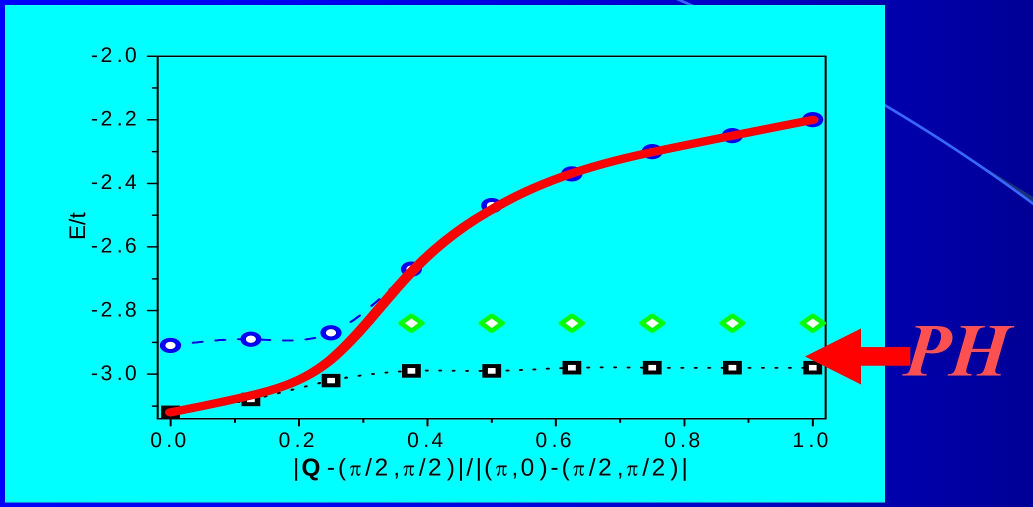
PH

Picture is more reach with high resolution

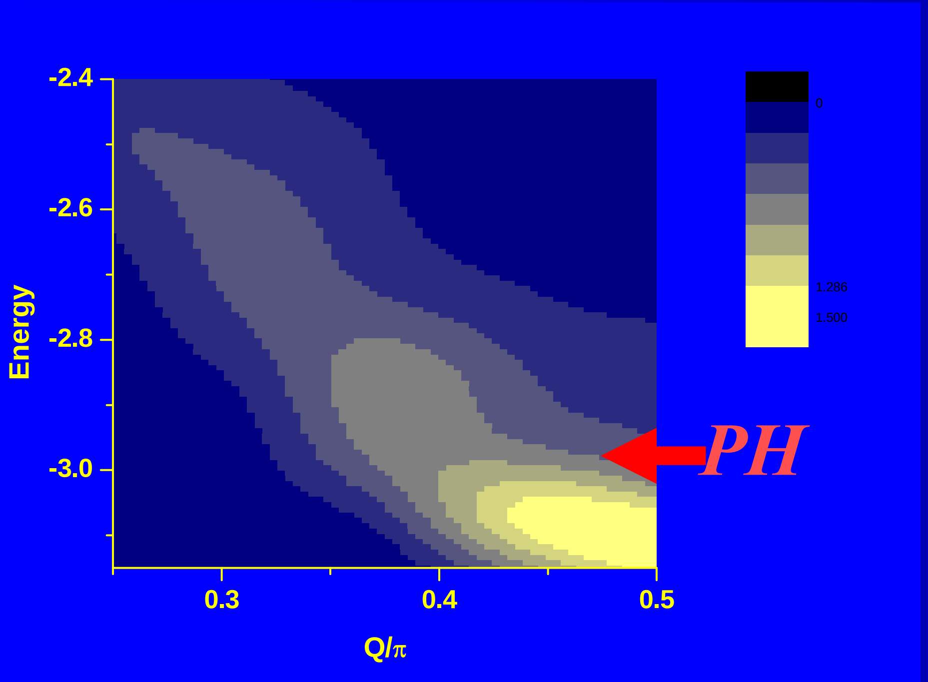


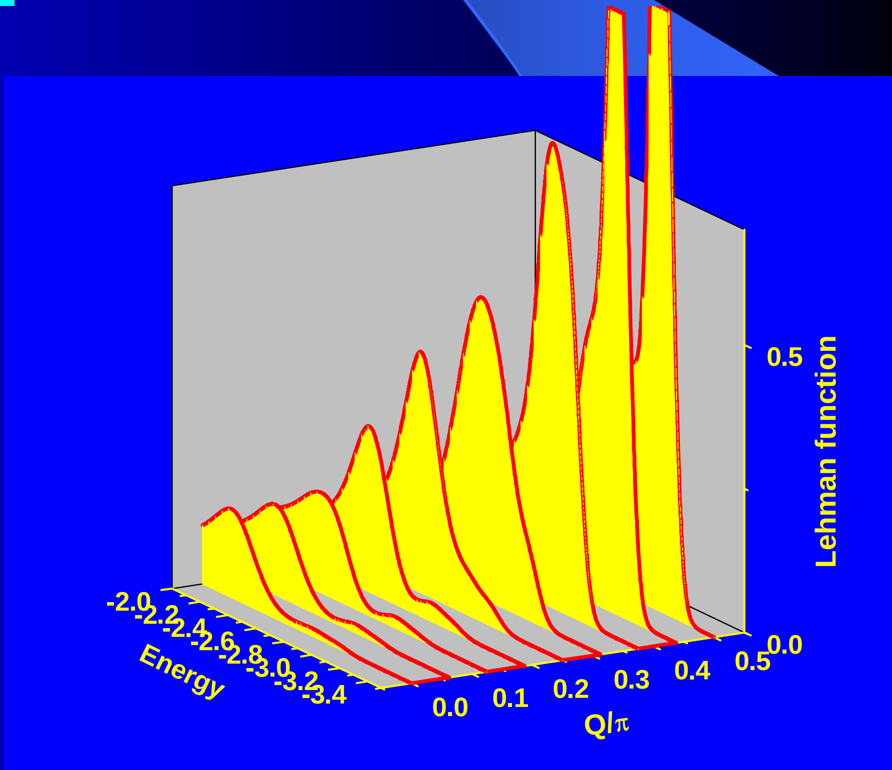


Spectra: (0, π) --- (π/2,π/2) at λ=0.5



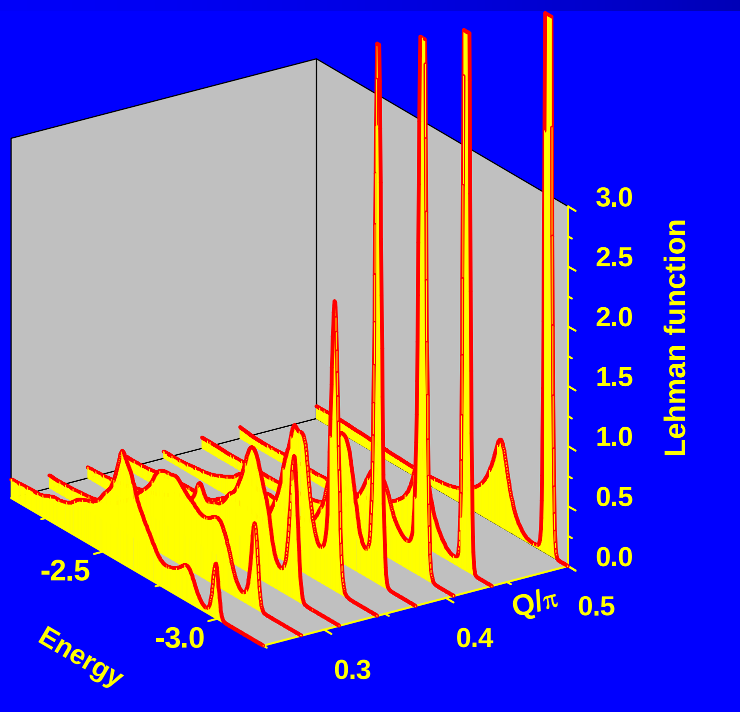
Picture recovers simple "Eliashberg" form with low resolution

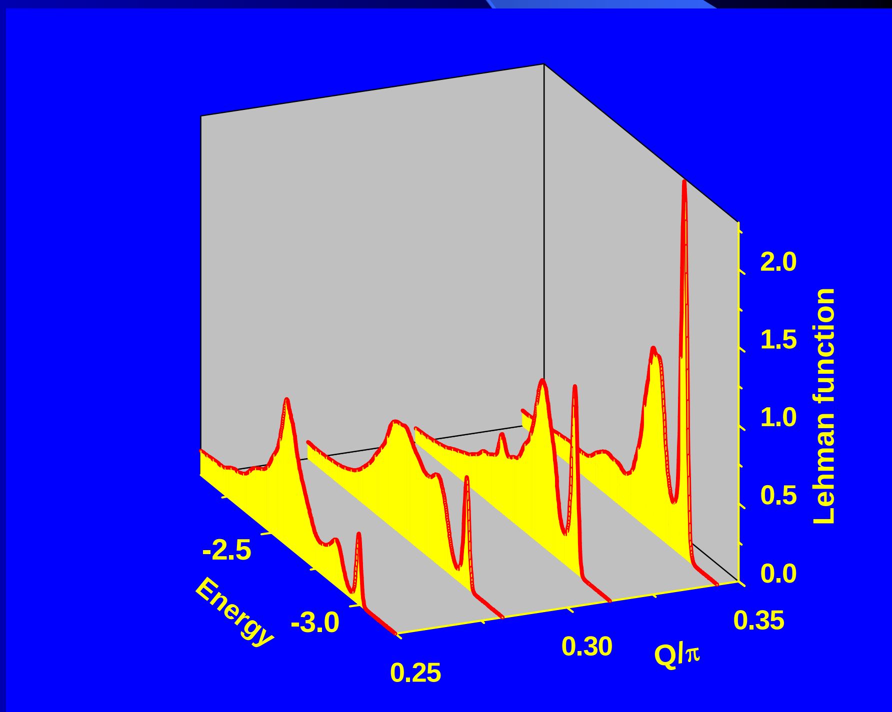




Spectra: (0, 0) --- (π/2,π/2) at λ=0.5

Picture reminds redistribution of weights between several resonances at phonon mode crossing with high resolution

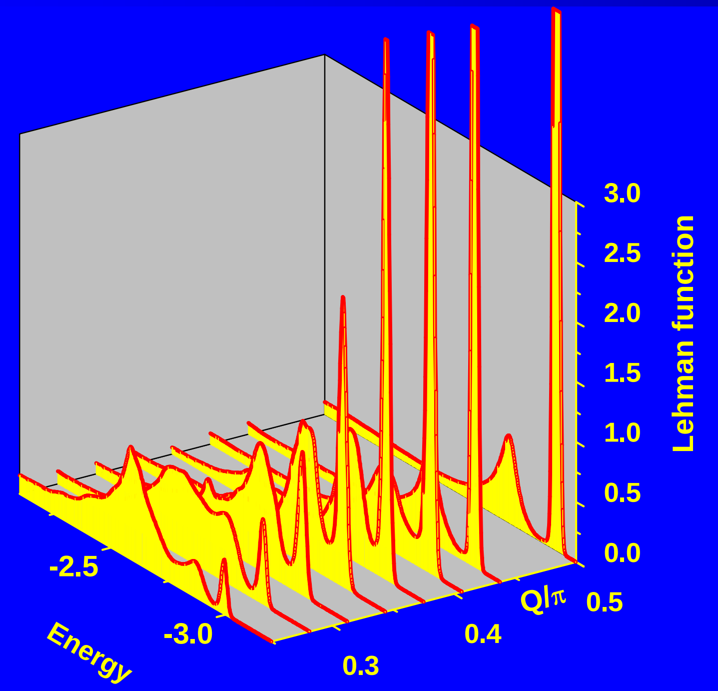


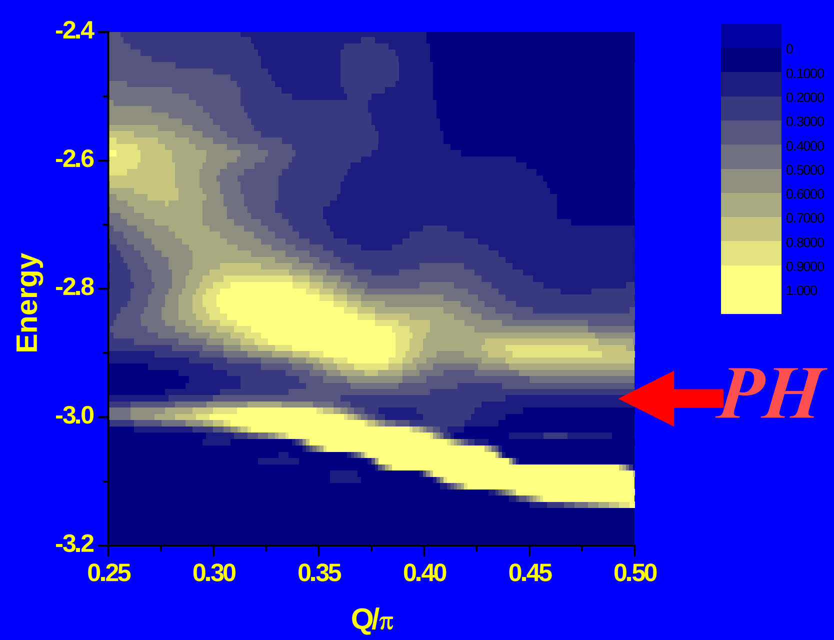


Spectra: (0, 0) --- (π/2,π/2) at λ=0.5

Picture reminds redistribution of weights between several resonances with high resolution

Special thanks to George Sawatzky





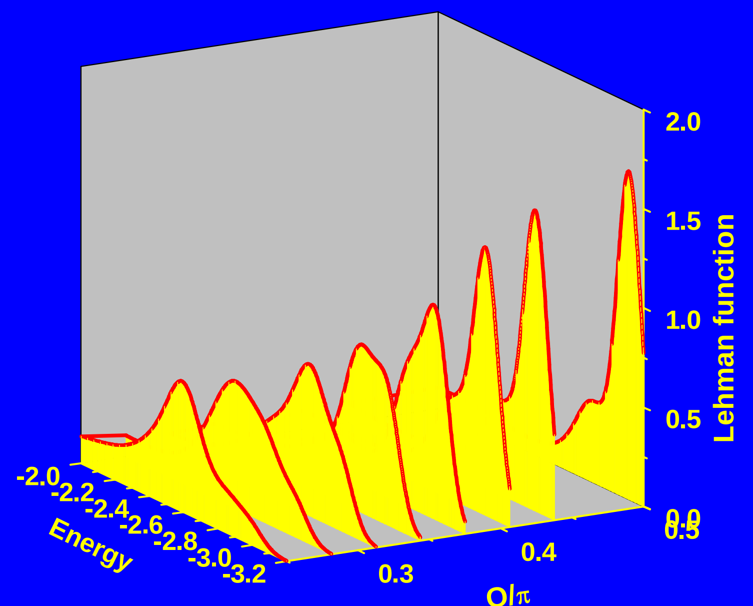
Spectra: (0, 0) --- (π/2,/2π) at λ=0.5

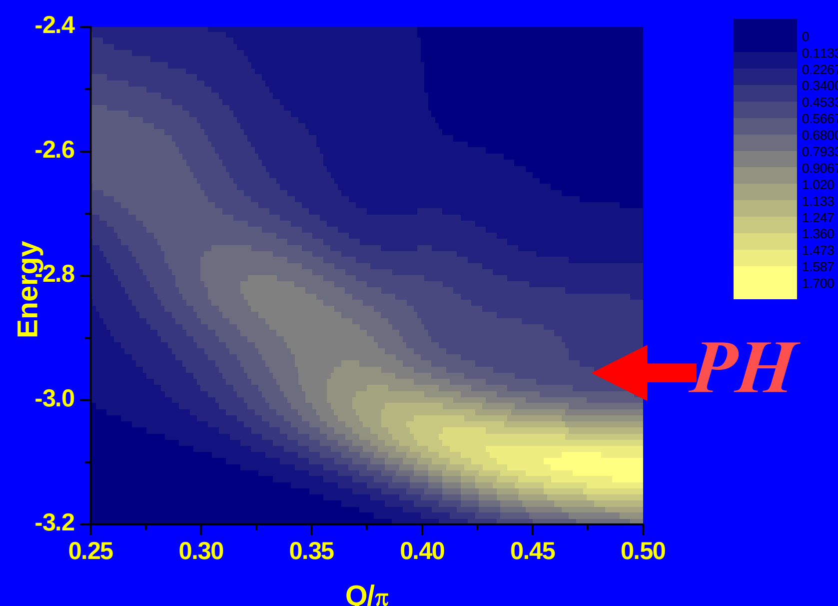
Tends back to "Eliashberg" behavior with low resolution

Either samples will be improved

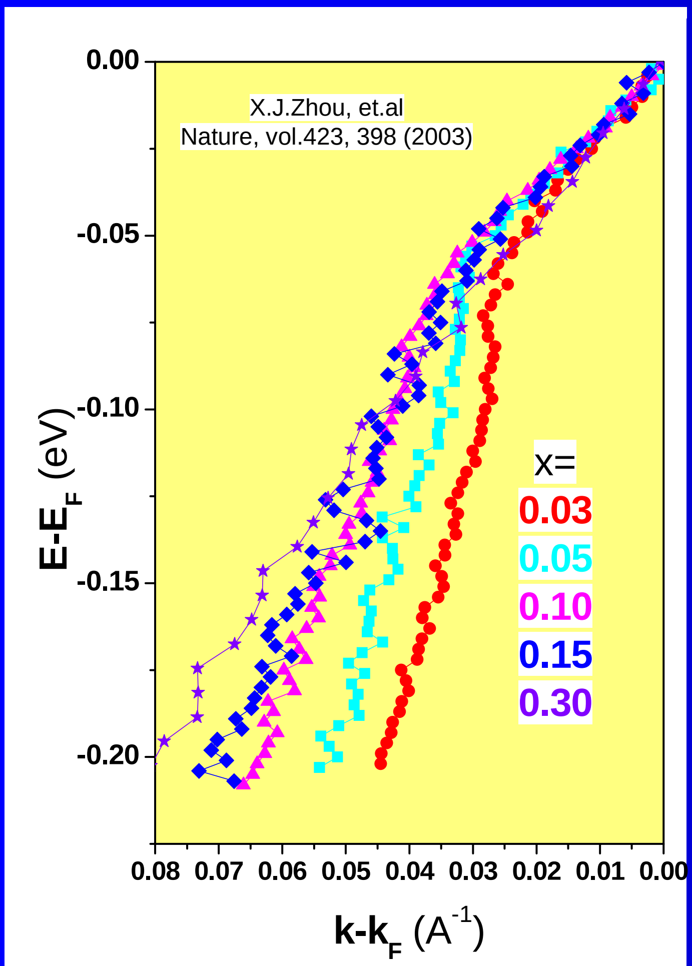
OR(?????)

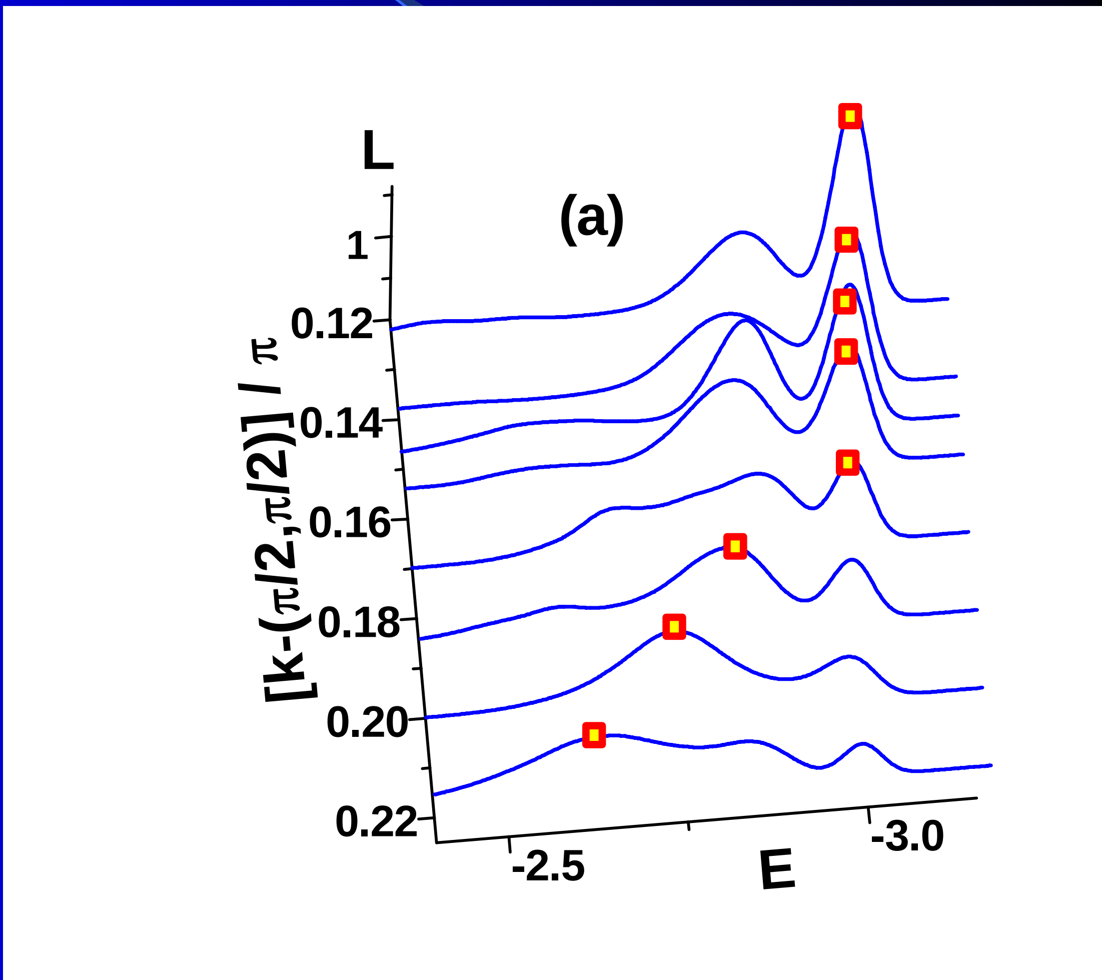
Theory will be spoiled by impurities

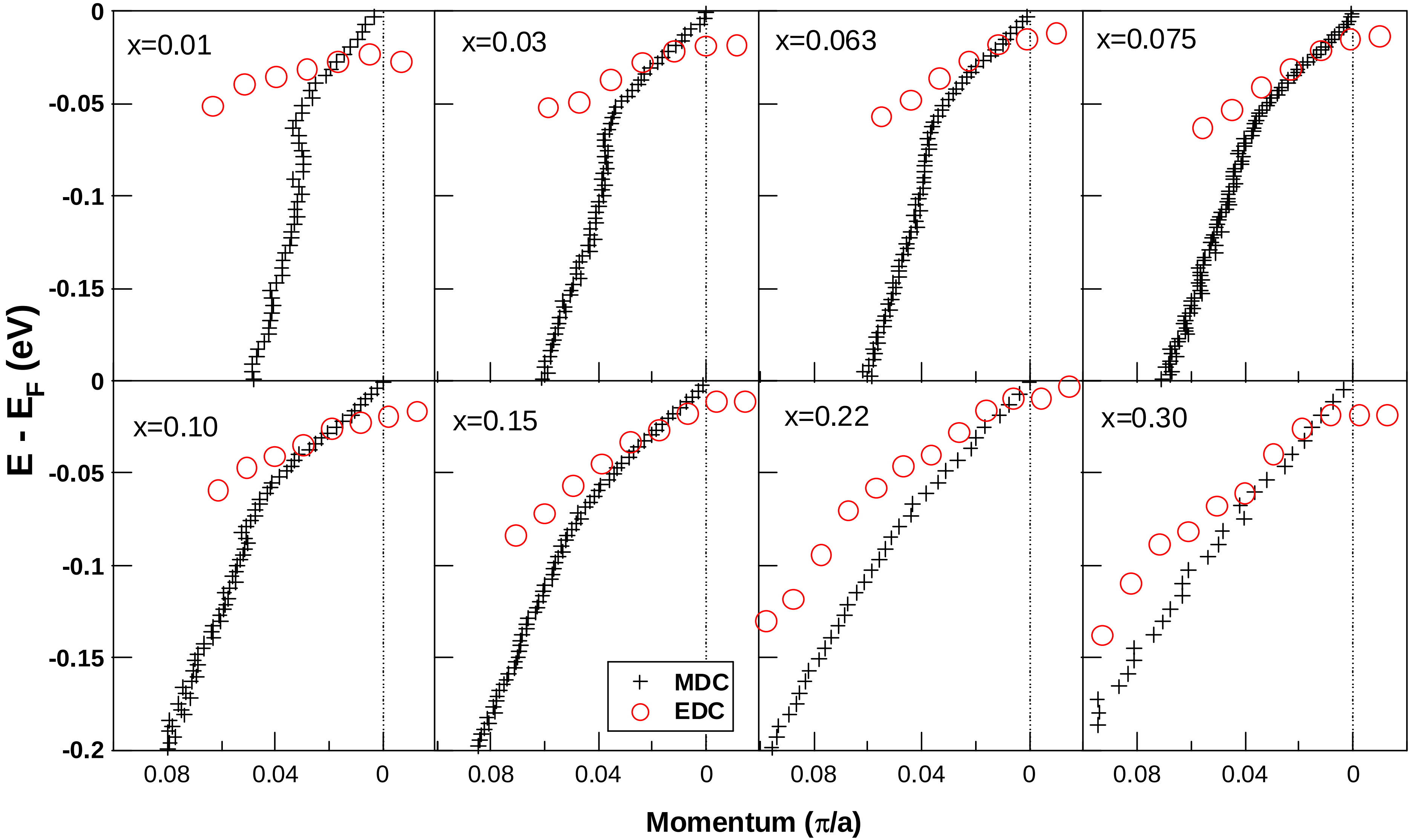




Kink exists in theoretical data and reproduces even the shape of the experimental dispersion






x=0.01
x=0.03
x=0.063
x=0.075
x=0.10
x=0.15
x=0.22
x=0.30
MDC
EDC
0
-0.05
-0.1
-0.15
-0.2
0.08
0.04
0
E - E_F (eV)
Momentum (π/a)

MDC and EDC dispersions

(1). In the traditional el-ph coupling, from simulations, under perfect energy and momentum resolution, EDC and MDC dispersions are identical;

(2). EDC dispersion is more sensitive to energy and momentum resolution. Our simulations find that under realistic energy and momentum resolution as we used, the MDC dispersion is more robust than EDC dispersion;

(3). EDC dispersion is also sensitive to disorder. As can be seen from x=0.03 data: EDC dispersion varies a lot between two samples, while the MDC dispersions are nearly the same;

(4). EDC dispersion is also affected by Fermi cutoff and “background”.

Therefore, for traditional el-ph coupling, MDC dispersion is more robust and better representative of the intrinsic dispersion.

(5). But, in polaron picture as we discussed in the present paper, since there is no simulation done, we can not tell which one is better between MDC and EDC dispersions.

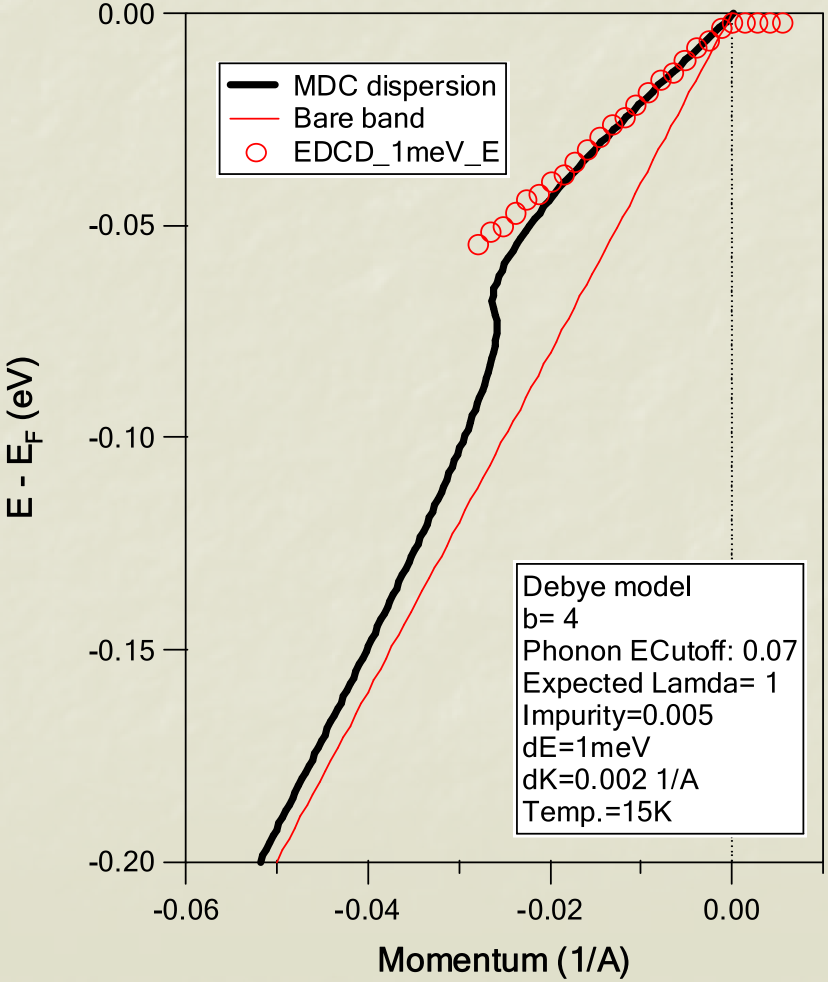
(6) From Fig. 4, the overall trend is that low-energy EDC and MDC velocities get closer with increasing doping. This effect may be beyond energy and momentum resolution effect.

(7). The justification of using EDC dispersion in the present paper is that calculation gives EDC dispersion.

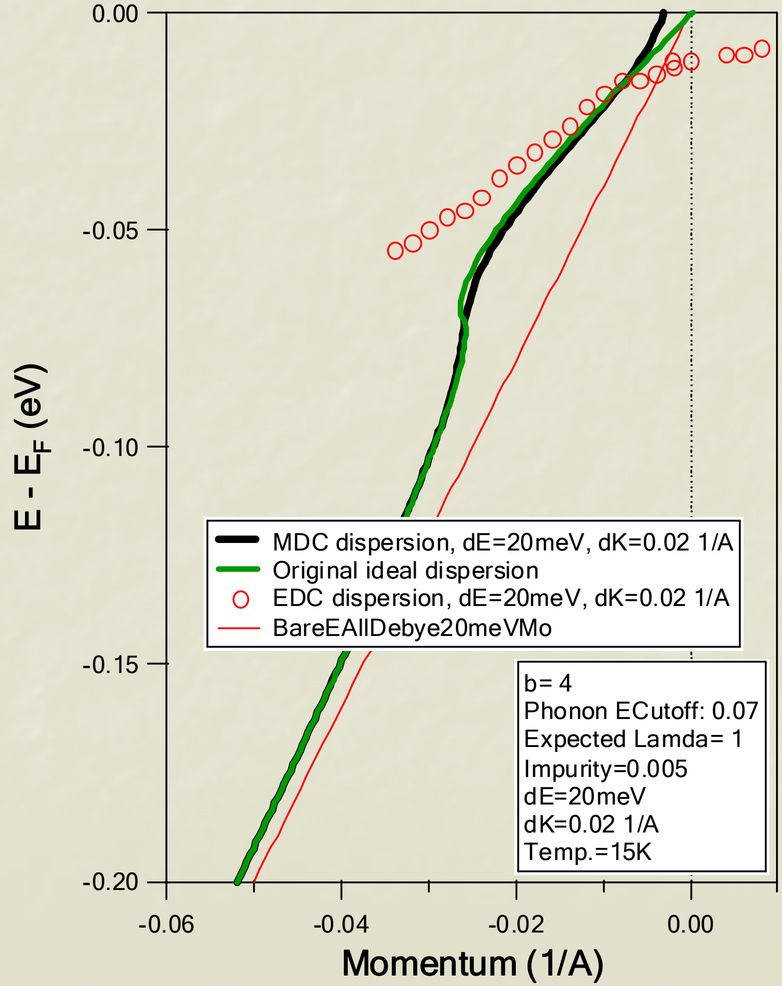
MDC and EDC dispersions: Why are they different? Which one is reliable?

2D Debye model, Cutoff=70 meV, lambda=1

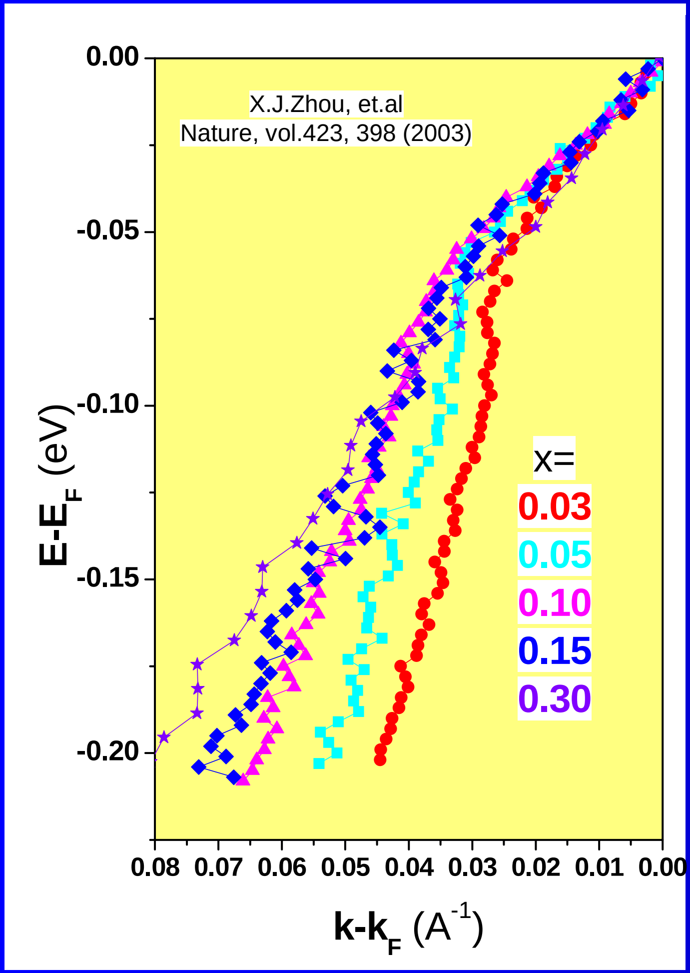
Perfect resolution

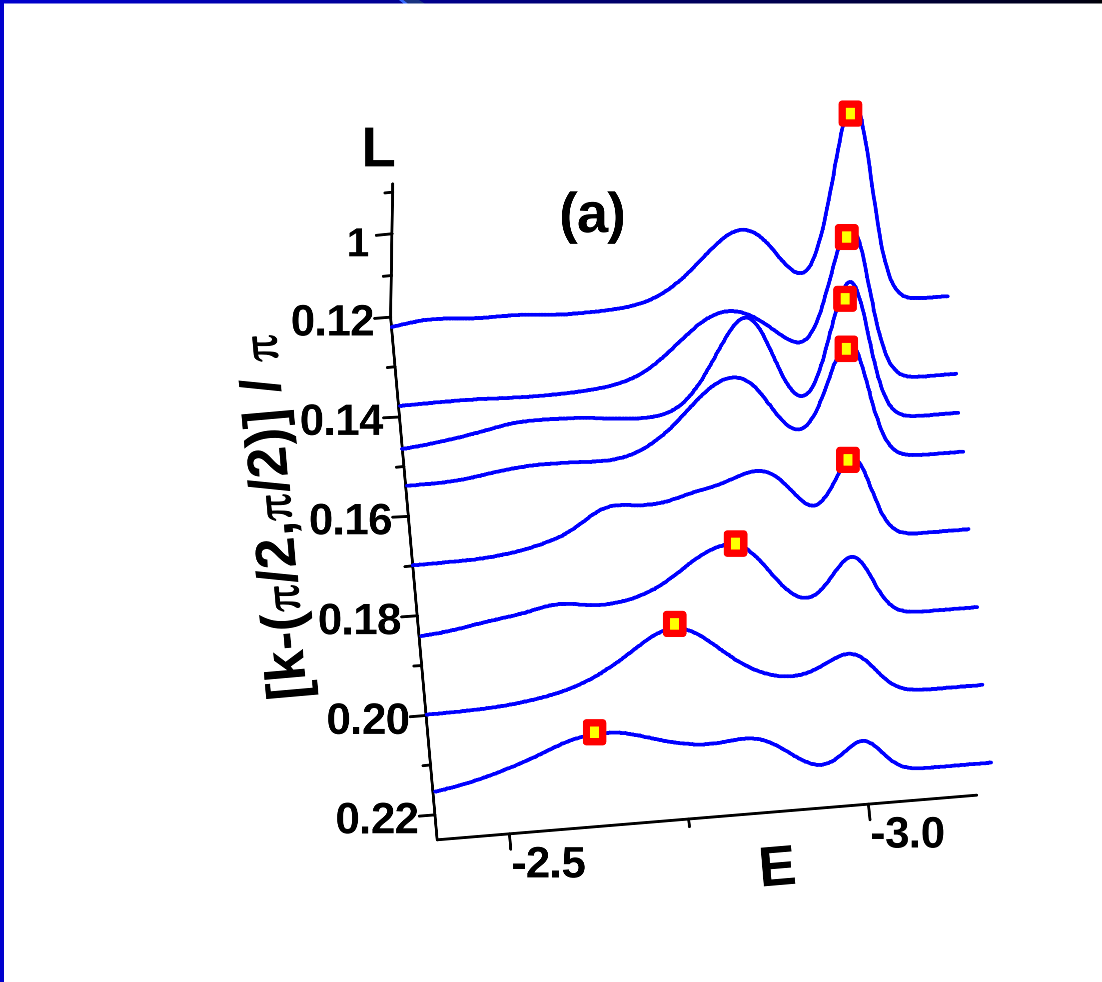


Realistic resolution

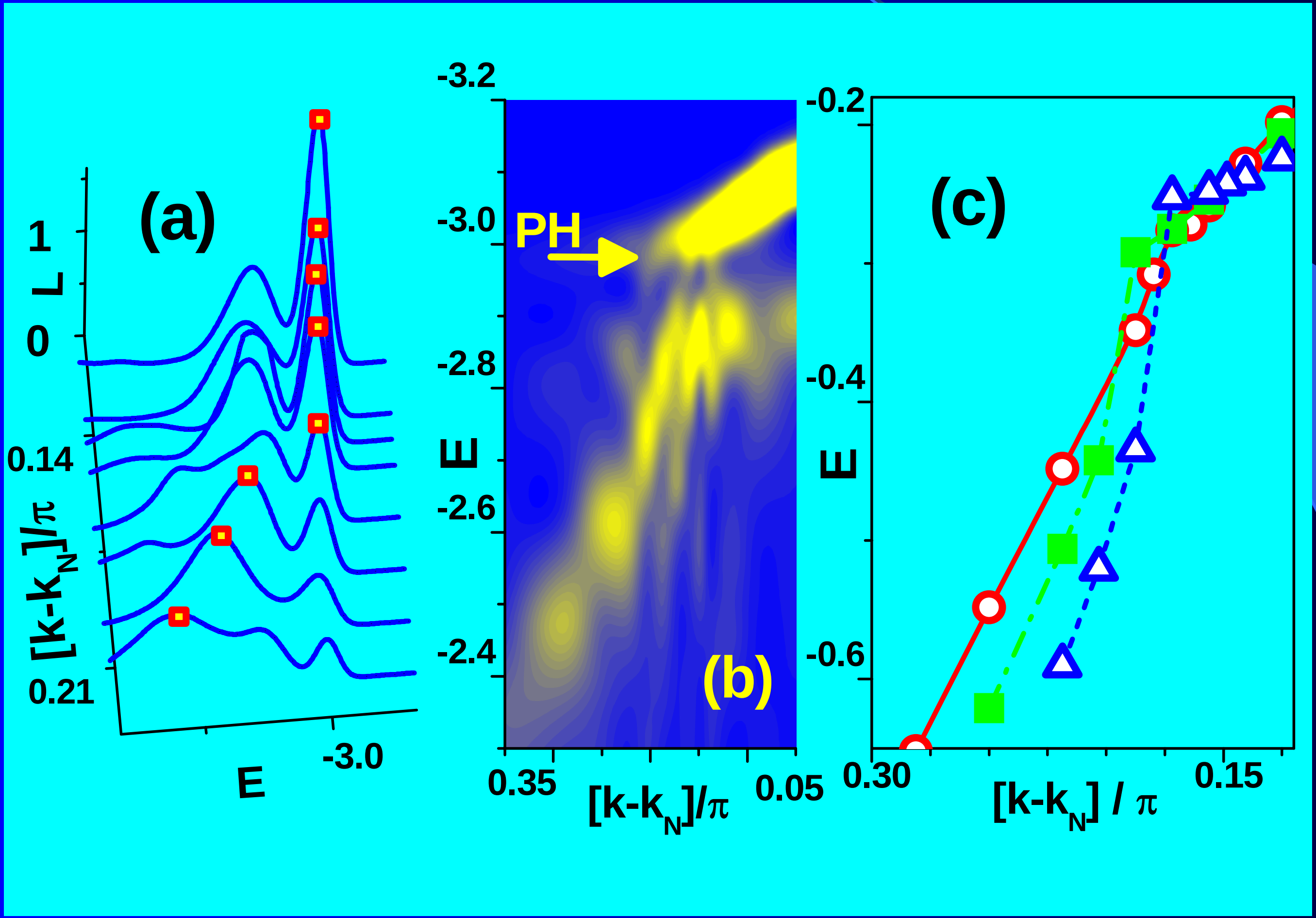


Kink exists in theoretical data and reproduces even the shape of the experimental dispersion



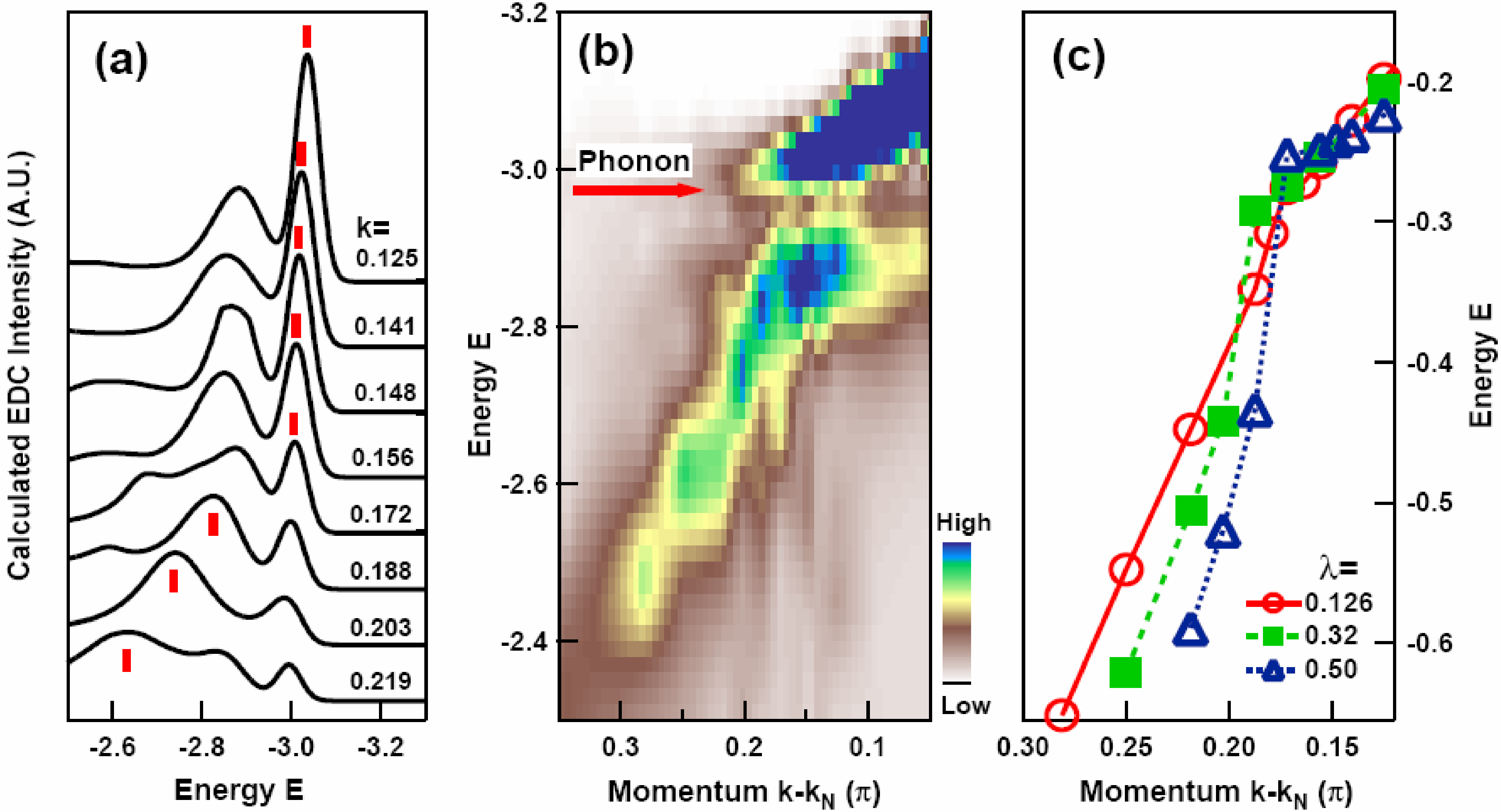


Kink exists in theoretical data and reproduces even the shape of the experimental dispersion

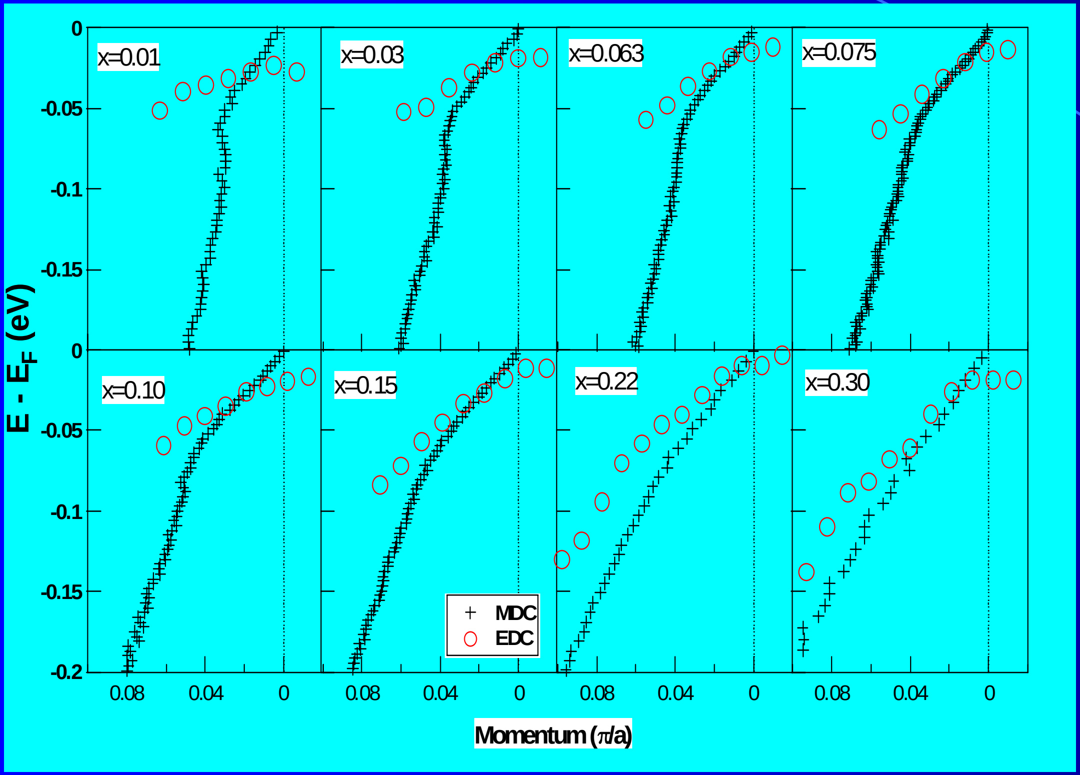


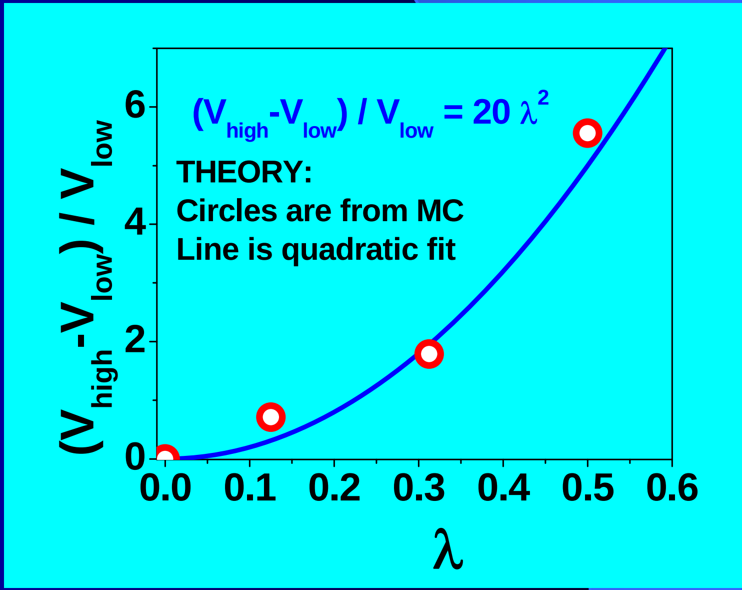
Energy and wave vector are counted from Fermi energy!

Theoretical data: theory or experiment?

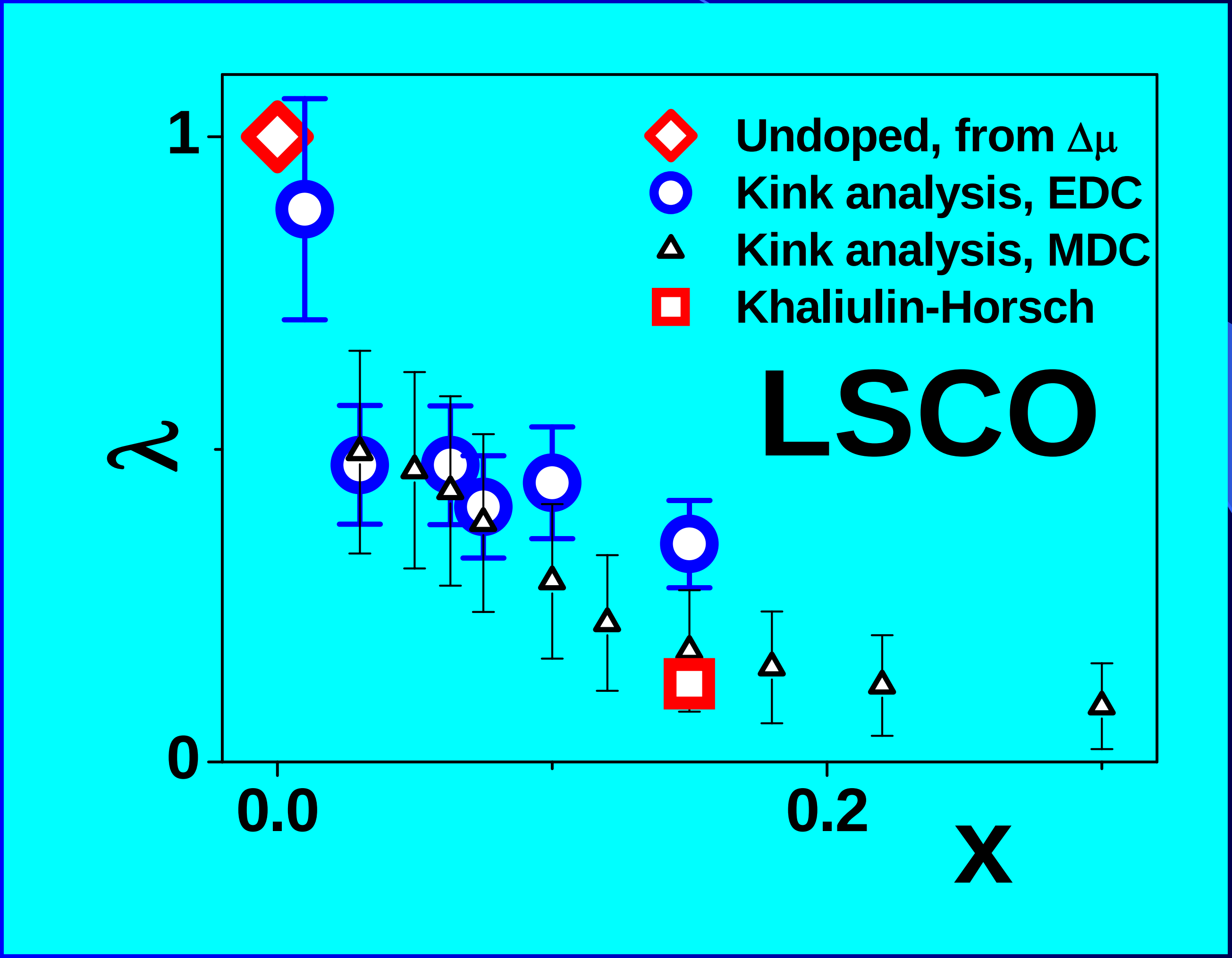


EDC and MDC Dispersion of LSCO

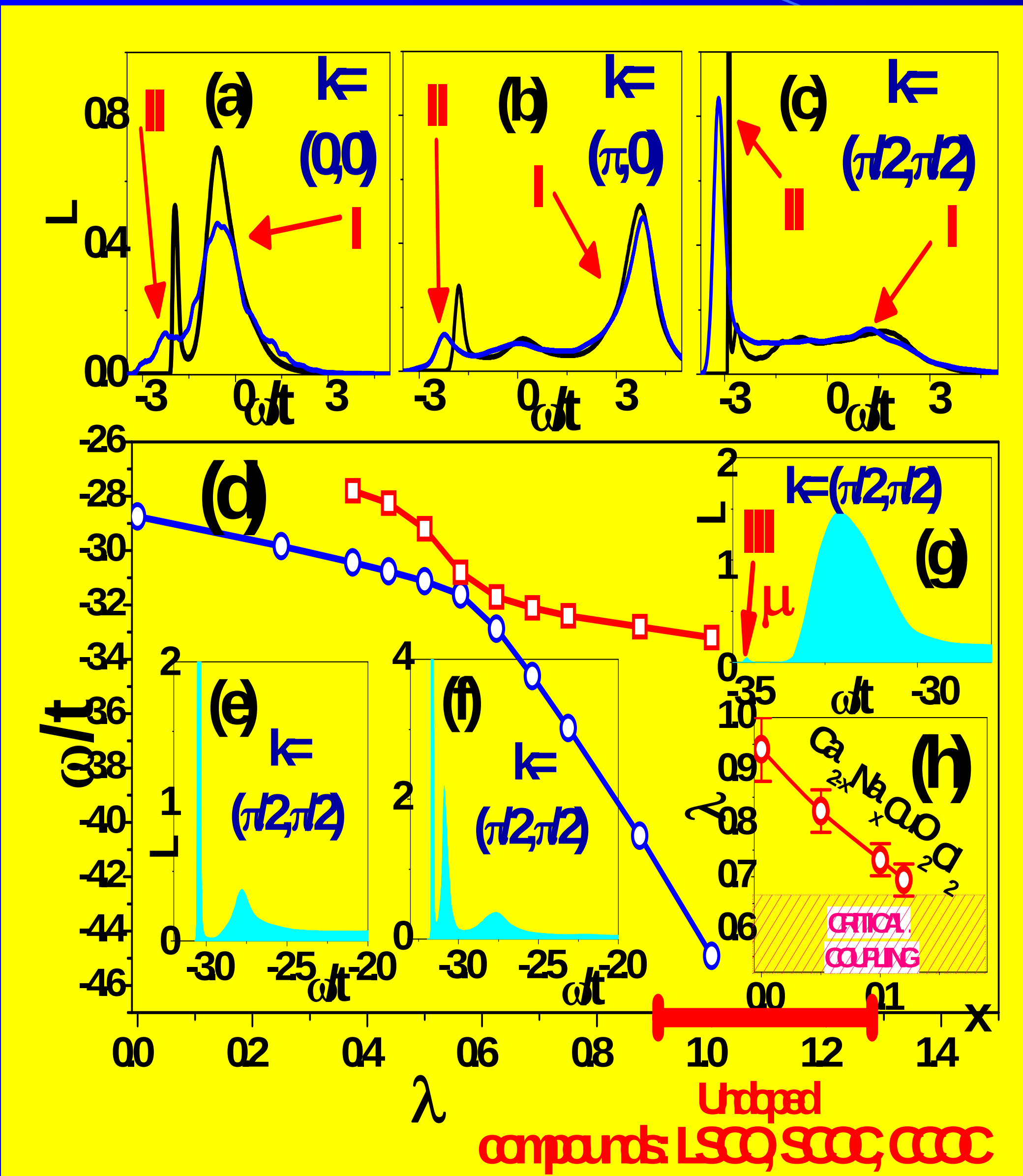


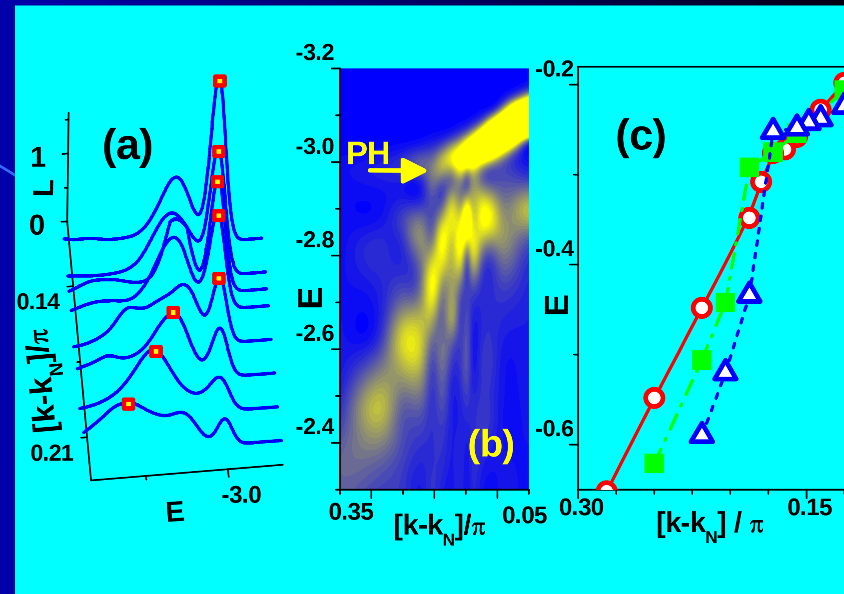


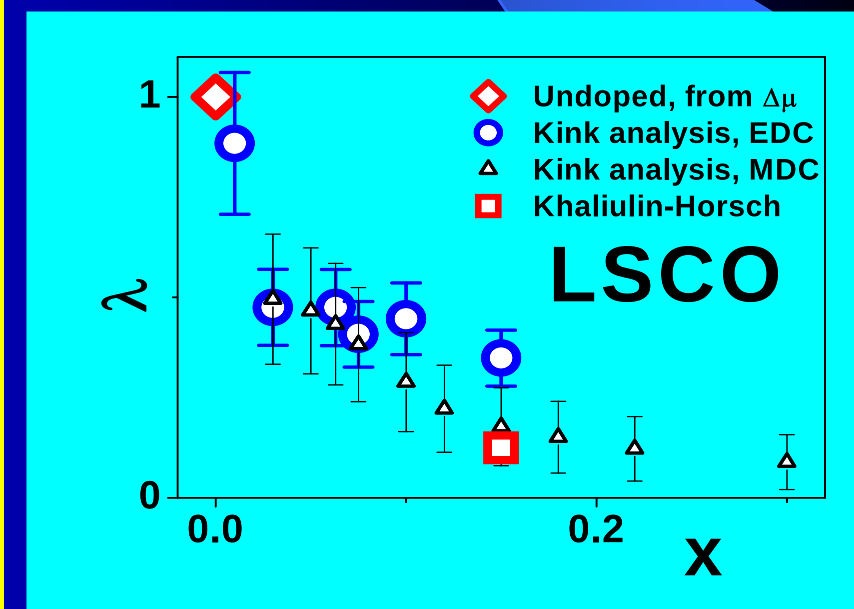
Dopping dependence of λ in LSCO



Summary


(a) k=(0,0)
(b) k=(π,0)
(c) k=(π/2,π/2)
I
II
L
ω/t
(d)
λ
(e) k=(π/2,π/2)
(f) k=(π/2,π/2)
(g) k=(π/2,π/2)
III
μ
(h)
Ca2-xNaxCuO2Cl2
CRITICAL COUPLING
x
Undoped
compounds: LSCO, SCOC, CCOC


(a)
(b)
(c)
PH
L
E
[k-kN]/π
[k-kN] / π


Undoped, from Δμ
Kink analysis, EDC
Kink analysis, MDC
Khaliulin-Horsch
LSCO
λ
x

CONCLUSIONS

1. In the strong coupling regime dispersionles polaron peak is invisible in ARPES but broad shake off peak traces the bare band dispersion

2. Relative width has universal behavior in the strong coupling regime

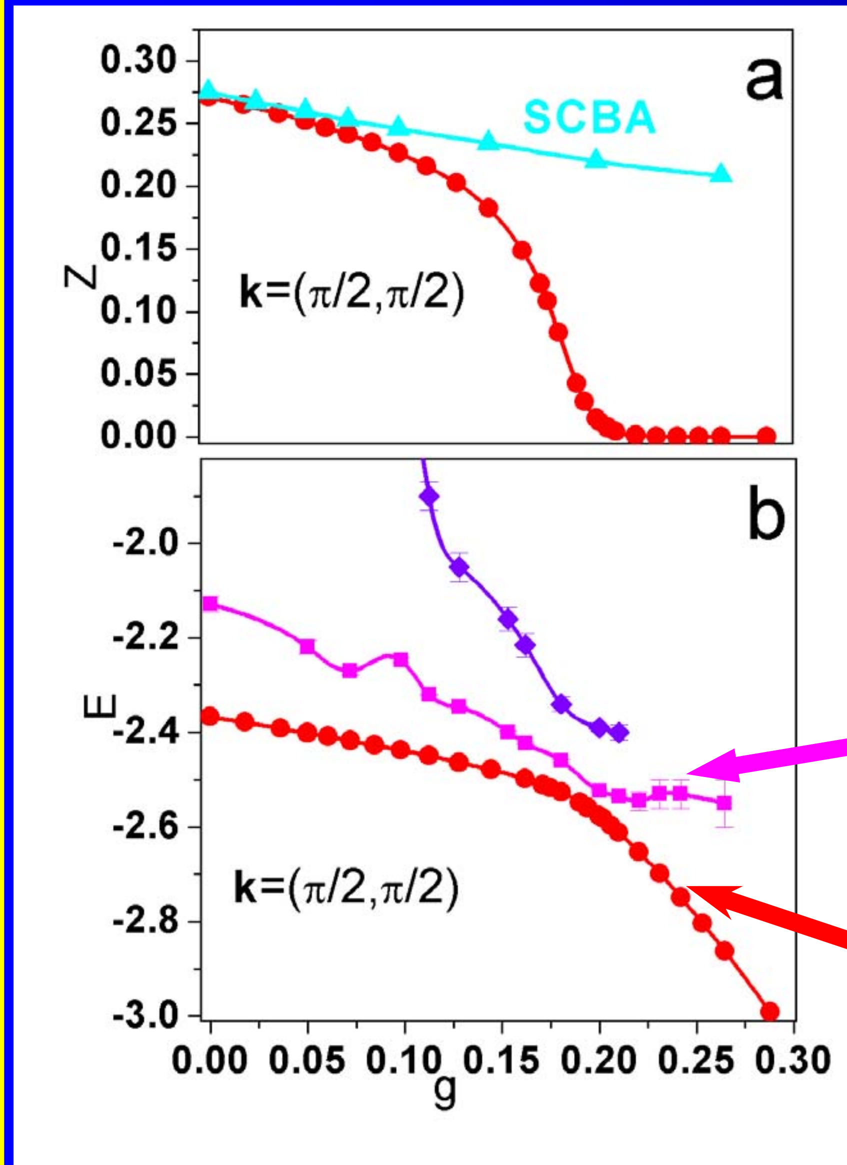
3. Compound $Sr_2CuO_2Cl_2$ is in the strong coupling regime with λ=1.2 which is considerably higher than critical coupling λ_c=0.58

4. Compound $Ca_{2-x}Na_xCuO_2Cl_2$ is in the strong coupling regime with λ=1.0. Coupling constant decreases with doping.

5. Experimentally observed kink is reproduced in intermediate and weak coupling regime. It's value helps to determine λ for $La_{2-x}Sr_xCuO_4$ which decreases with doping.

Isotope effect

t-J model

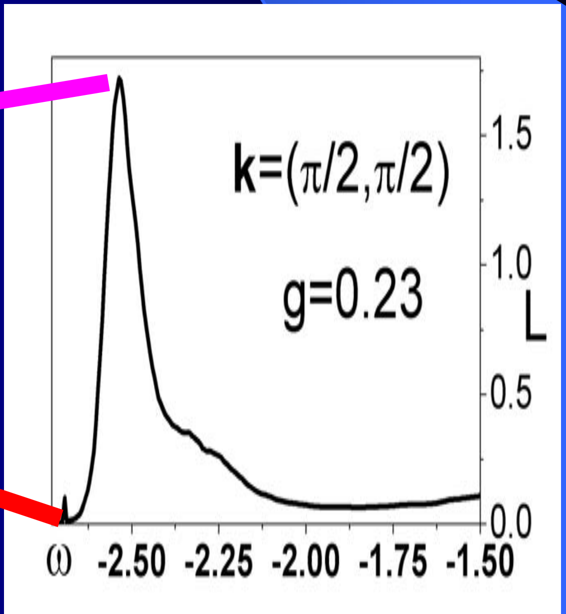


We expect unusual isotope effect in the strong coupling regime.

1. Independent Einstein oscillator model gives qualitative explanation of the isotope effect.
2. The actual magnitude of the isotope effect is one order of magnitude larger due to closeness to self-trapping point.

Weak lattice deformation

Strong lattice deformation



Isotope effect in the independent oscillators model

$$H_{int} = \sigma / (\omega^{(ph)} m)^{1/2} \dots$$

$$\kappa = (m_0/m_{isotope})^{1/2} = \omega_{isotope}^{(ph)}/\omega_0^{(ph)}$$

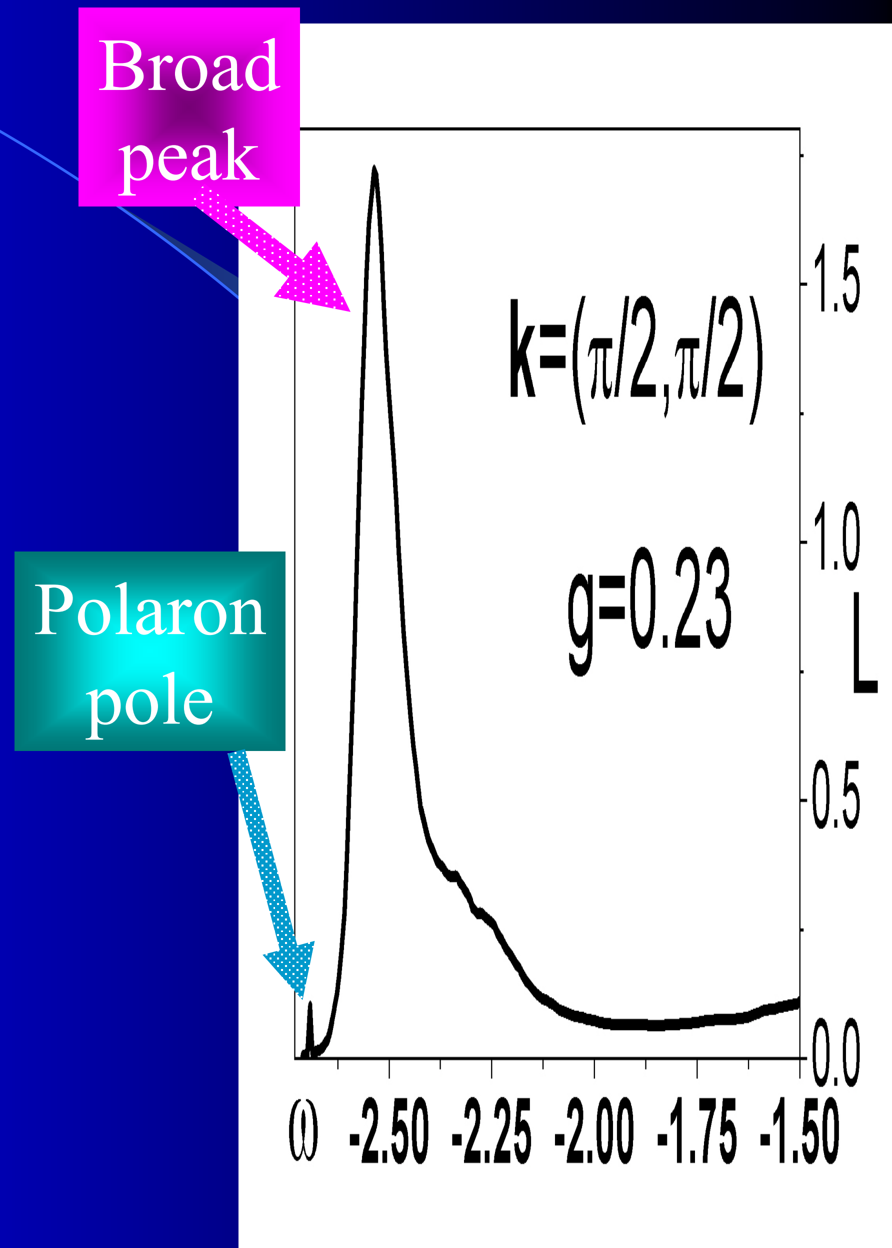
σ : does not depend on isotope

κ : measure of the mass substitution

Energy of polaron pole does not depend on isotope: $E_0 = -\sigma^2$

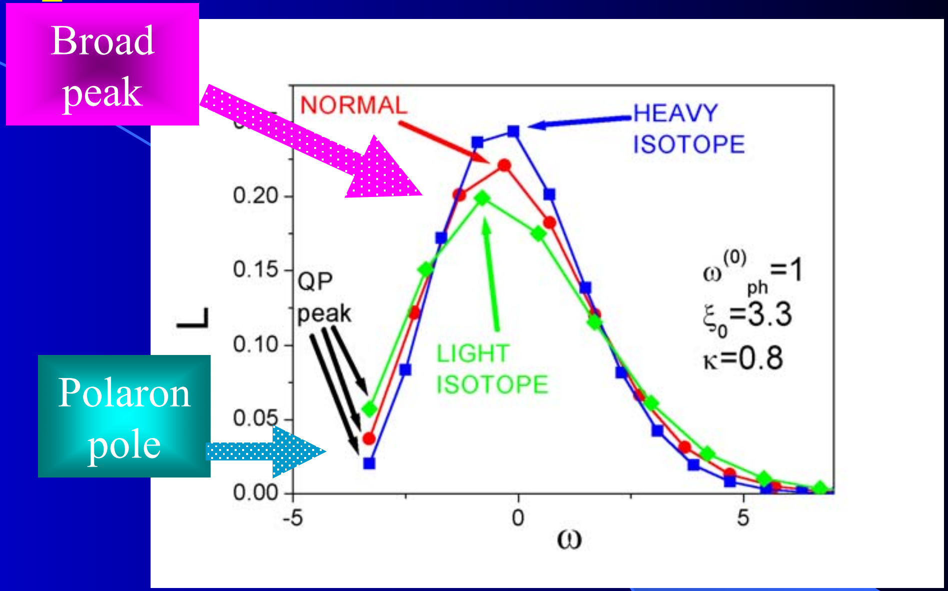
Z-factor strongly depends on Isotope:

$$Z = \exp\{-\sigma^2/[\omega_0^{(ph)}\kappa]\}$$

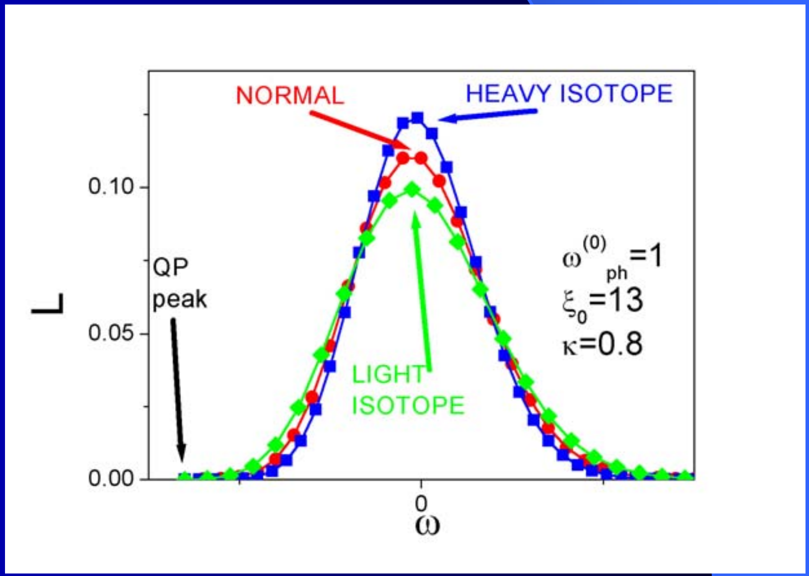


Isotope effect in the independent oscillators model

In the intermediate coupling regime broad peak is more narrow and shifts to higher energies for heavier isotope



Note, that *very large* $\kappa = 0.8$ mass change is required to see significant shift [Experimental: $\kappa_{exp} = 0.94$]



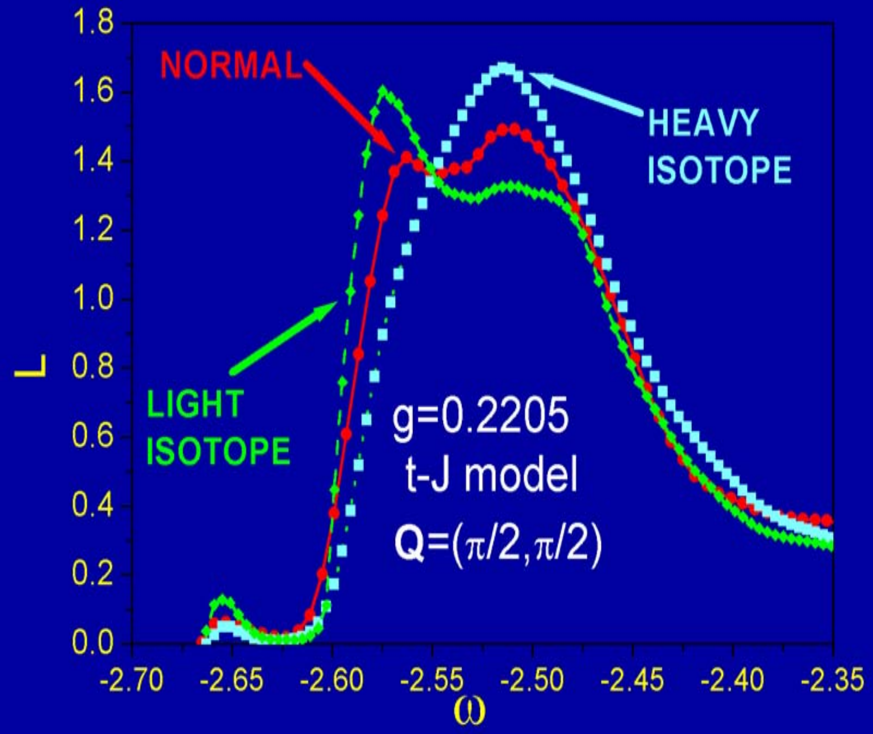
In the strong coupling regime broad peak is more narrow for heavier isotope

Isotope effect in the t-J model

Vicinity of the self-trapping point

$\kappa_{exp} = 0.94$

In the vicinity of the self-trapping point system is very sensitive to isotope substitution.
Even very small
$\kappa_{exp} = 0.94$
gives significant effect

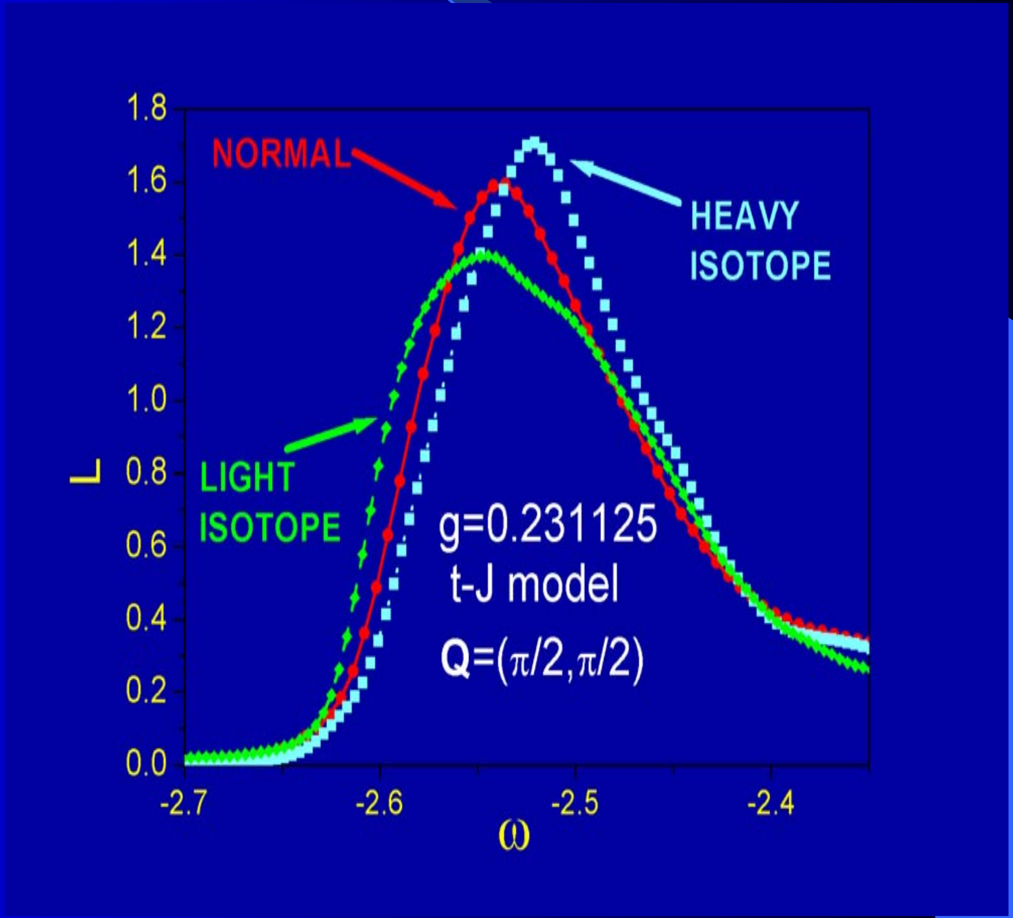


Isotope effect in the t-J model

Strong coupling regime

$\kappa_{exp} = 0.94$

In the strong coupling regime (Z-factor is almost zero) system is still very sensitive to isotope substitution.
Even very small $\kappa_{exp} = 0.94$ gives significant effect



1. Independent Einstein oscillator model gives qualitative explanation of the isotope effect.
2. The actual magnitude of the isotope effect is one order of magnitude larger due to closeness to self-trapping point.

1. Closeness to the self-trapping point increases sensitivity of the system to the isotope substitution

2. The t-J model is in the strong coupling regime while still far away from independent Einstein oscillator model regime