

# Angle Resolved Photoemission Spectroscopy

Dan Dessau  
University of Colorado, Boulder  
Dessau@Colorado.edu



# ARPES for studies of superconductivity.

## Measurements of

- Band structures (E vs. k), Fermi surfaces, and orbital symmetries.
  - Particularly important for correlated electron systems where band theory has limited applicability
- Superconducting gaps as a function of k, T, doping
- Pseudogaps as a function of k, T, doping
- Self-energy effects/dynamics (many-body interactions, electron-electron, electron-boson) as a function of k, T, doping
- Non-equilibrium physics using ultrafast pump-probe ARPES

## Compared to other spectroscopies:

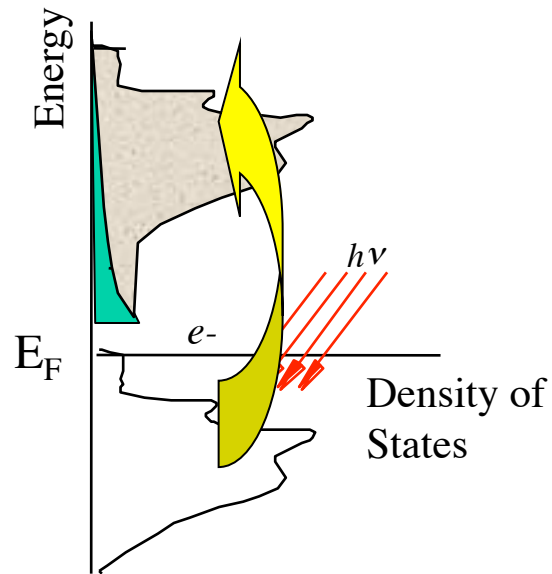
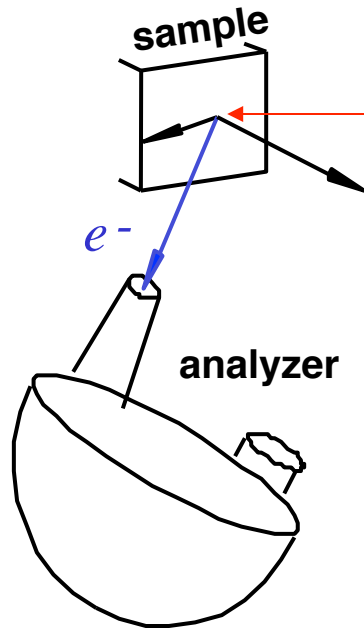
- The k resolution is unique. Arguably the most direct of all spectroscopies.
- Surface sensitive. Requires high quality surfaces for studies of “bulk” physical effects. Laser-ARPES has improved this somewhat.
- Energy resolution ( $\sim 1$ -20 meV scale) and base temperatures (2-15K) still somewhat limited.
- Spatially averaged (typically 50 microns and up). NanoARPES with 10 nm spatial scale is coming.
- Only measures the occupied states, though at elevated temperatures some states above  $E_F$  are thermally occupied.
- Still developing rapidly.

# Plan

- Discussion of the technique. Main principles early on. More detailed or subtle issues later, as needed.
- Cover a number of case studies, mostly from the p-type cuprates Bi2212 and Bi2201. These have the best cleaved surfaces and have been the most studied by ARPES and STM. They are also “dirtier” than many other cuprates.
  - Some discussion of n-type cuprates if time allows. Minimal on other p-type cuprates.
- Focus on the case studies where ARPES has made the largest initial impacts, and/or where it is uniquely suited to answer a critical question or open a new line of thought. Partially historical in nature.
- Early studies focused more on peak tracking, using older ideas of FL theory (even if FL theory fails). Most recent studies are able to bring real quantitative accuracy, even in the presence of disorder. Are directly connecting to transport, thermodynamics, etc.
- Topics: Evolution of electronic structure from the parent Mott state, Fermi surfaces and Fermi arcs, superconducting gaps, pseudogaps, self-energy effects, etc.

# Introduction to the ARPES technique (basics)

# Photoemission Spectroscopy



High K.E. Low B.E.

Low K.E. High B.E.

Primary electrons – no scattering events.  
Contain information of the electron  
spectral function

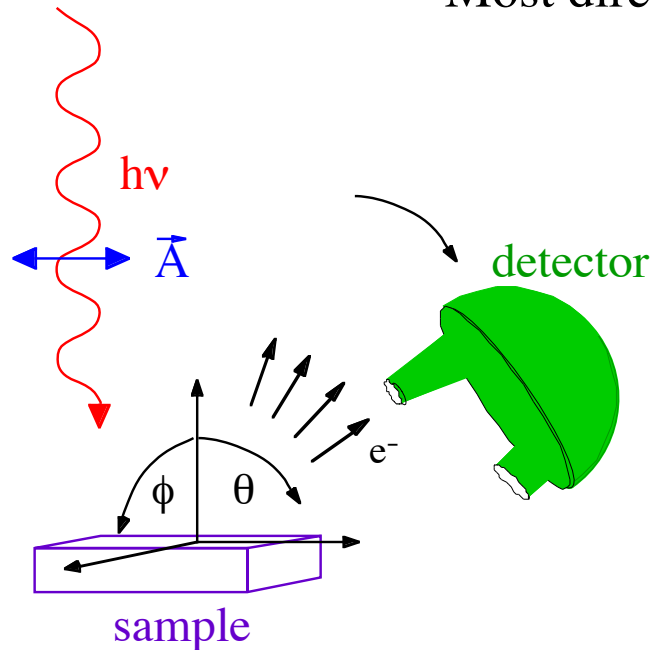
Secondary electrons (inelastic  
background) – increases with decreasing  
kinetic energy.

$$E_{kin} = \hbar\omega - \Phi - |E_B|$$

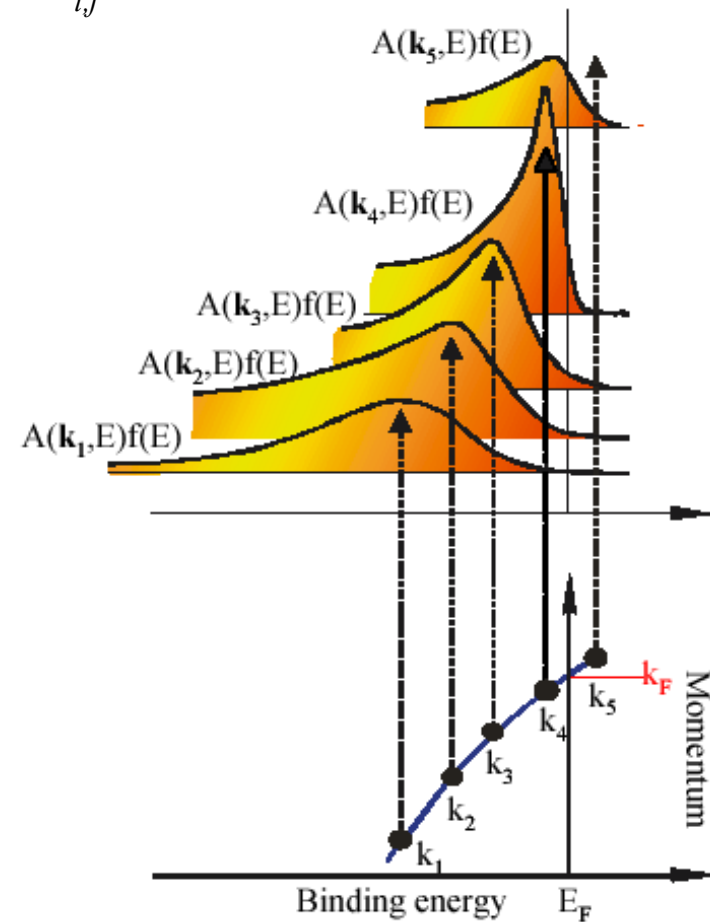
# Angle Resolved Photoemission (ARPES)

## A momentum resolved spectroscopy

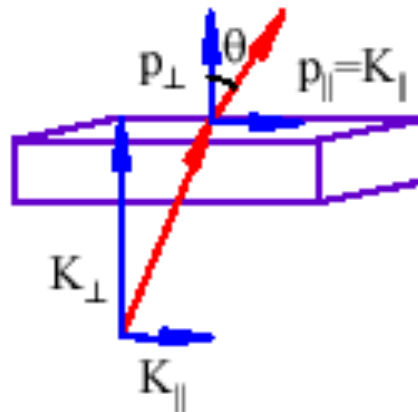
Most direct way to measure E vs. k of a solid.



$$\text{Intensity} \propto \sum_{i,f} \left| \langle f | \vec{p} \cdot \vec{A} | i \rangle \right|^2 A(\vec{k}, E) f(E)$$

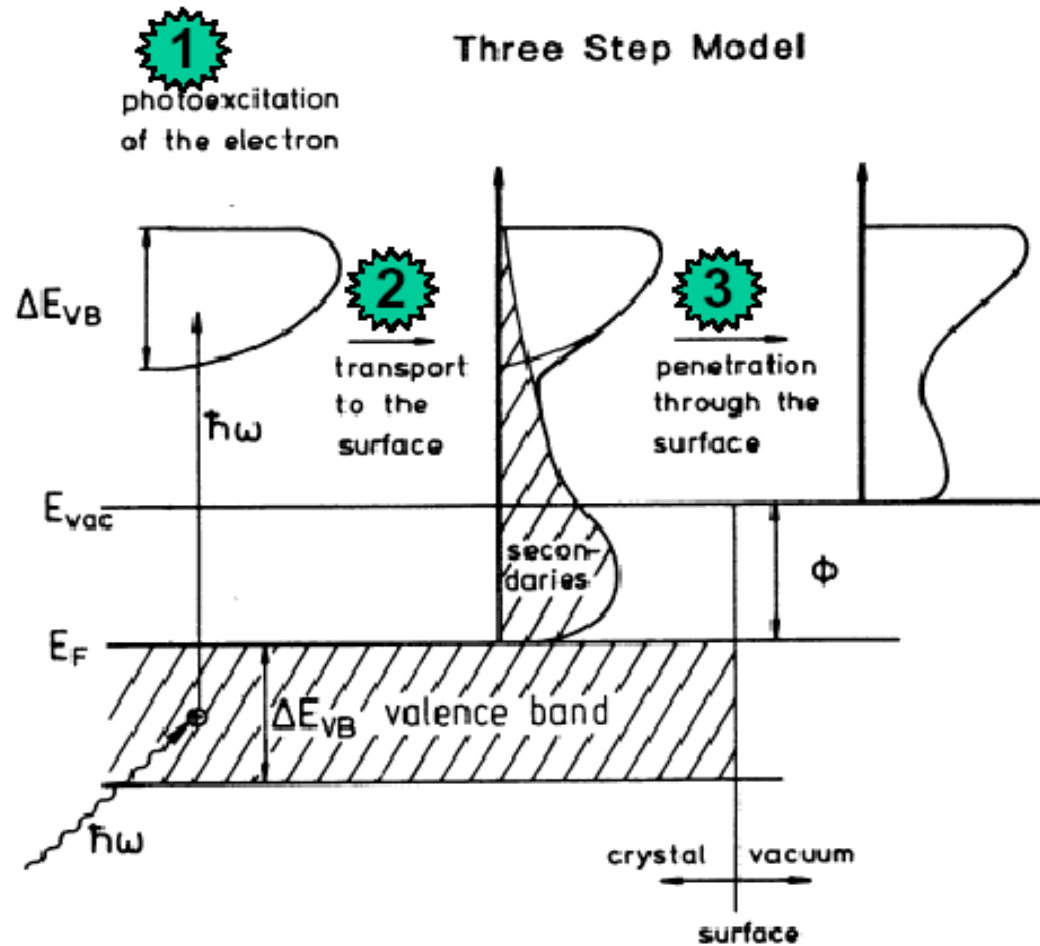


Electron momentum  
Parallel to the surface is  
conserved



# Three Step Model

## W.E. Spicer

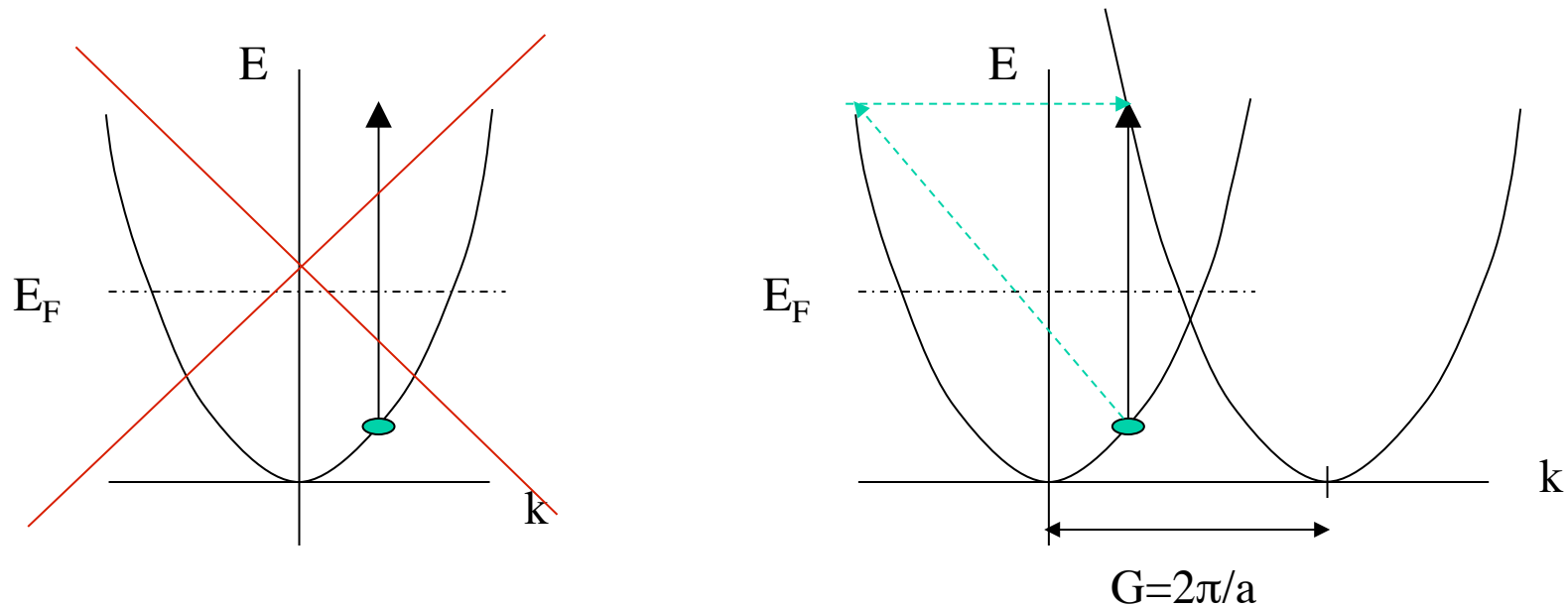


“One-step” models in which the photoemission process is considered as a single quantum mechanical event are more accurate, but not as illuminating.

# Momentum Conservation

Photons of a few hundred eV or less carry negligible momentum compared to the typical electron momentum scales in a solid.

Therefore we consider “vertical” transition processes. For a free electron parabola there would be no final state and the process is forbidden.



The vertical transition is allowed by considering the extended zone scheme and employing a reciprocal lattice vector  $G=2\pi/a$  (the lattice degree of freedom takes care of the “missing” momentum).



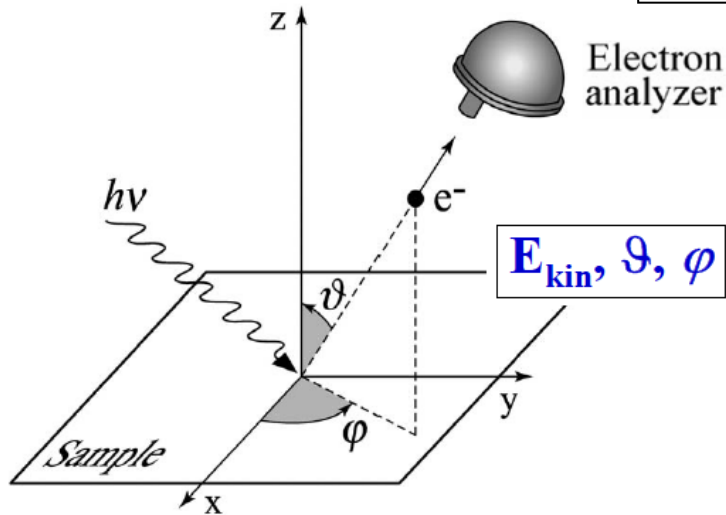
## 2D compounds

- Can ignore  $k_z$  dispersion.
- Need not vary photon energy to map out Fermi surface and high symmetry directions.
- Less final state broadening. Intrinsic initial-state linewidths can be studied.
- Usually much better cleaved surfaces

# Angle Resolved Photoemission (ARPES)

→ k-resolved electronic structure

$$E_{kin} = h\nu - \Phi - E_i$$



$$\mathbf{K} = \mathbf{p} / \hbar = \sqrt{2mE_{kin}} / \hbar$$

$$K_x = \frac{1}{\hbar} \sqrt{2mE_{kin}} \sin \vartheta \cos \varphi$$

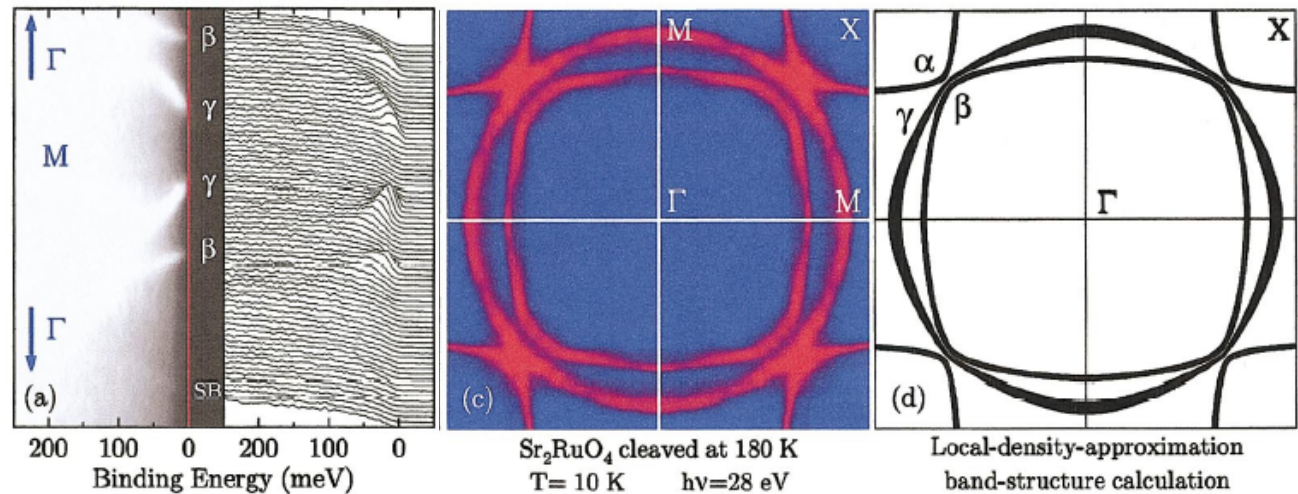
$$K_y = \frac{1}{\hbar} \sqrt{2mE_{kin}} \sin \vartheta \sin \varphi$$

$$K_z = \frac{1}{\hbar} \sqrt{2mE_{kin}} \cos \vartheta$$

Peak tracking - measure E vs. k, Fermi surfaces, etc.

Example 2D compound

$\text{Sr}_2\text{RuO}_4$  Fermi Surface  
Damascelli and Shen  
PRL 2000

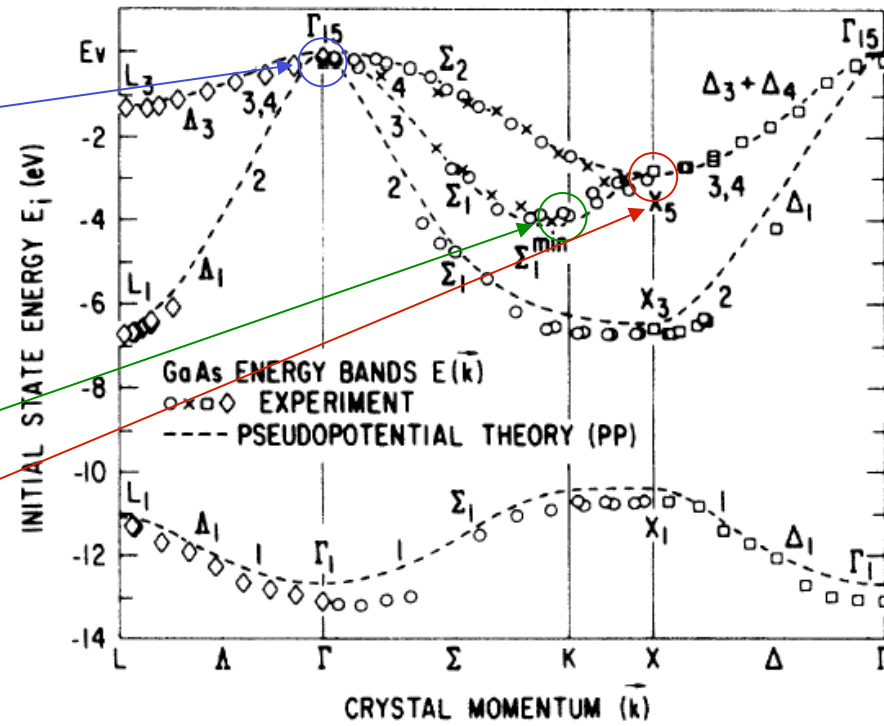
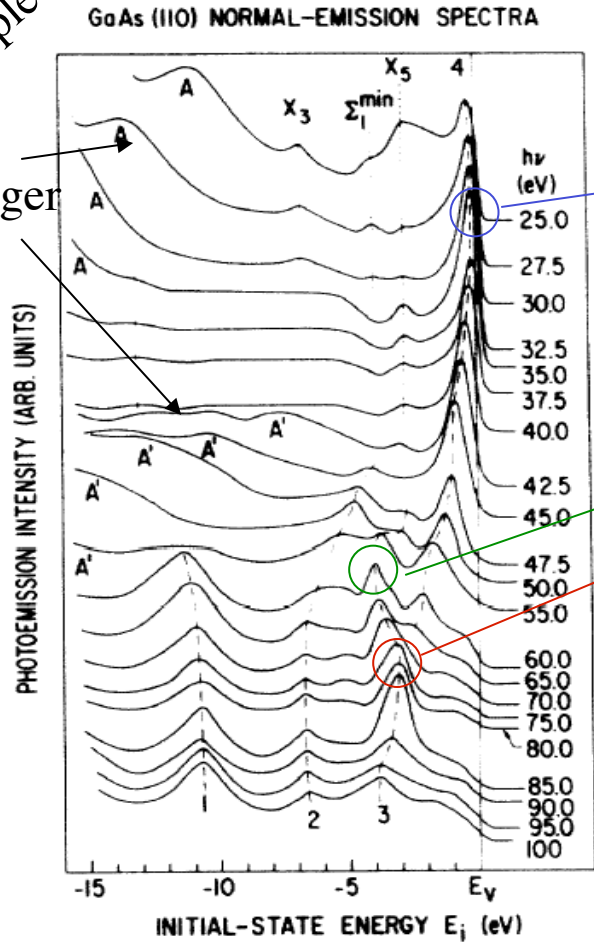


### Angle-resolved photoemission, valence-band dispersions $E(\vec{k})$ , and electron and hole lifetimes for GaAs

T.-C. Chiang, J. A. Knapp,\* M. Aono,<sup>†</sup> and D. E. Eastman  
 IBM Thomas J. Watson Research Center, Yorktown Heights, New York 10598  
 (Received 3 December 1979)

Example 3D compound

Auger



Angle-resolved photoemission, valence-band dispersions  $E(\vec{k})$ , and electron and hole lifetimes for GaAs

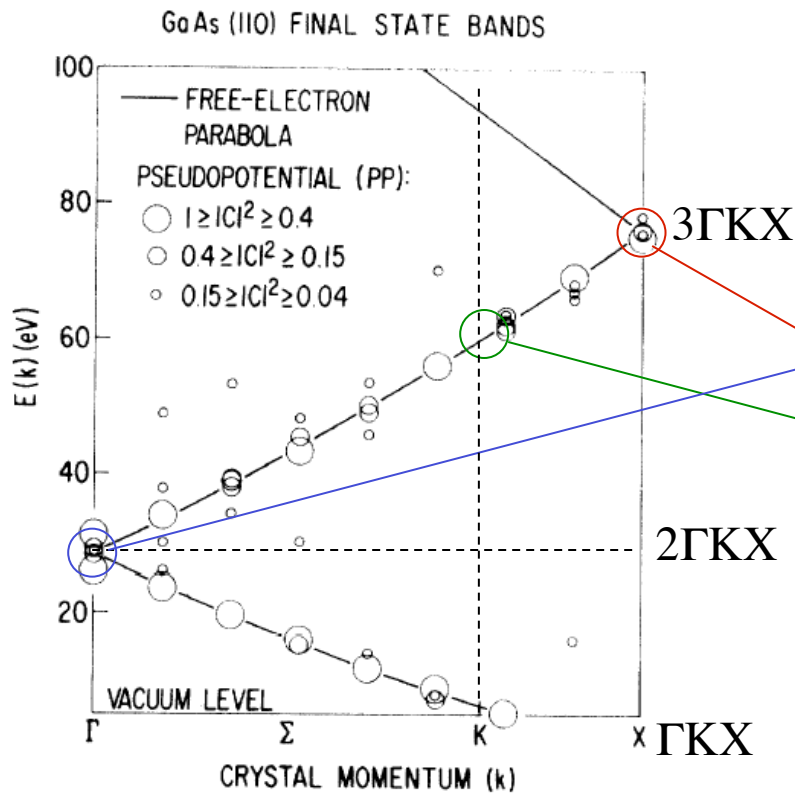
T.-C. Chiang, J. A. Knapp,\* M. Aono,† and D. E. Eastman  
 IBM Thomas J. Watson Research Center, Yorktown Heights, New York 10598  
 (Received 3 December 1979)

Example 3D compound

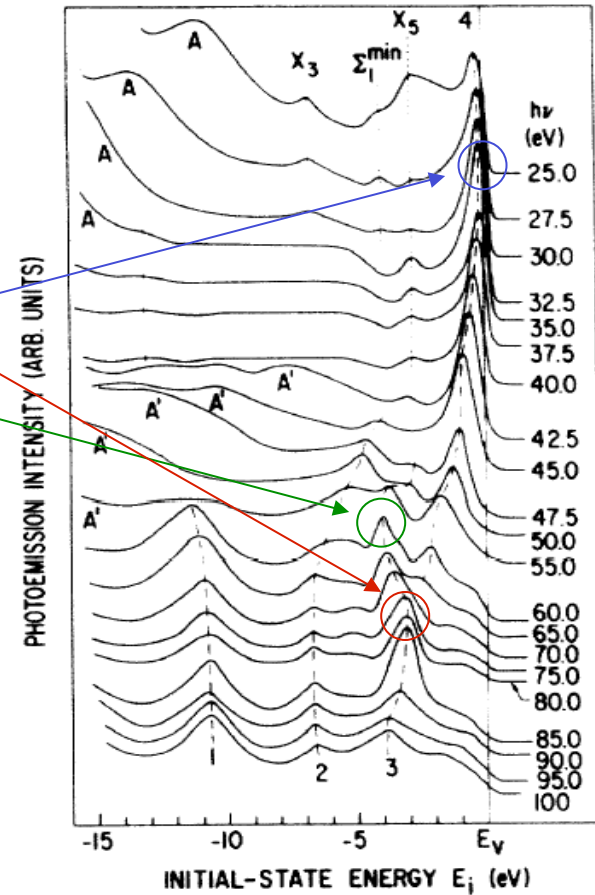
Normal emission: theta=0

$$\hbar k_{\parallel} = 0$$

$$\hbar k_{\perp} = [2m(E_i + e\Phi - E_0)]^{1/2}$$



GaAs (110) NORMAL-EMISSION SPECTRA



## Matrix Element for Photoemission

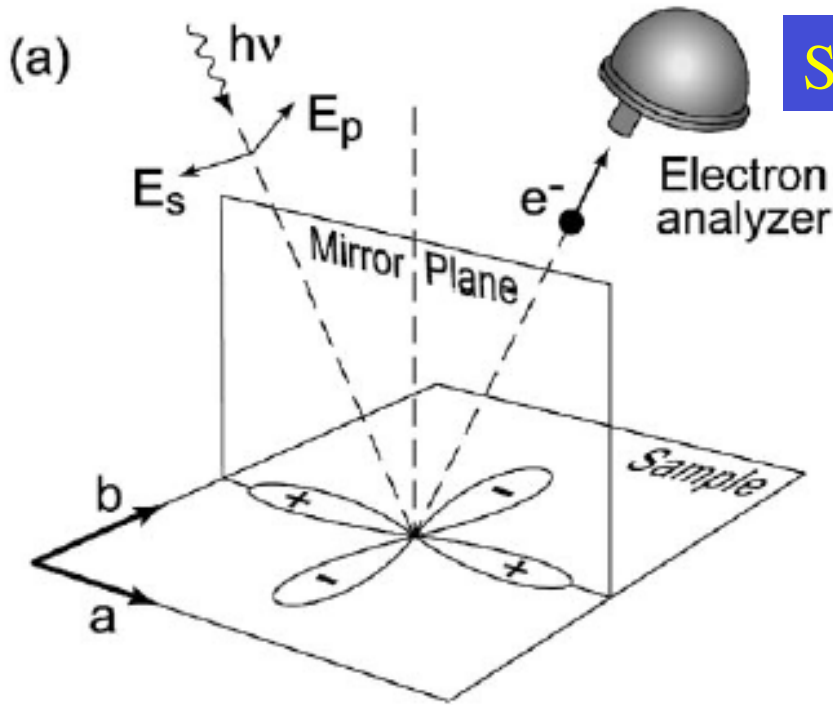
**Perturbation Theory gives Fermi's Golden Rule for transition probability**

$$w = \frac{2\pi}{\hbar} \left| \langle \psi_f | H_{\text{int}} | \psi_i \rangle \right|^2 \delta(E_f - E_i - \hbar\omega)$$

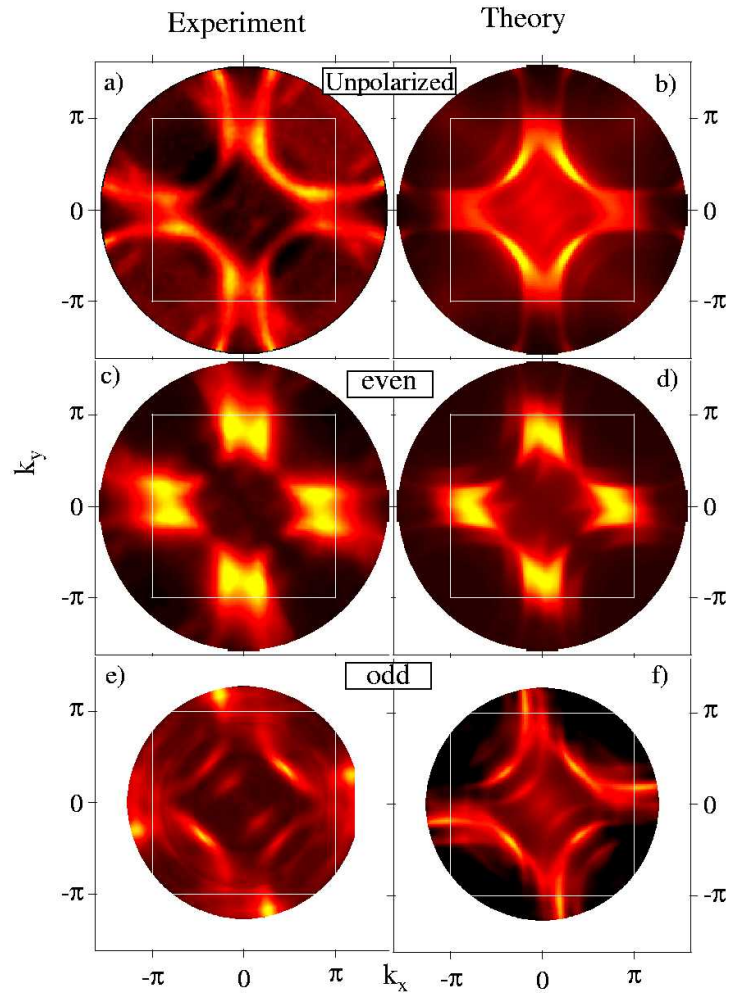
**For dipole allowed transitions,**

$$H_{\text{int}} = \frac{e}{mc} \mathbf{A} \cdot \mathbf{p}$$

# Symmetry Analysis



E field



Bansil group.

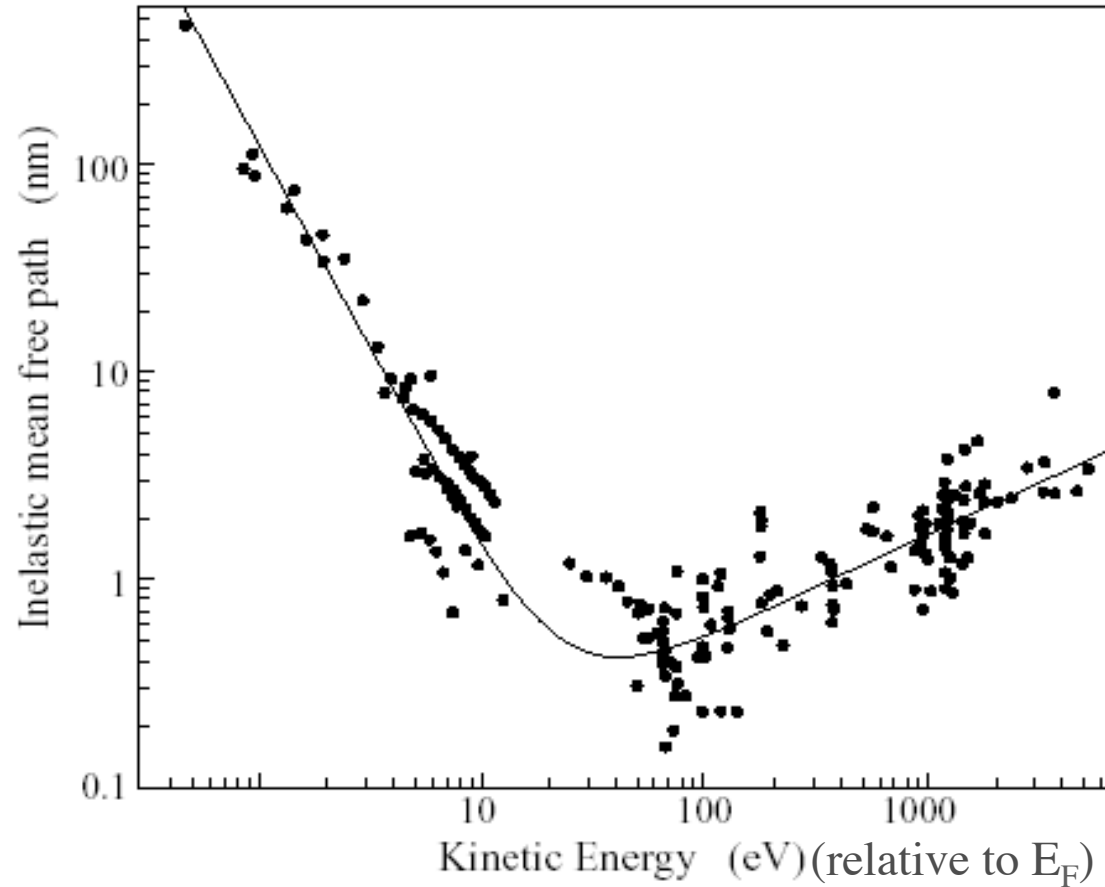
$$\langle \phi_f^{\mathbf{k}} | \mathbf{A} \cdot \mathbf{p} | \phi_i^{\mathbf{k}} \rangle \begin{cases} \phi_i^{\mathbf{k}} \text{ even } \langle + | + | + \rangle \Rightarrow \mathbf{A} \text{ even} \\ \phi_i^{\mathbf{k}} \text{ odd } \langle + | - | - \rangle \Rightarrow \mathbf{A} \text{ odd.} \end{cases}$$

The matrix element is integrated over all space.  
 The integration axis of interest here is perpendicular to a chosen mirror plane.  
 If net odd symmetry, then the matrix element integrates to exactly zero.

Powerful method for selecting out the spectral contribution from various initial-state symmetry states/orbitals.

# Surface sensitivity – electron kinetic energy “Universal Curve”

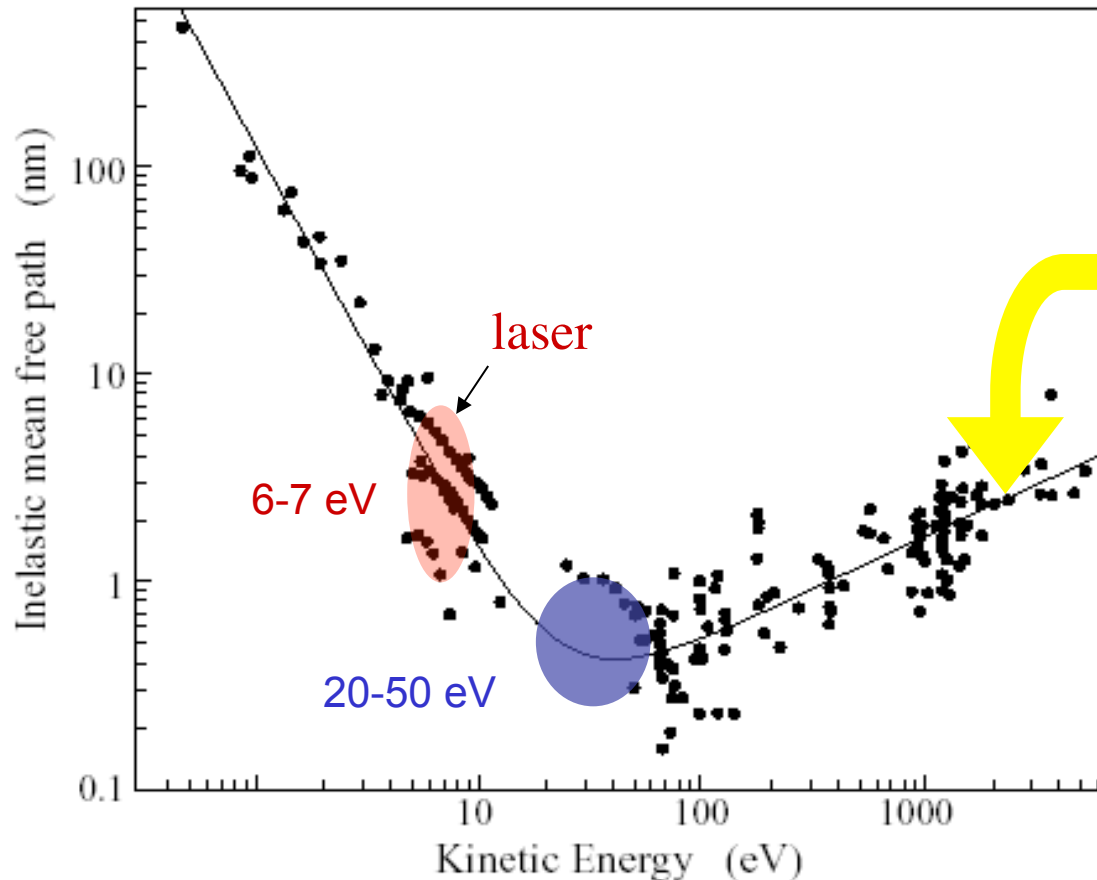
Can be an advantage or a disadvantage!



←  
Decreasing phase space for  
excitations (plasmons, e-h  
pairs, etc.)

→  
Decreasing interaction  
times.

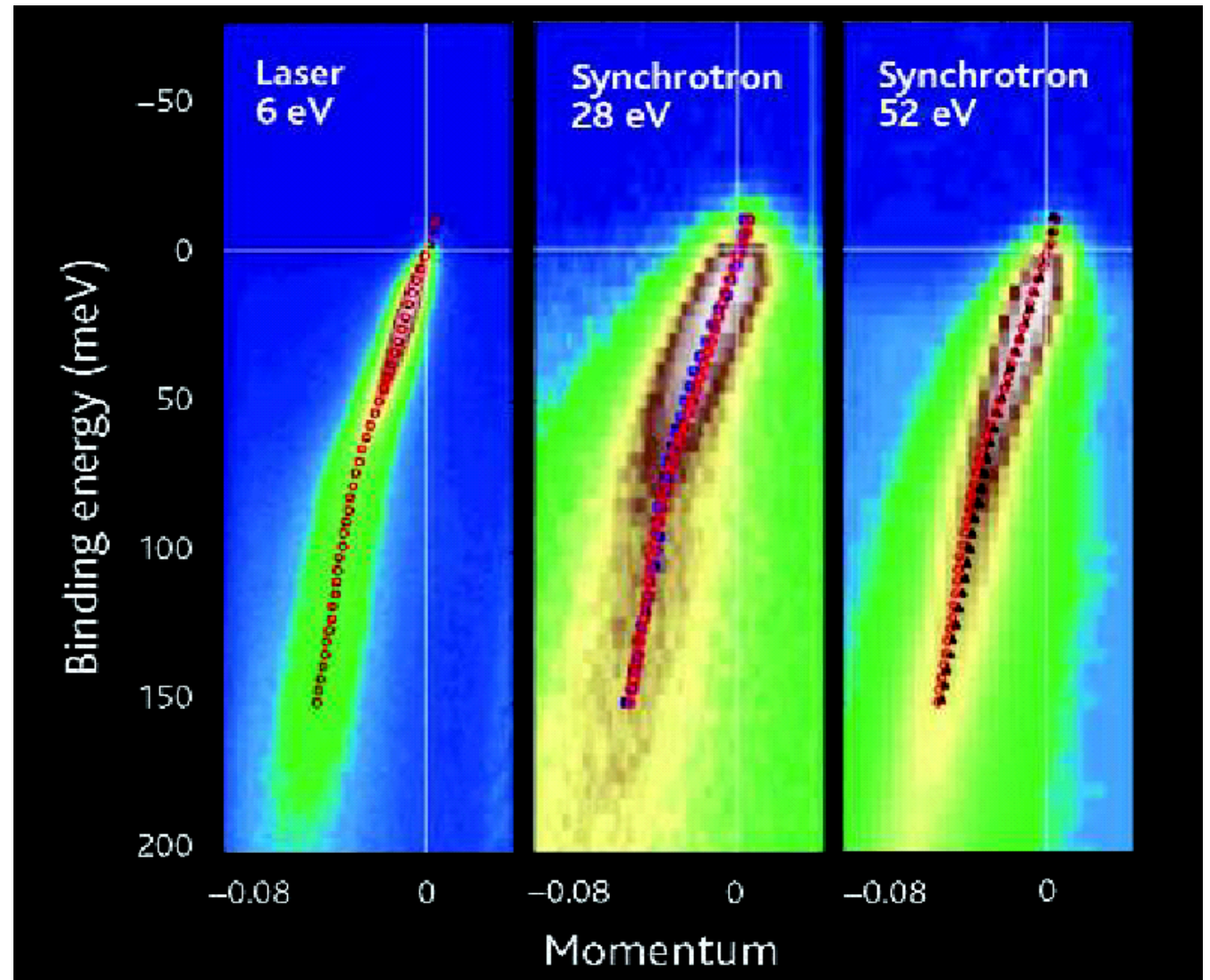
## Surface sensitivity – electron kinetic energy



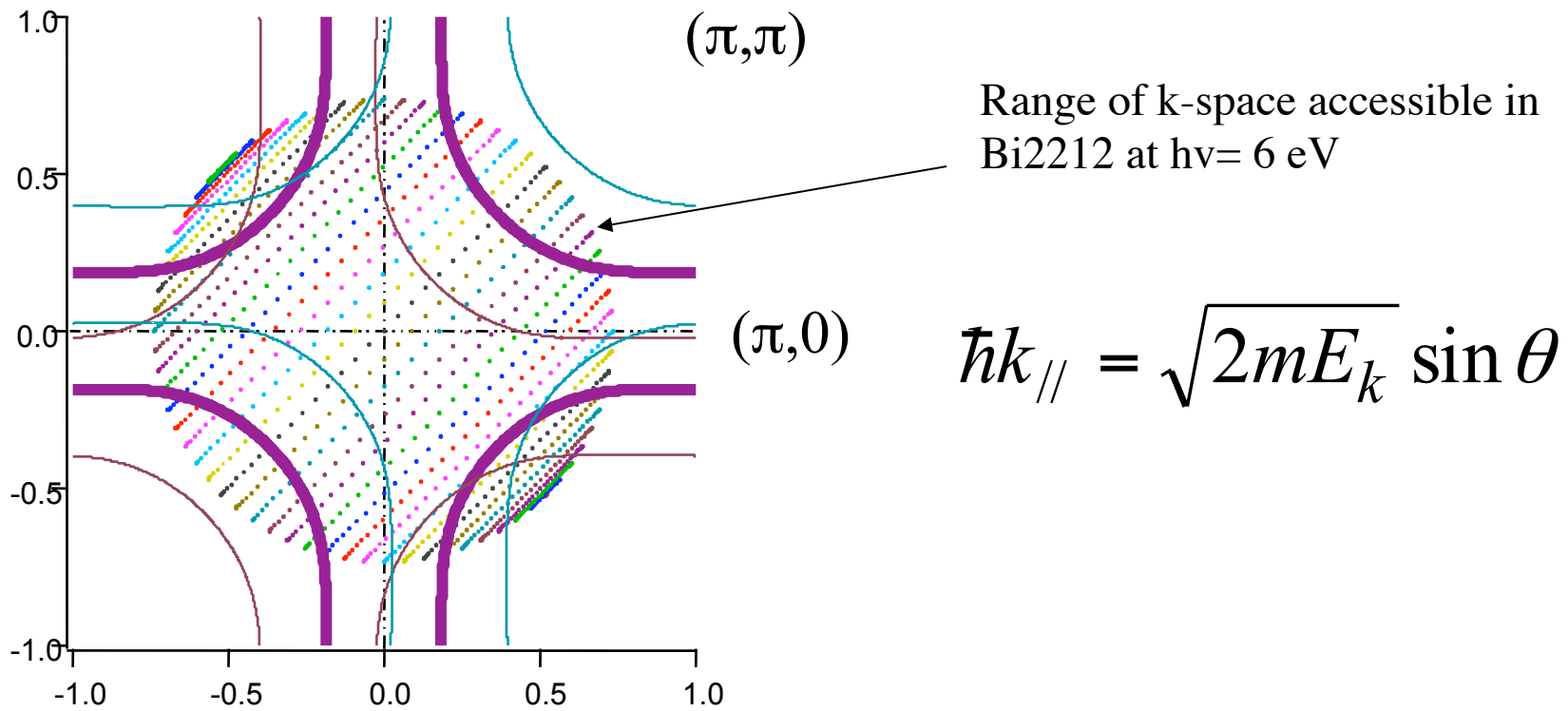
→ Laser-ARPES is 3-10 times more bulk sensitive than standard ARPES  
Very helpful for studies of “bulk” physics.



ARPES dispersion  
along the nodal line  
of  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$   
 $T \sim 20\text{K}$

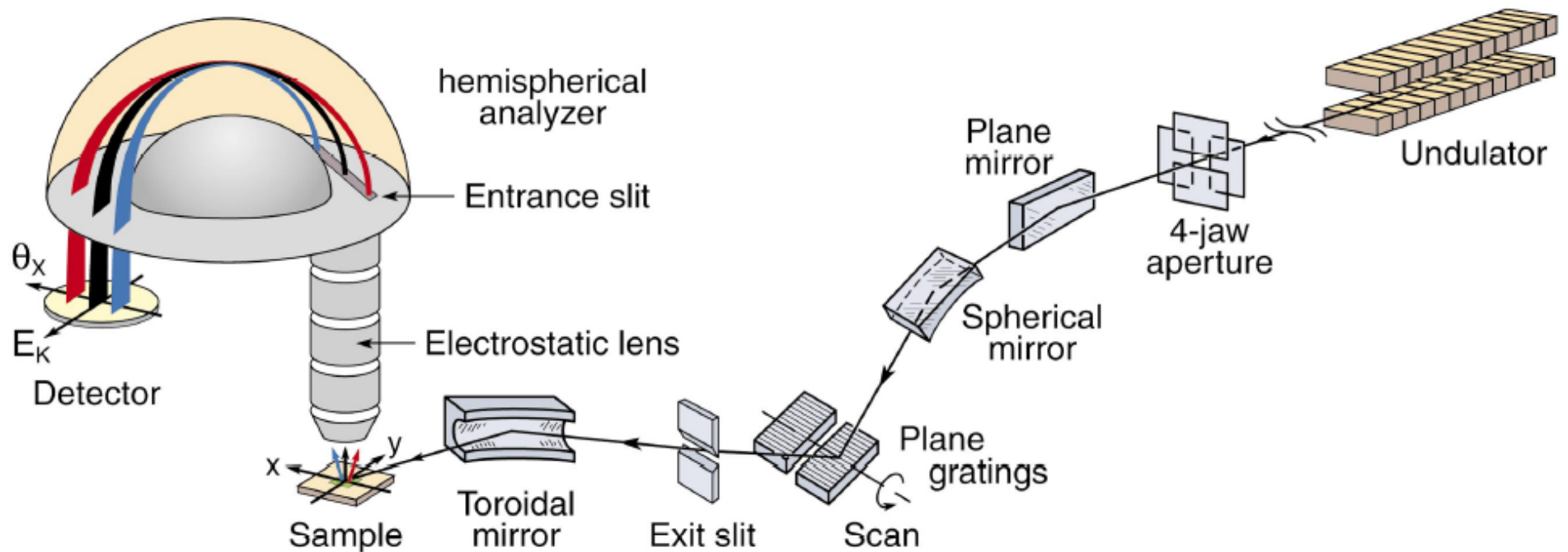


## Resolution and k-space effect



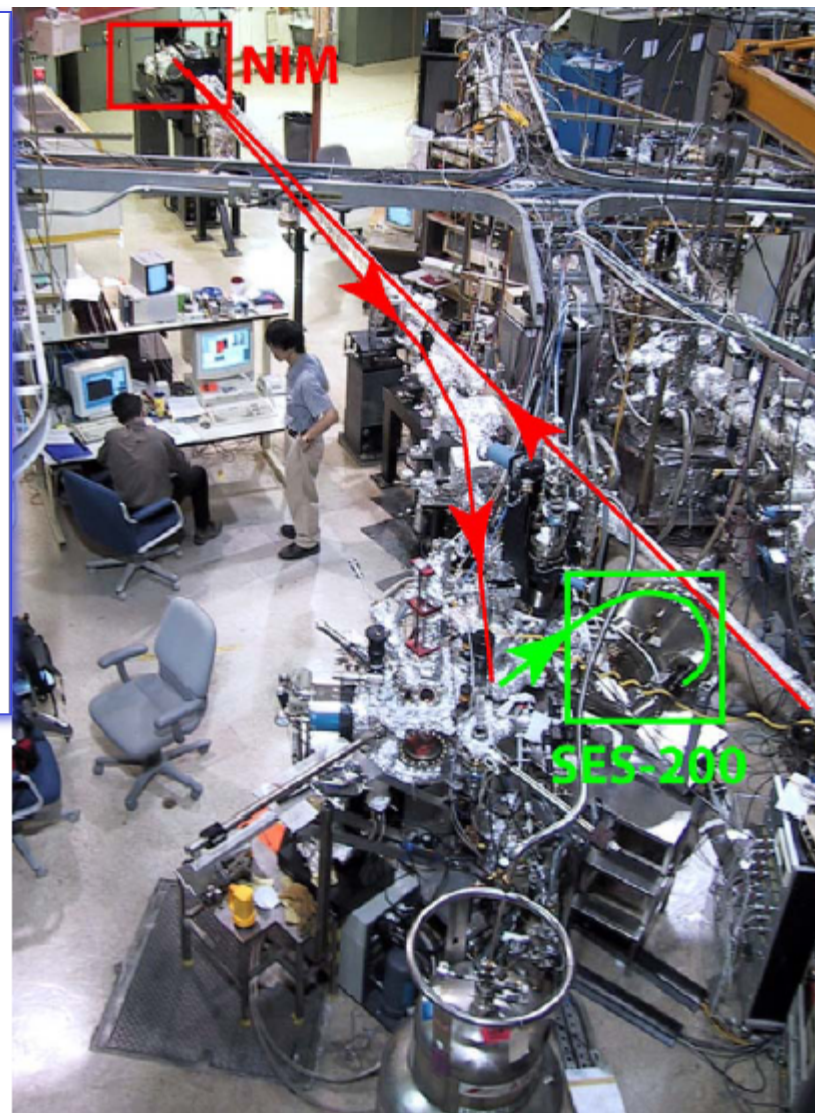
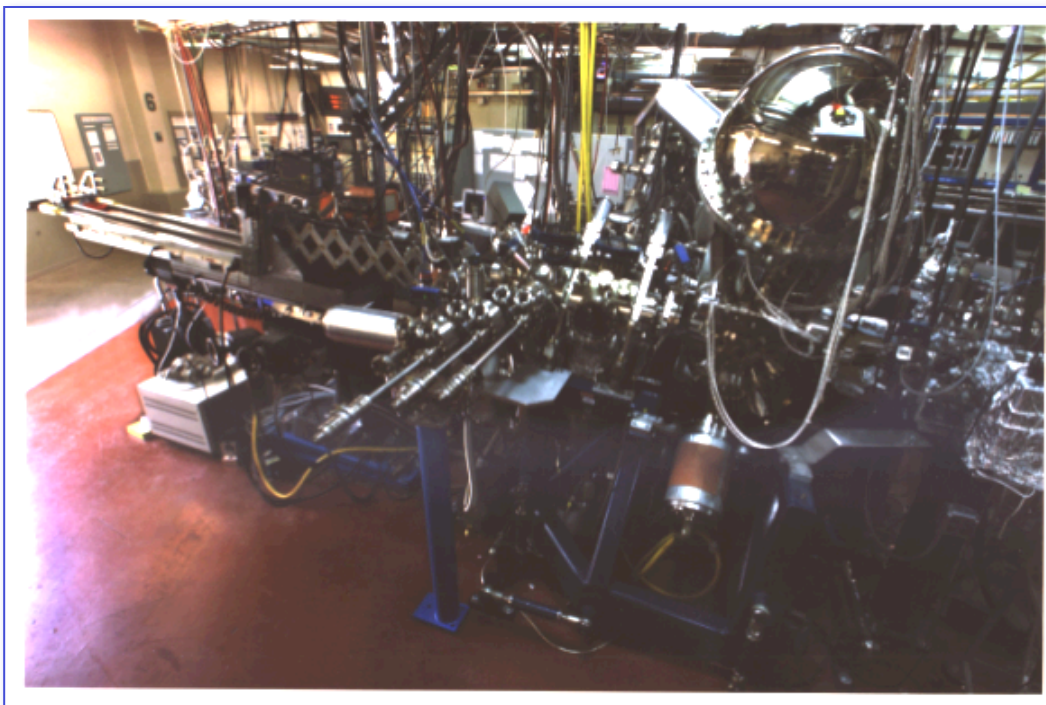
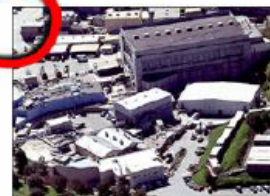
- For the same angular resolution, the k resolution at low E is superior.
- k resolution translates to E widths if the peak is dispersive.  
For nodal states &  $\pm .15$  degree angular resolution,  
5 meV broadening for  $h\nu = 6$  eV, 38 meV for  $h\nu = 52$  eV.
- However – relatively small range of k-space accessible.

# Typical synchrotron beamline for ARPES





STANFORD SYNCHROTRON RADIATION LABORATORY

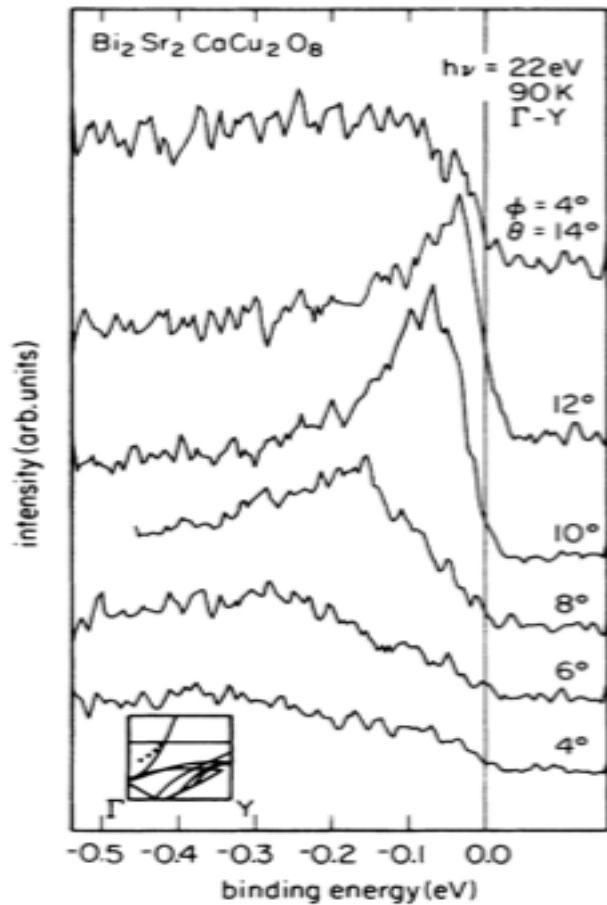


- UHV analysis chamber ( $10^{-11}$  Torr)
- 5 or 6 axis, He cooled sample manipulators
- Load-Lock transfer system
- Samples may be cleaved in UHV

Band dispersions, Fermi surfaces, etc.

# ARPES compared to LDA band structure.

Normal state near-optimal Bi2212 along the nodal line.

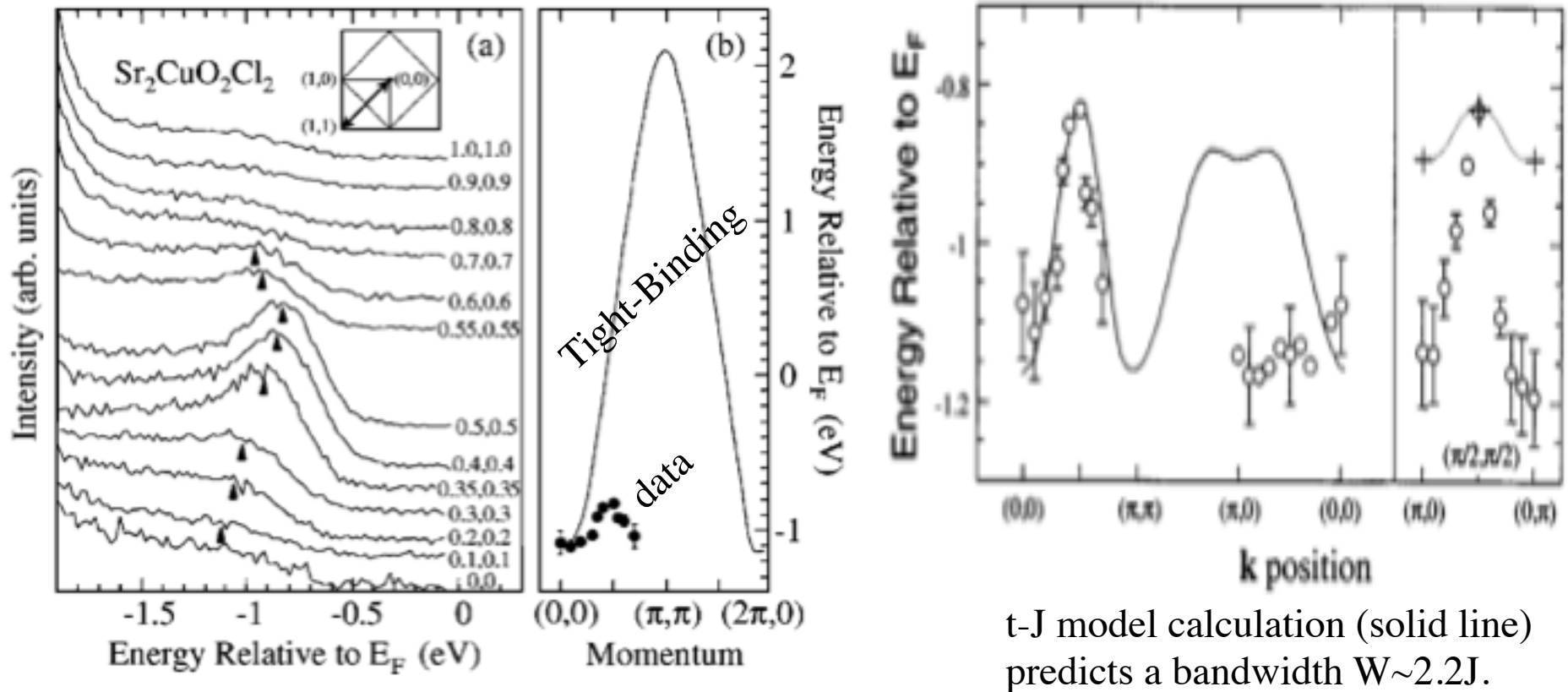


~ a factor of two mass enhancement compared to LDA.

C.G. Olson et al., PRB 1990

# *E* versus *k* Relations and Many Body Effects in the Model Insulating Copper Oxide $\text{Sr}_2\text{CuO}_2\text{Cl}_2$

Wells et al. 1994, 1995



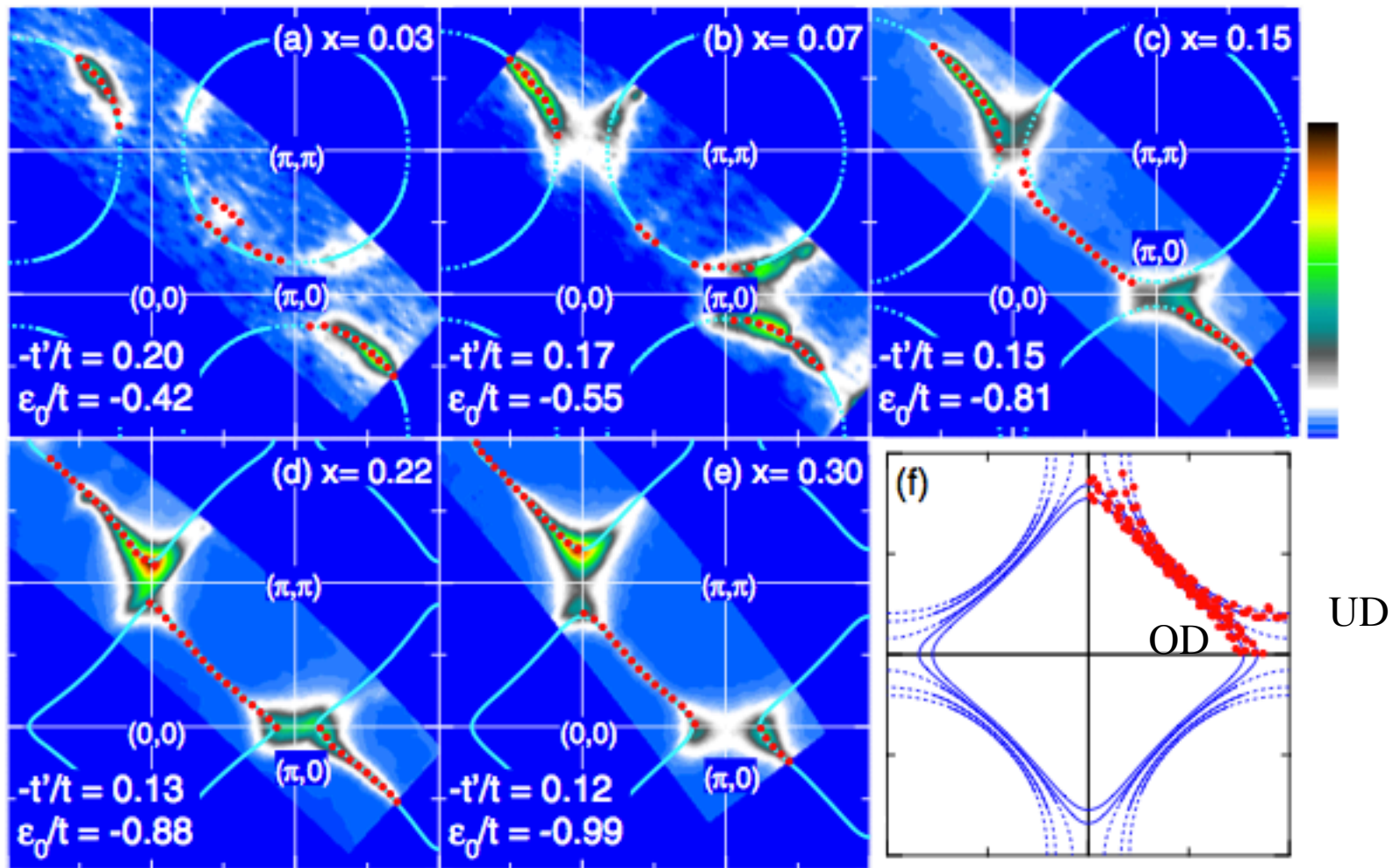
$t$ - $J$  model calculation (solid line)  
predicts a bandwidth  $W \sim 2.2J$ .

It is natural to expect that doping with holes should give a small pocket centered at  $(\pi/2, \pi/2)$

# Fermi surface mapping vs hole doping level in $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$

J. Phys.: Condens. Matter **19** (2007) 125209

T Yoshida *et al*



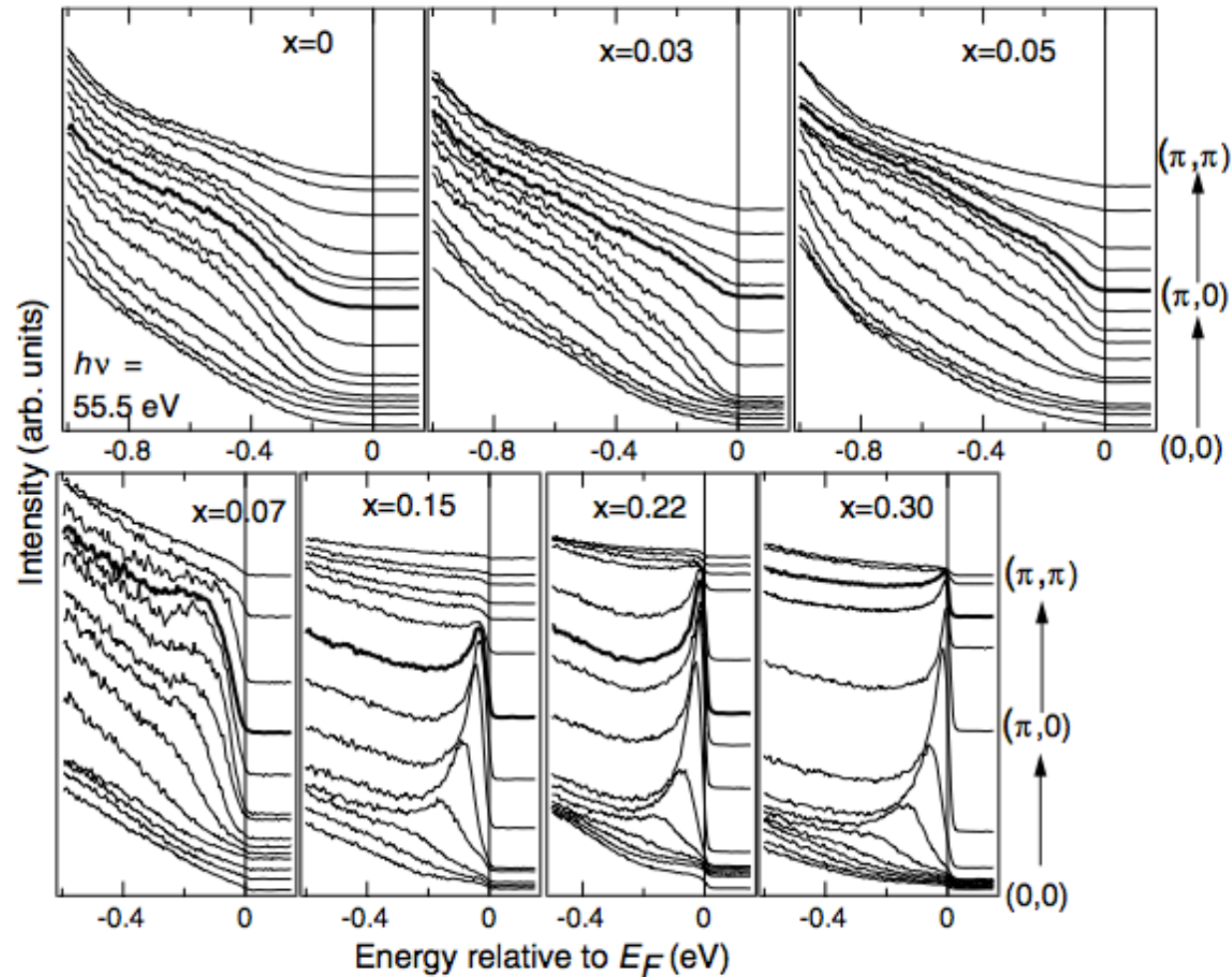
There is a locus of low energy states that is large and centered at the zone corner (UD) or the zone center (OD).



# Nodal cut band dispersion vs hole doping level in $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$

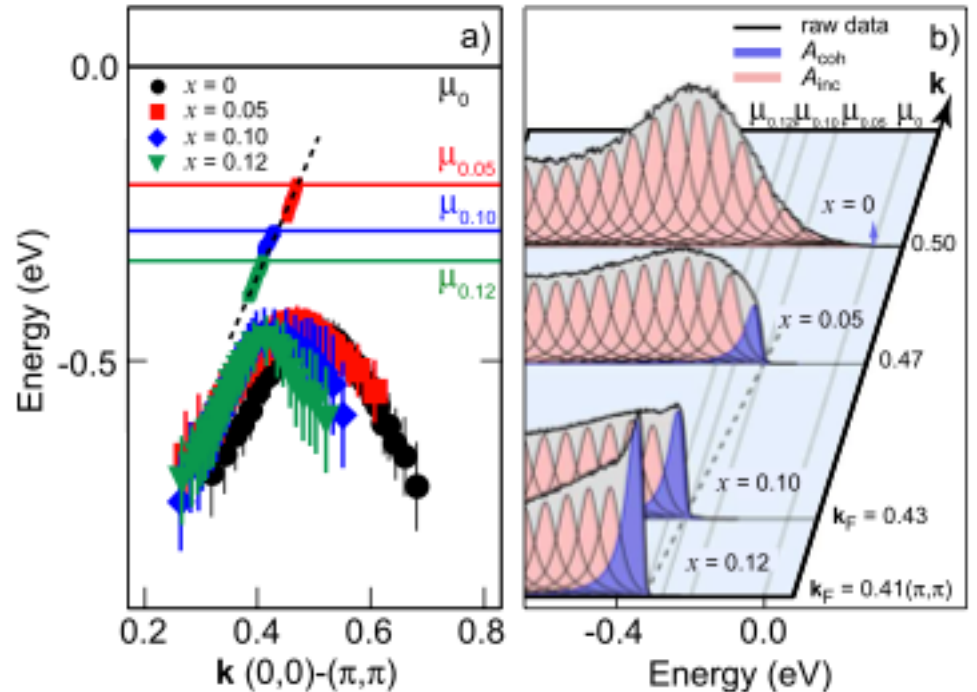
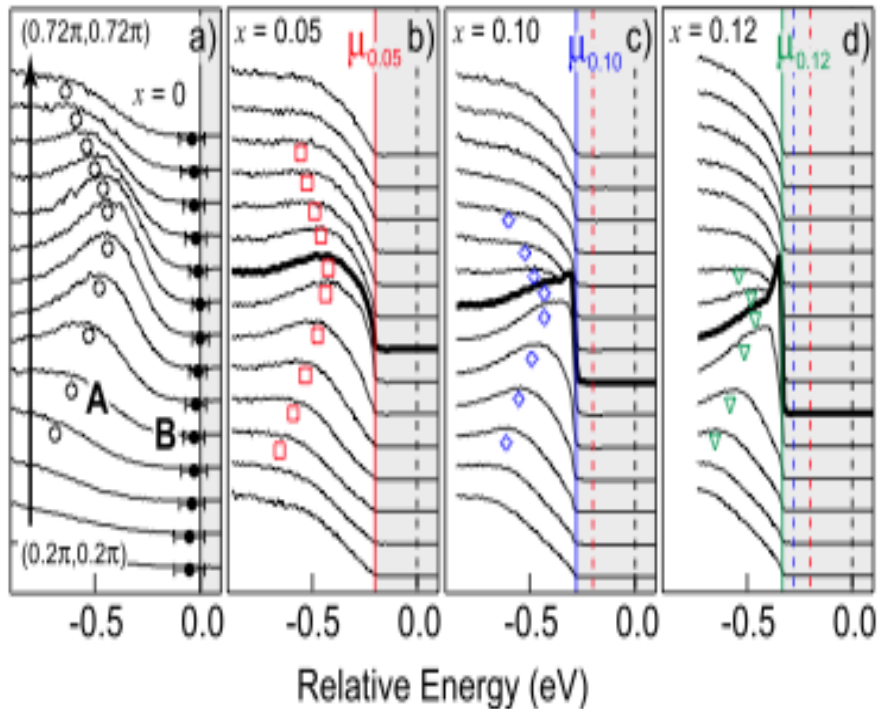
J. Phys.: Condens. Matter **19** (2007) 125209

T Yoshida *et al*



The spectral peaks are very broad and low intensity for UD. A very different type of doping evolution than for a normal semiconductor. Also not what is naively expected for doping the Mott insulator (no small pocket).

# Na-doped $\text{Ca}_2\text{CuO}_2\text{Cl}_2$



K. Shen, Z-X Shen, PRL 2004

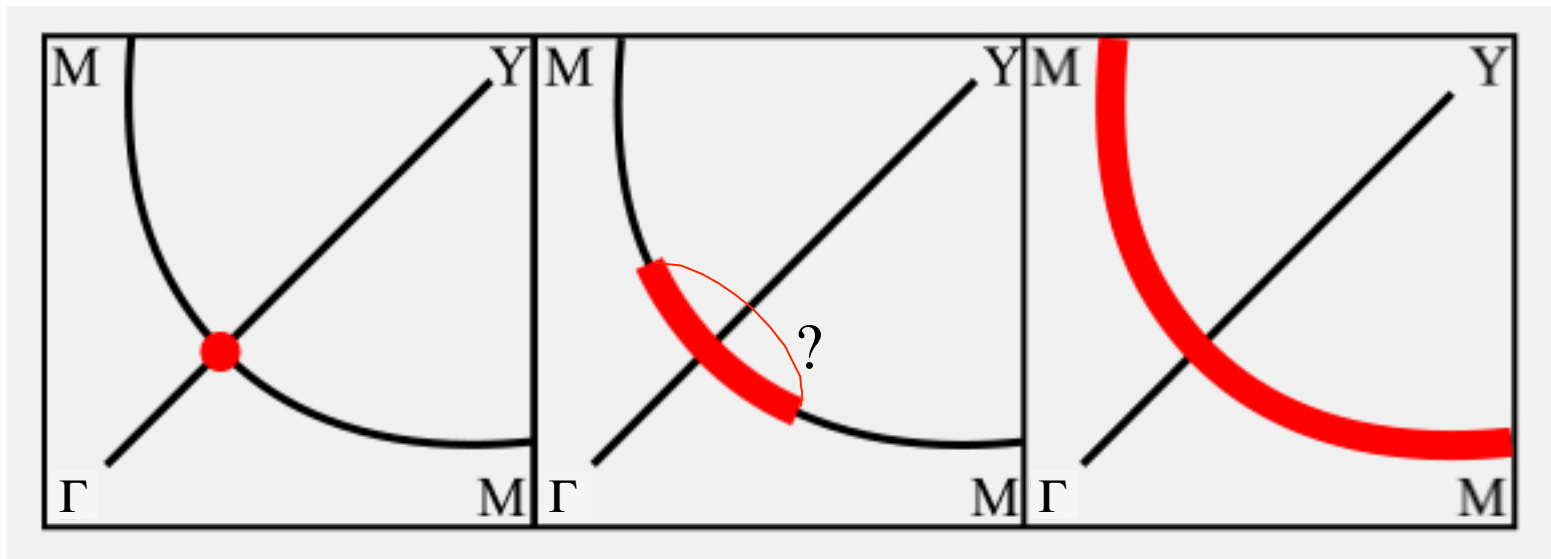
Interpretation put forward: The majority of the dispersive peak is an incoherent superposition of many Franck-Condon-broadened loss peaks. The zero-loss peak with weight  $Z$  is the quasiparticle, with  $Z$  vanishingly small for low doping.

Q: Why is the dispersion of the sharp peak independent of doping? This is to first-order inconsistent with a varying  $Z$ .

# Fermi arcs

Another aspect of the Fermi surface that deviates from conventional is that of the “Fermi arcs”, which are small discontinuous portions centered around the nodal directions.

The origin and phenomenology is still heavily debated, but nominally these are argued to be long and connected at high T or OD, and short/disconnected at low T, UD.

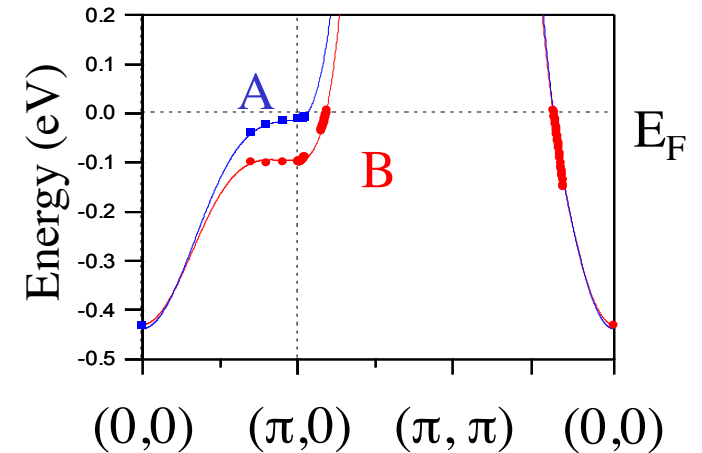
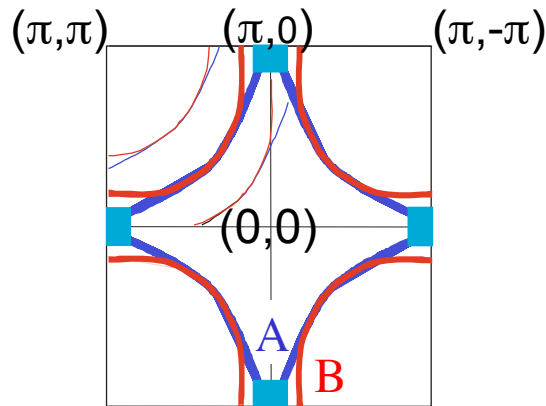


Truly truncated? Closed by a weak “shadow” piece on the back side? Made of quasiparticles?

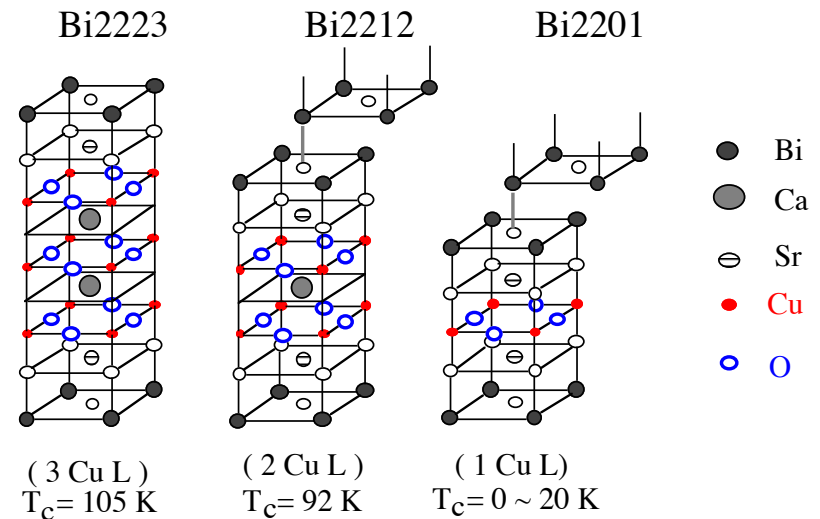
Will cover later in more detail.

# Bilayer Splitting in double-layer cuprates

BILAYER SPLITTING = 2 PIECES OF FS **Bonding** plus **Antibonding** band  
 Due to electronic coupling between the pair of  $\text{CuO}_2$  planes per unit cell  
 Superstructure bands exist as well.



$\Delta E \sim 100 \text{ meV.}$

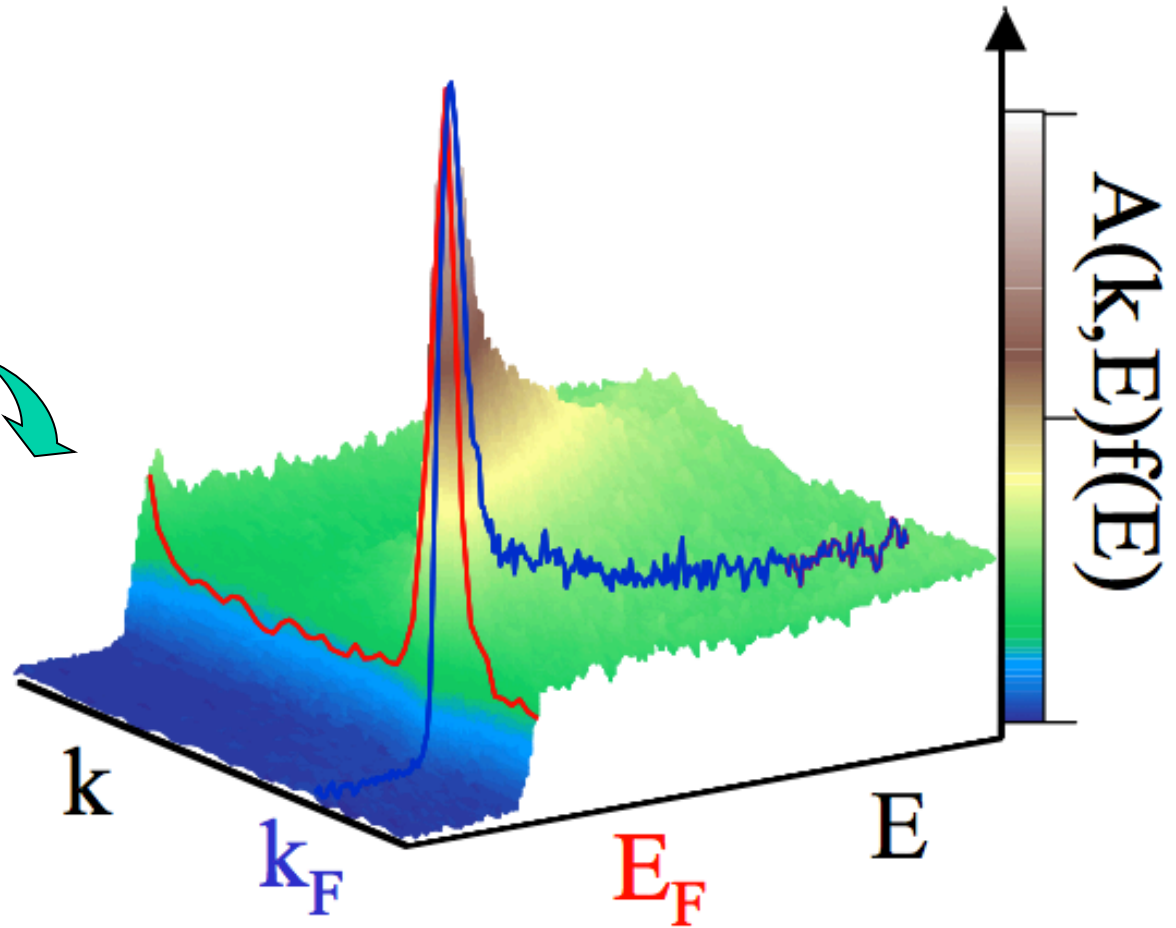
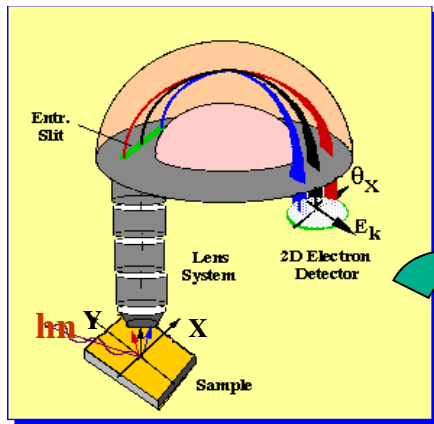


Y.D. Chuang et al, Phys. Rev. Lett. **87**, 117002 (2001))

2D detection (in energy and momentum)

EDCs and MDCs

## Two dimensional electron detection



Energy Distribution Curve  
(EDC)

Momentum Distribution  
Curve (MDC)

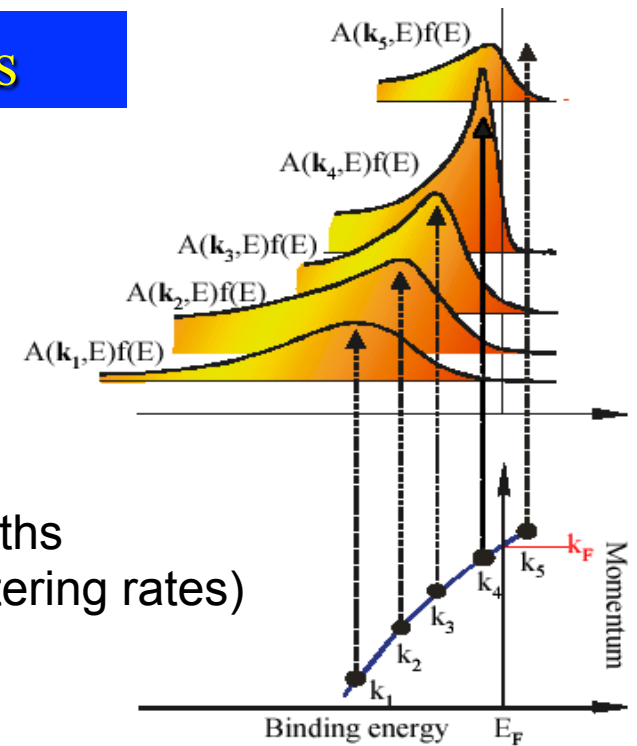
# ARPES peak widths and lineshapes

Spectral Function  $A(\mathbf{k}, \omega) = -\text{Im } G(\mathbf{k}, \omega)$

$$A(\mathbf{k}, \omega) = -\frac{1}{\pi} \frac{\Sigma''(\mathbf{k}, \omega)}{[\omega - \epsilon_{\mathbf{k}} - \Sigma'(\mathbf{k}, \omega)]^2 + [\Sigma''(\mathbf{k}, \omega)]^2}$$

Renormalized dispersion  
(e.g. kinks, mass renormalization)

Peak widths  
(Lifetimes or scattering rates)



Peak widths and lineshapes in cuprates are not understood.  
Marginal Fermi Liquid vs. Fermi Liquid?  
Is there a real qp peak in cuprates or not?

Shen & Schrieffer PRL 1997

Laughlin PRL, 1997

Casey, Dessau, Anderson Nat Phys 2008

& many many others.

When the peak is absent or broad, can we utilize the standard concepts of solids?

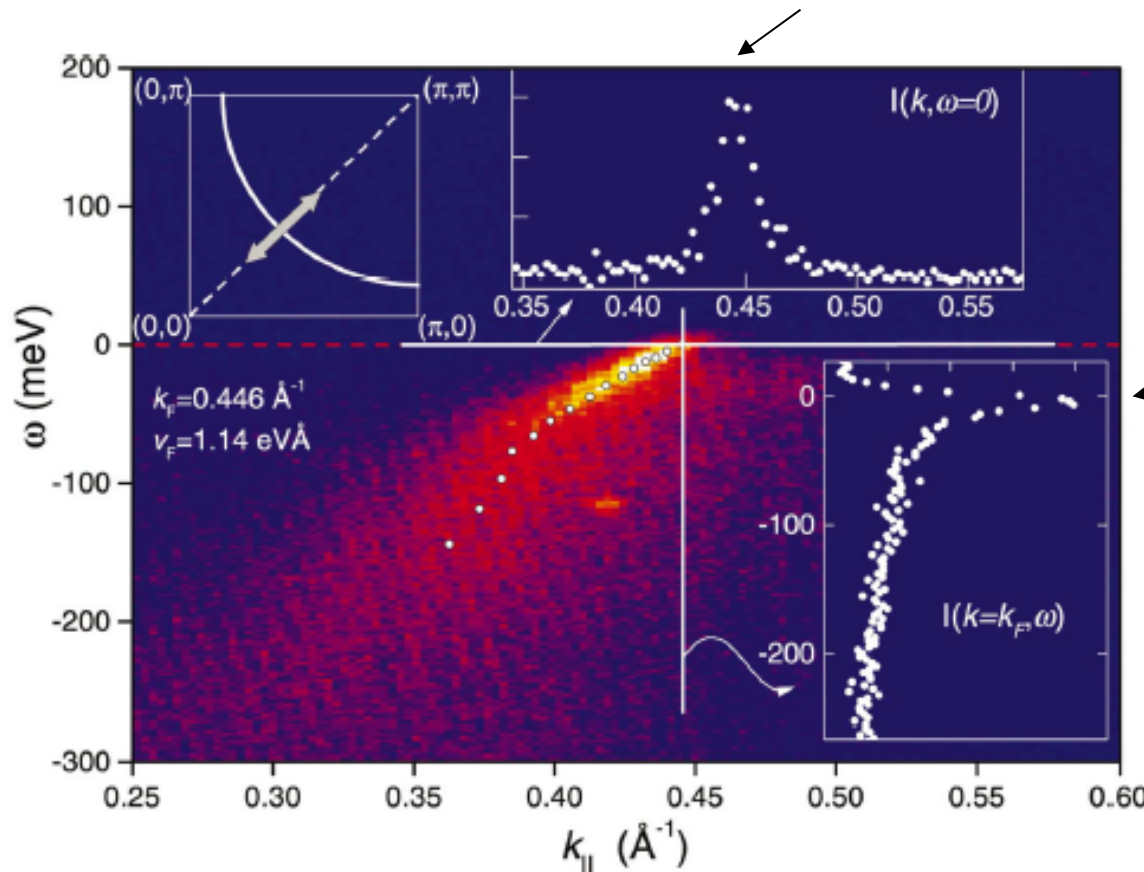
# 2D detection: high $T_c$ superconductor $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$

T. Valla,<sup>1</sup> A. V. Fedorov,<sup>1</sup> P. D. Johnson,<sup>1</sup> B. O. Wells,<sup>1,4</sup>  
 S. L. Hulbert,<sup>2</sup> Q. Li,<sup>3</sup> G. D. Gu,<sup>5</sup> N. Koshizuka<sup>6</sup>

24 SEPTEMBER 1999 VOL 285 SCIENCE

Momentum Distribution Curve (MDC)

Peak width  $\Delta k = 1/\lambda$ :  $\lambda$ =electron mean free path.



Energy Distribution Curve (EDC)

Peak width  $\Delta E = \hbar\bar{\nu}/\tau$   
 $1/\tau \sim$  scattering rate  
 $\tau \sim$  quasiparticle lifetime

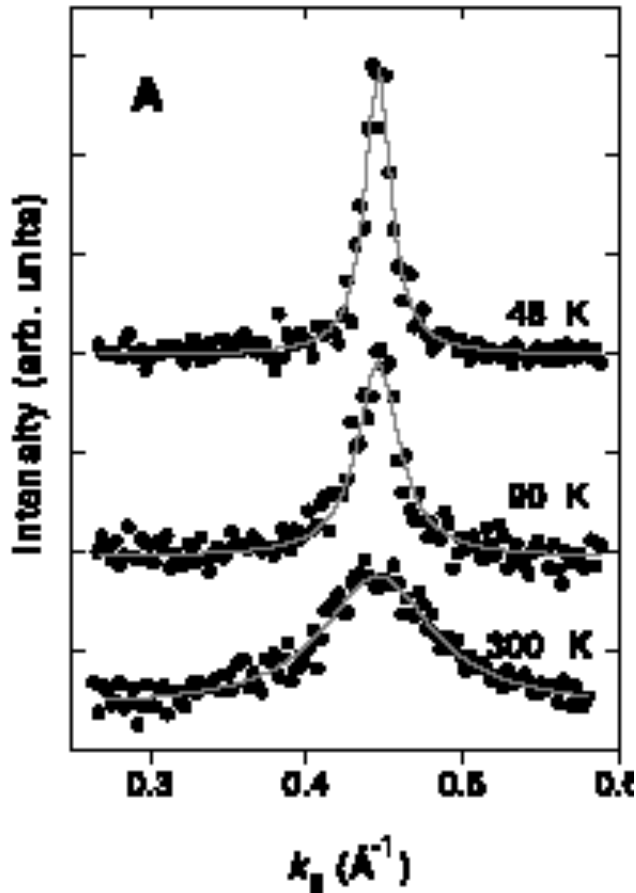
$$\Delta E = \Delta k * dE/dk = \Delta k * v$$

MDCs are usually more symmetric than EDCs (simple Lorentzian). → easier to fit



## 2D detection on the high Tc superconductor $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$

Valla et al., Science (1999)



Lorentzian MDC fits as a function of temperature. Broader peaks at higher T  $\rightarrow$  shorter photohole lifetimes.

Origin: Electron-electron scattering?  
Electron-phonon? Electron-impurity?

These are in general self-energy effects, and should show up in both the real and imaginary parts of the self-energy.

In general: MDC better for large velocities, EDC better for very small velocities.  
Since  $\Sigma$  usually a much stronger function of E than k, MDCs usually simpler.

# ARPES on Cuprates II

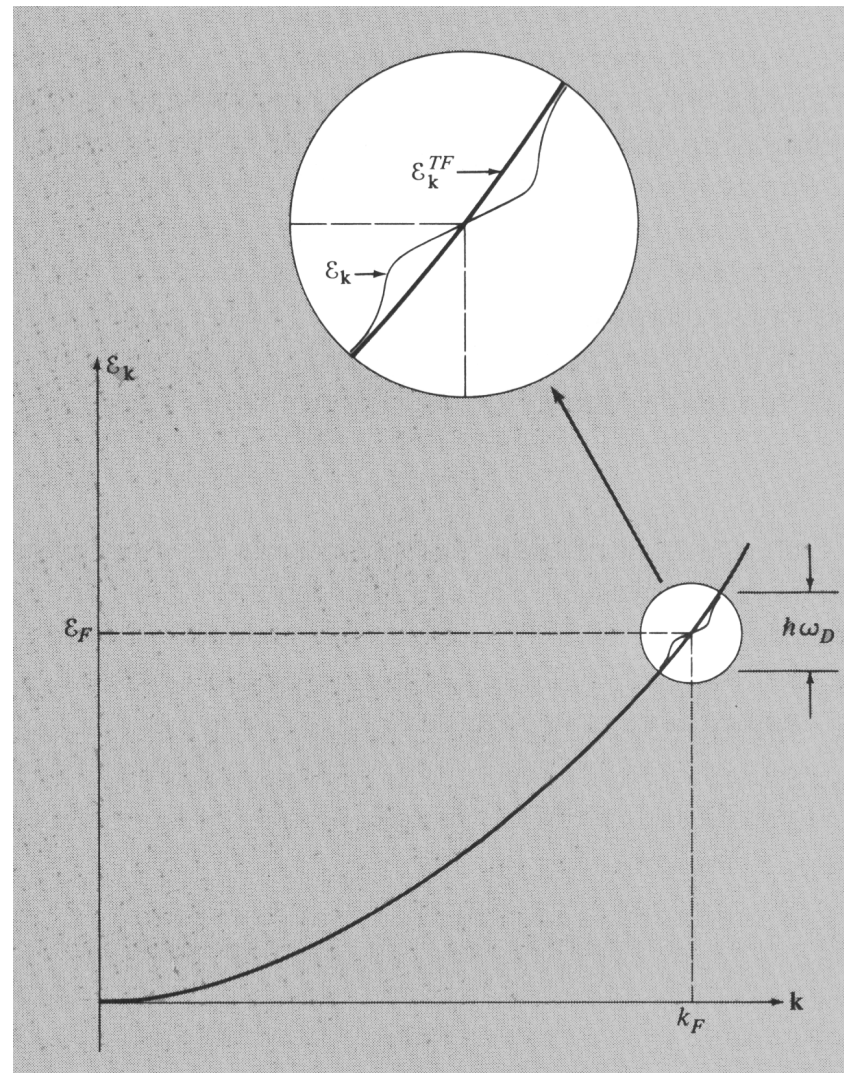
Dan Dessau

University of Colorado, Boulder

Dessau@Colorado.edu

- Kinks or dispersion anomalies (mostly SC state, beyond gap)  
Nodal  $\sim 65$  meV. Most clear in SC state.  
Antinodal  $\sim 40$ - $65$  meV as a function of doping. SC only  
  
Low E nodal kink  $\sim 10$  meV. SC only  
High E anomaly (all T, all k)  $\sim 300$  meV
- SC gaps
- Pseudogaps, arcs
- Self energy effects inside the gap

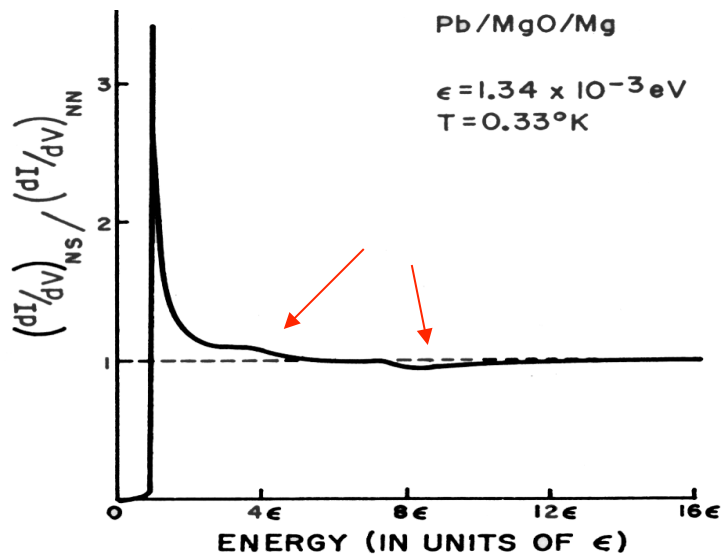
Changes in the carrier mass due to electron-phonon (or other electron-boson) coupling only affects the near- $E_F$  states  
From Ashcroft and Mermin, Solid State Physics, 1976



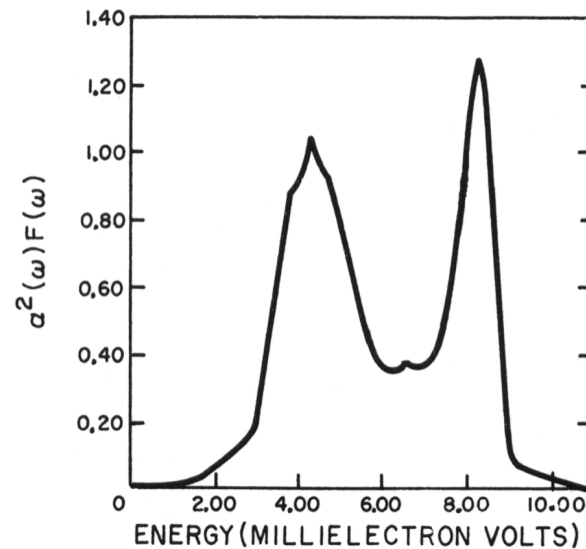
# Self energies in conventional superconductors Via Structure in the tunneling density of states

==> Confirmation that phonons mediate the pairing  
From Nobel Lecture, John Bardeen, 1972

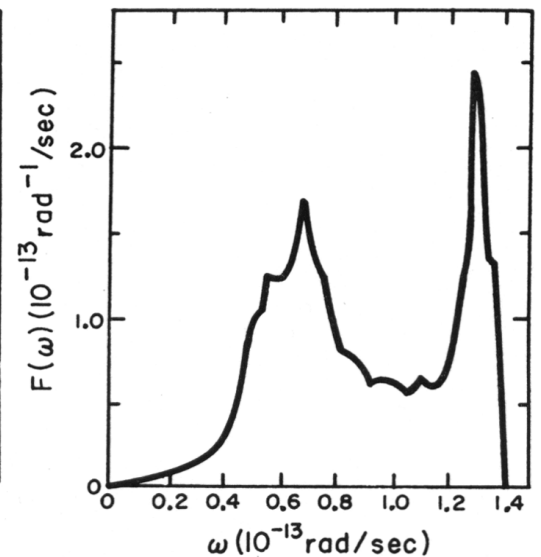
Tunneling Spectrum (Density of States)



Phonon spectrum (times coupling constant) extracted from tunneling data



Phonon spectrum measured from Neutron scattering



Tunneling spectroscopy on High  $T_c$ : Gap is k-dependent (d-wave).

--> Superposition of many gap sizes, structures, etc.

## Many-Body Effects in Angle-Resolved Photoemission: Quasiparticle Energy and Lifetime of a Mo(110) Surface State

T. Valla,<sup>1</sup> A. V. Fedorov,<sup>1</sup> P. D. Johnson,<sup>1</sup> and S. L. Hulbert<sup>2</sup>

$$A(\mathbf{k}, \omega) \propto \frac{\text{Im}\Sigma(\mathbf{k}, \omega)}{[\omega - \varepsilon_{\mathbf{k}} - \text{Re}\Sigma(\mathbf{k}, \omega)]^2 + [\text{Im}\Sigma(\mathbf{k}, \omega)]^2} \quad \text{“spectral function”} = \text{ARPES weight } (\mathbf{k}, \omega)$$

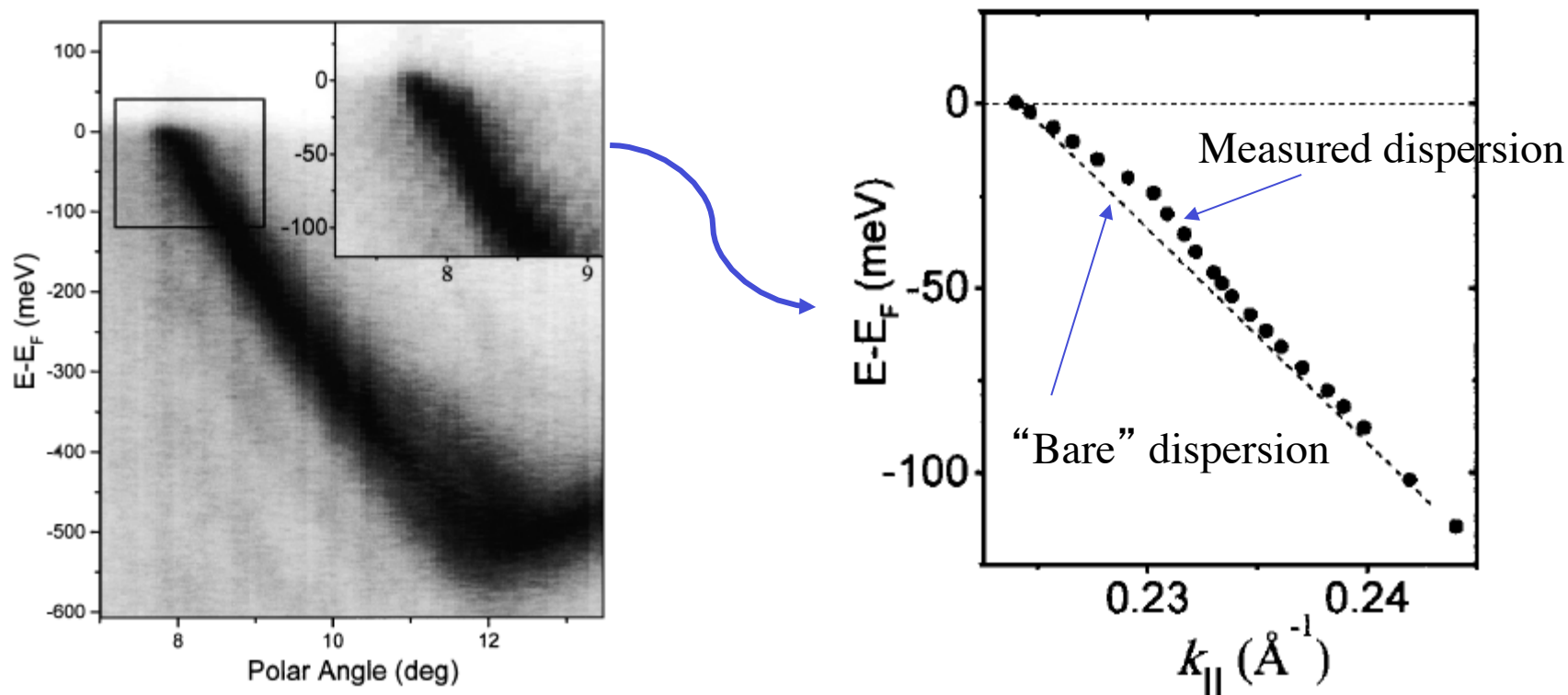
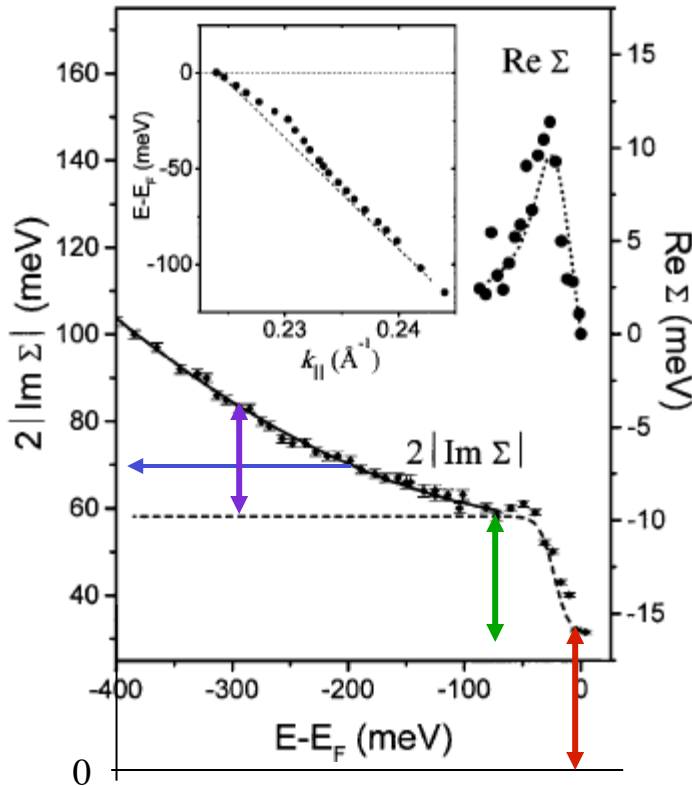


FIG. 1. ARPES intensity plot of the Mo(110) surface recorded along the  $\bar{\Gamma}$ - $\bar{N}$  line of the surface Brillouin zone at 70 K. Shown in the inset is the spectrum of the region around  $k_F$  taken with special attention to the surface cleanliness.

“Kink effect”

$$A(\mathbf{k}, \omega) \propto \frac{\text{Im}\Sigma(\mathbf{k}, \omega)}{[\omega - \varepsilon_{\mathbf{k}} - \text{Re}\Sigma(\mathbf{k}, \omega)]^2 + [\text{Im}\Sigma(\mathbf{k}, \omega)]^2}$$

FWHM of  
quasiparticle peak



$\text{Im}\Sigma$  = width of spectral peak  
Measurable in the same spectra.

$\text{Im}\Sigma$  and  $\text{Re}\Sigma$  related through Kramers-Kronig relations (weighted integral over all energies).

Electron-electron scattering

Coupling to phonons

Impurities, finite resolution,  
final state effects, etc.

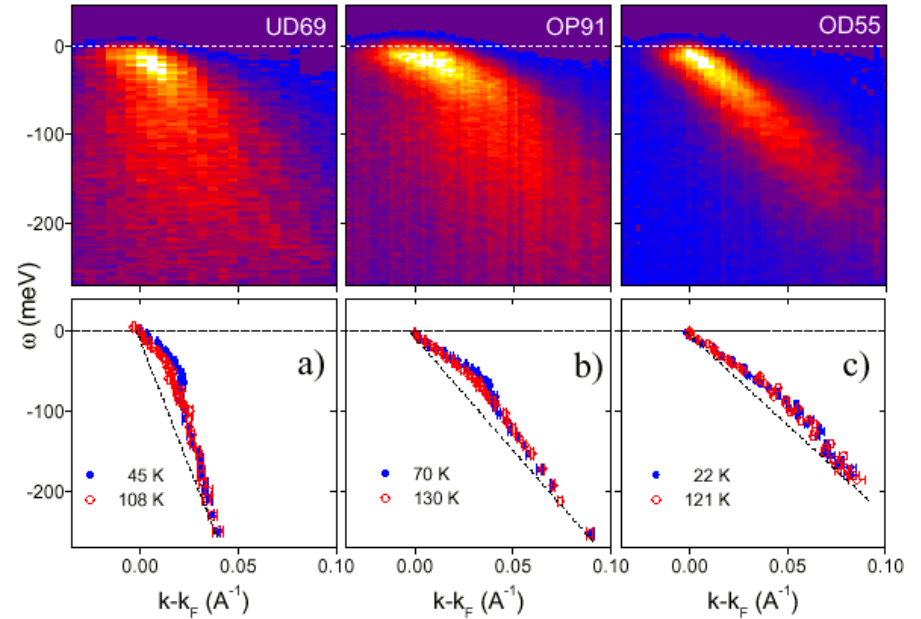
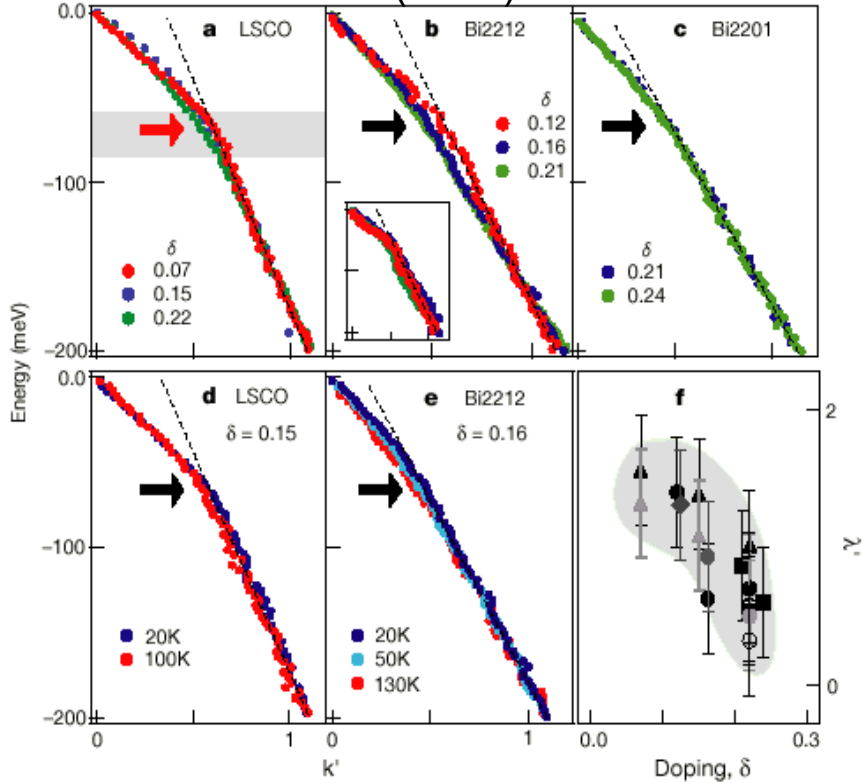
In principle the ARPES spectral function contains all the info about the single-particle many-body fermionic interactions. This plus bosonic measurements from neutrons or inelastic x-rays should give a nearly complete picture of the many-body physics.

# kinks in cuprates ( $\pi, \pi$ ) direction (nodal direction of d-wave gap)

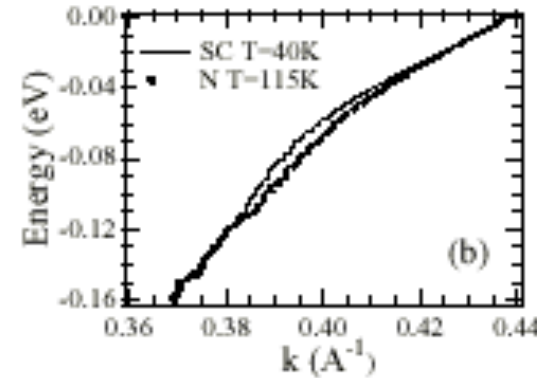
Stanford Group  
Lanzara et al.  
Nature (2001)

Kink energy scale  $\sim 65$  meV

Brookhaven Group  
Johnson et al.  
PRL (2001).



Argonne Group  
Kaminski et al.  
PRL (2001)

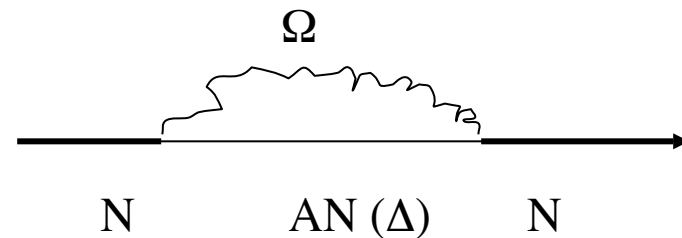
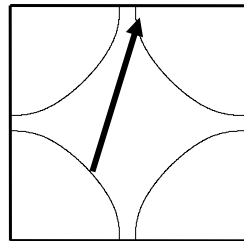


Origin of boson that is causing this kink?  
Phonon?  
“41 meV” Neutron magnetic resonance mode?

## Electron-Boson Coupling and SC Gap Referencing (SC state)

Self-energy term has an intermediate set of states at  $k'$  that are summed over. The set of  $k'$  is not a-priori known.

- If nodal-antinodal (e.g. magnetic resonance mode,  $B_{1g}$  phonon) then gap referencing (to an average around the FS) needed. Mode should shift by gap average upon entering SC state. Mode  $\sim 30-40$  meV.



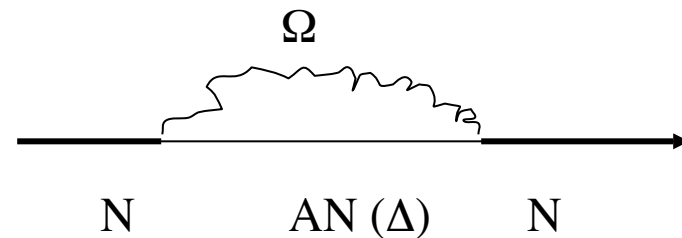
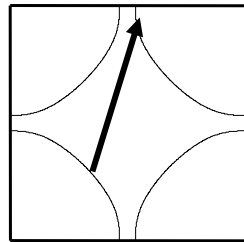
Most data is inconsistent with an energy shift of the kink energy (same kink energy in N and SC state, or no kink in the N state).



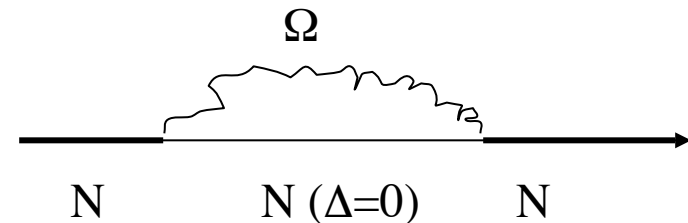
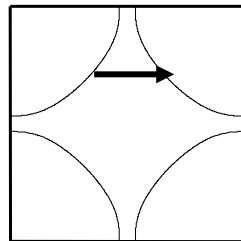
## Electron-Boson Coupling and Gap Referencing (SC state)

Self-energy term has an intermediate set of states at  $k'$  that are summed over. The set of  $k'$  is not known.

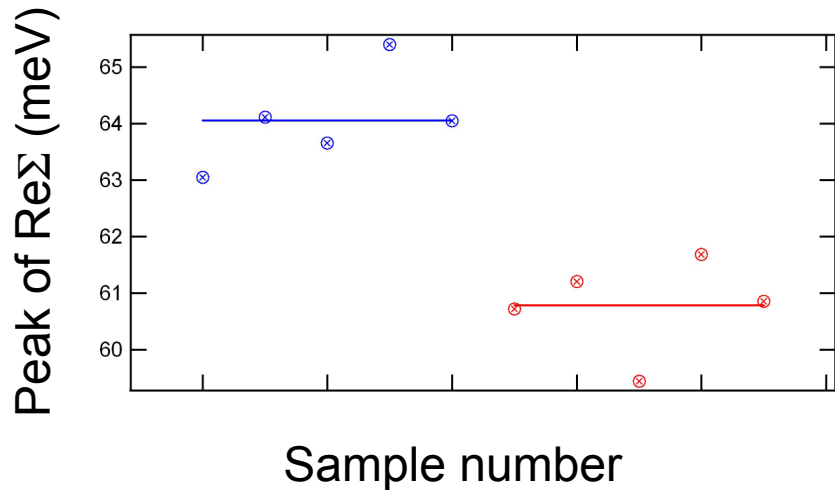
- If nodal-antinodal (e.g. magnetic resonance mode,  $B_{1g}$  phonon) then gap referencing (to an average around the FS) needed. Mode should shift by gap average upon entering SC state. Mode  $\sim 30-40$  meV.



- If nodal-nodal (e.g. LO phonon) then no gap referencing needed. Mode energy = nodal kink energy = 65 meV.

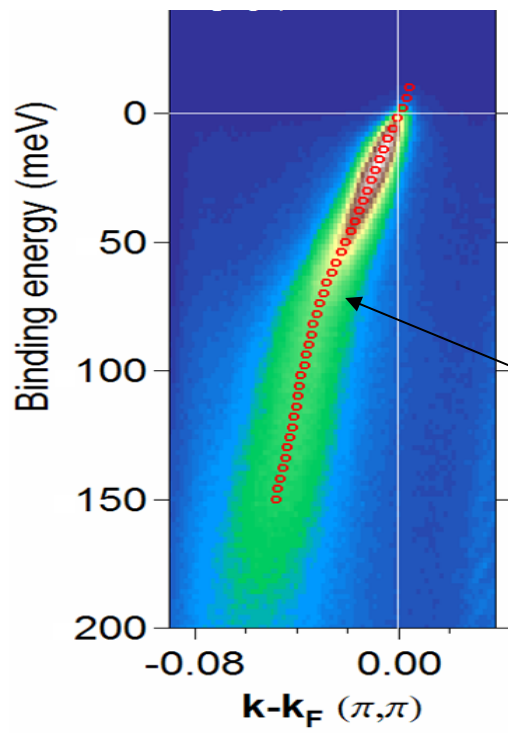


# Isotope Effect study of the nodal kink (SC state)

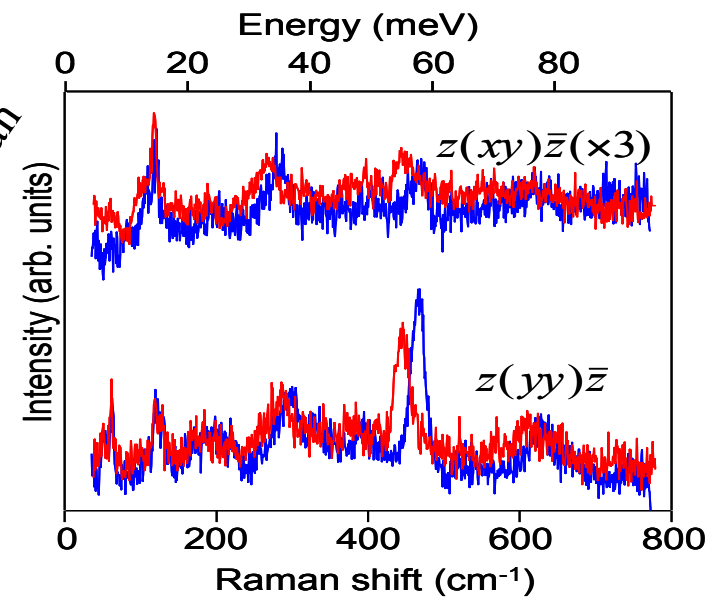


—  $^{16}\text{O}$   
—  $^{18}\text{O}$

Kink softening of  $3.4 \pm 0.5$  meV

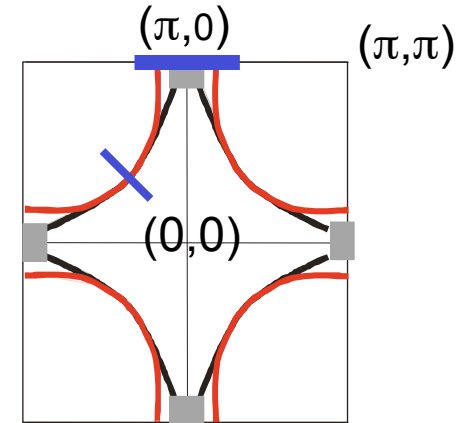
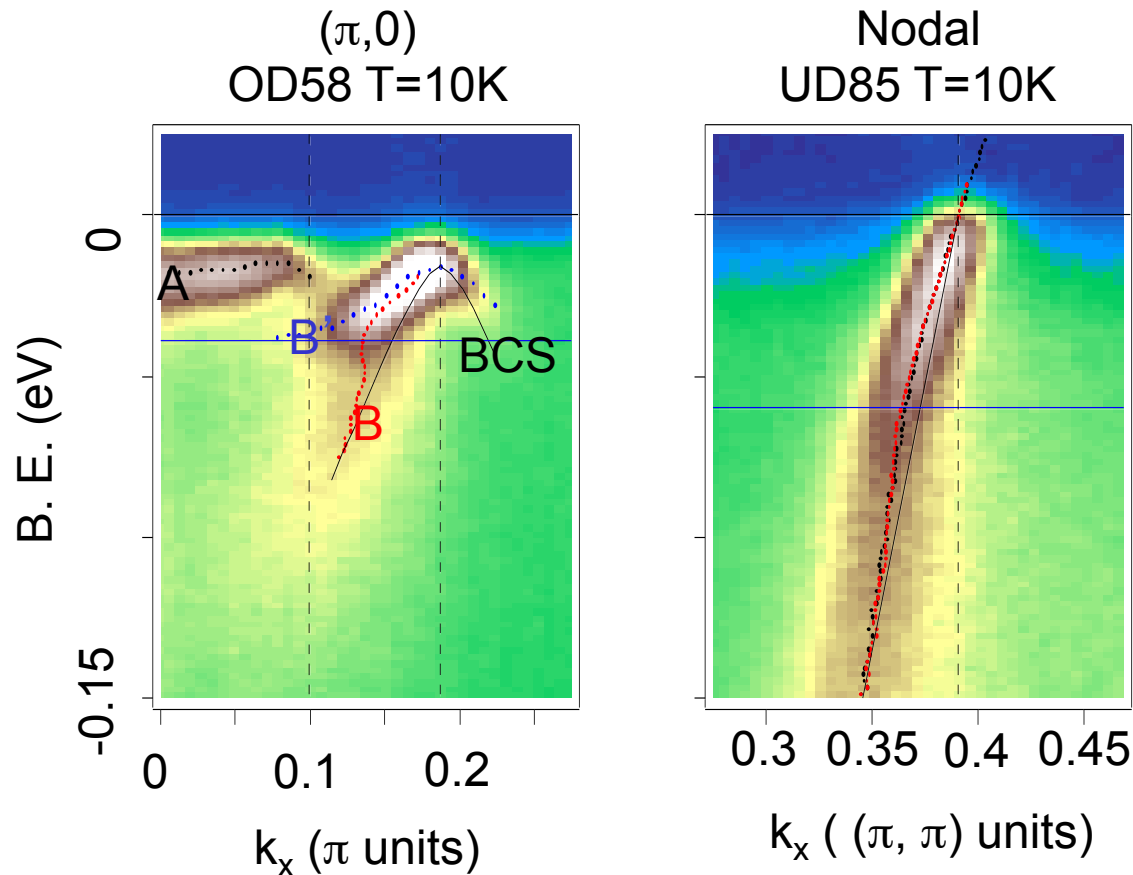


Phonons from Raman



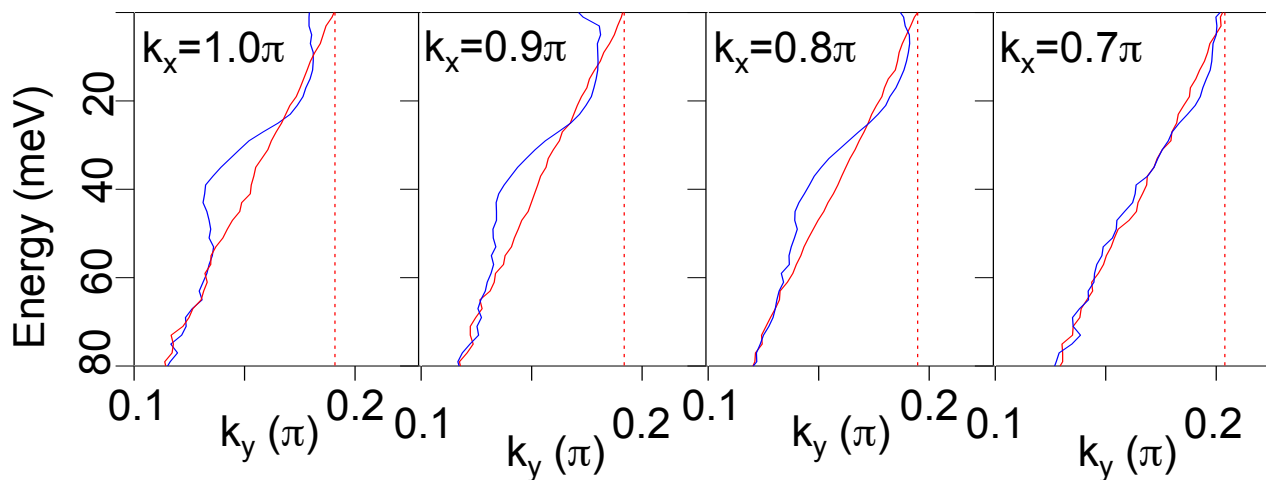
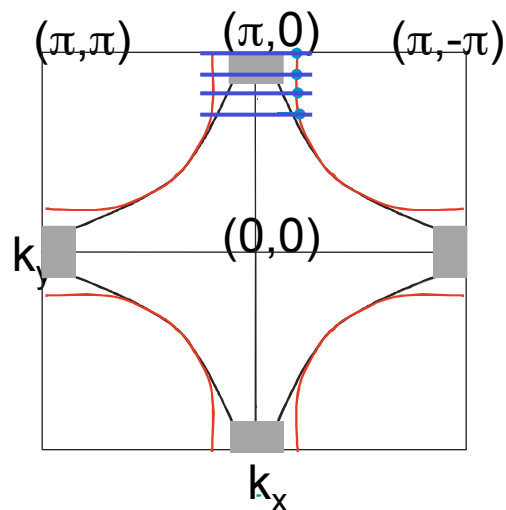
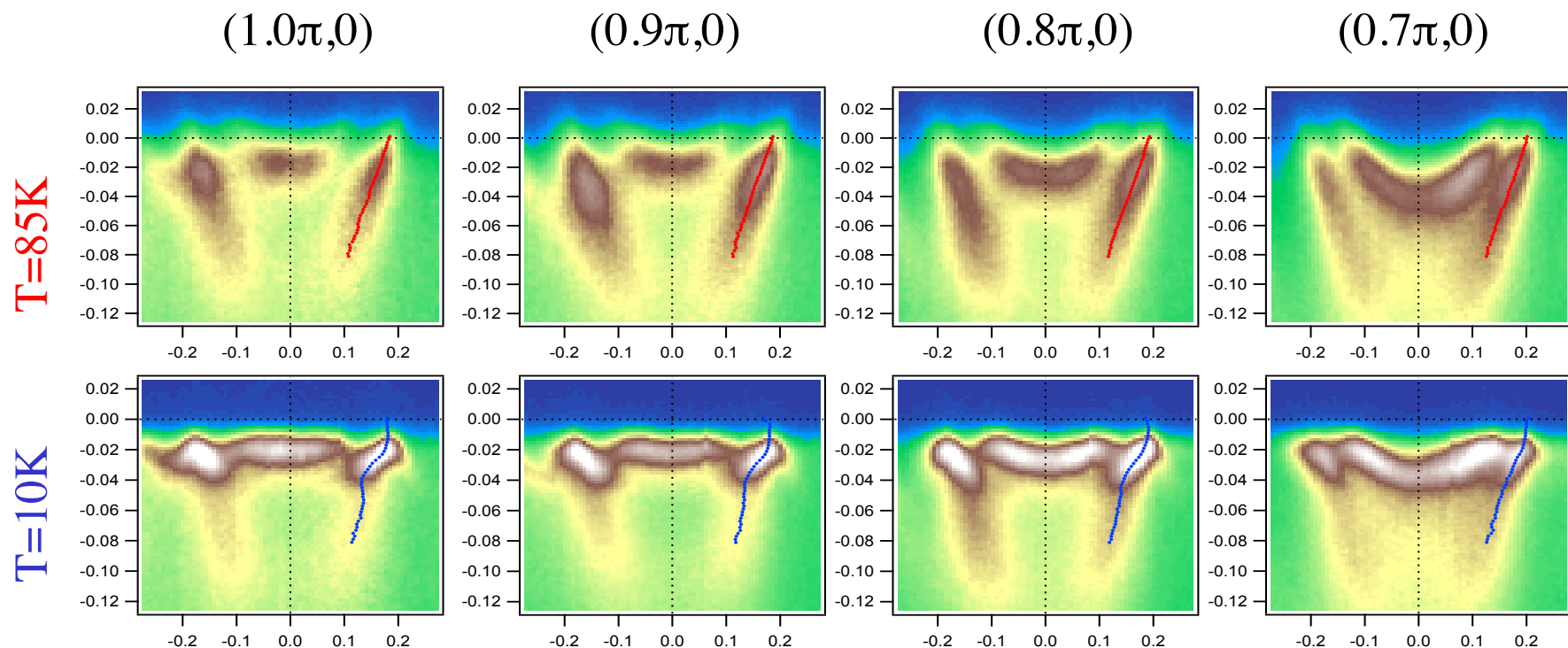
Nodal kink positively fingerprinted as having a major contribution from electron-phonon coupling.

$(\pi,0)$  kink vs. nodal kink

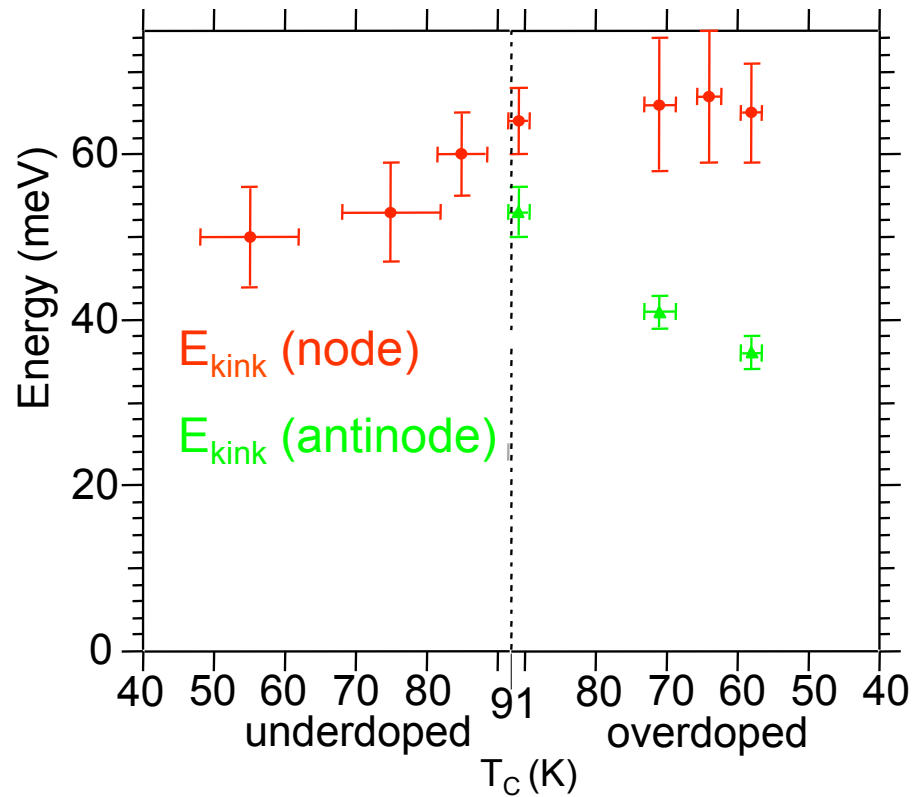


$(\pi,0)$  kink is much stronger than nodal kink,  
shows much stronger T dependence, and is at a different (lower) energy.

k-dependence of the kink near  $(\pi,0)$   $T_c=71\text{K}$  OD Bi2212



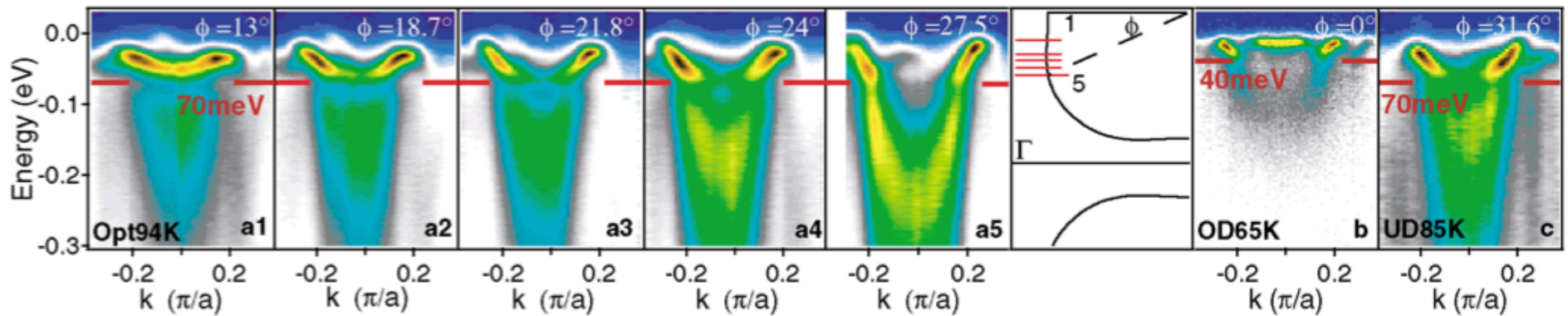
## Doping dependence of kink energies (Bi2212)



Gromko et al., Phys. Rev. B **68**, 174520 (2003).

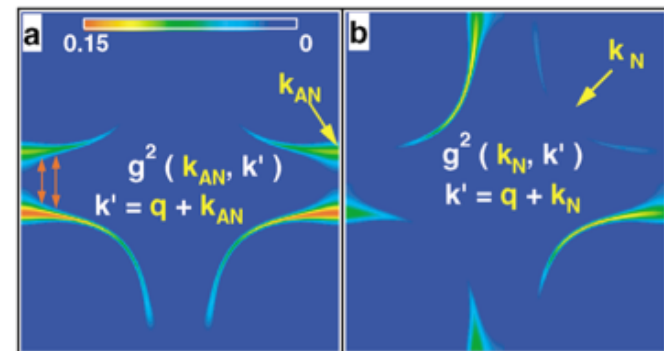
- **Nodal** and **Antinodal** kinks have different energy scales, different k-dependence, different T dependences ==> different phenomena.

## Other studies on the $(\pi,0)$ kink



“Phenomenological agreements with neutron and Raman experiments suggest that this mode is the  $B_{1g}$  oxygen bond-buckling phonon.”

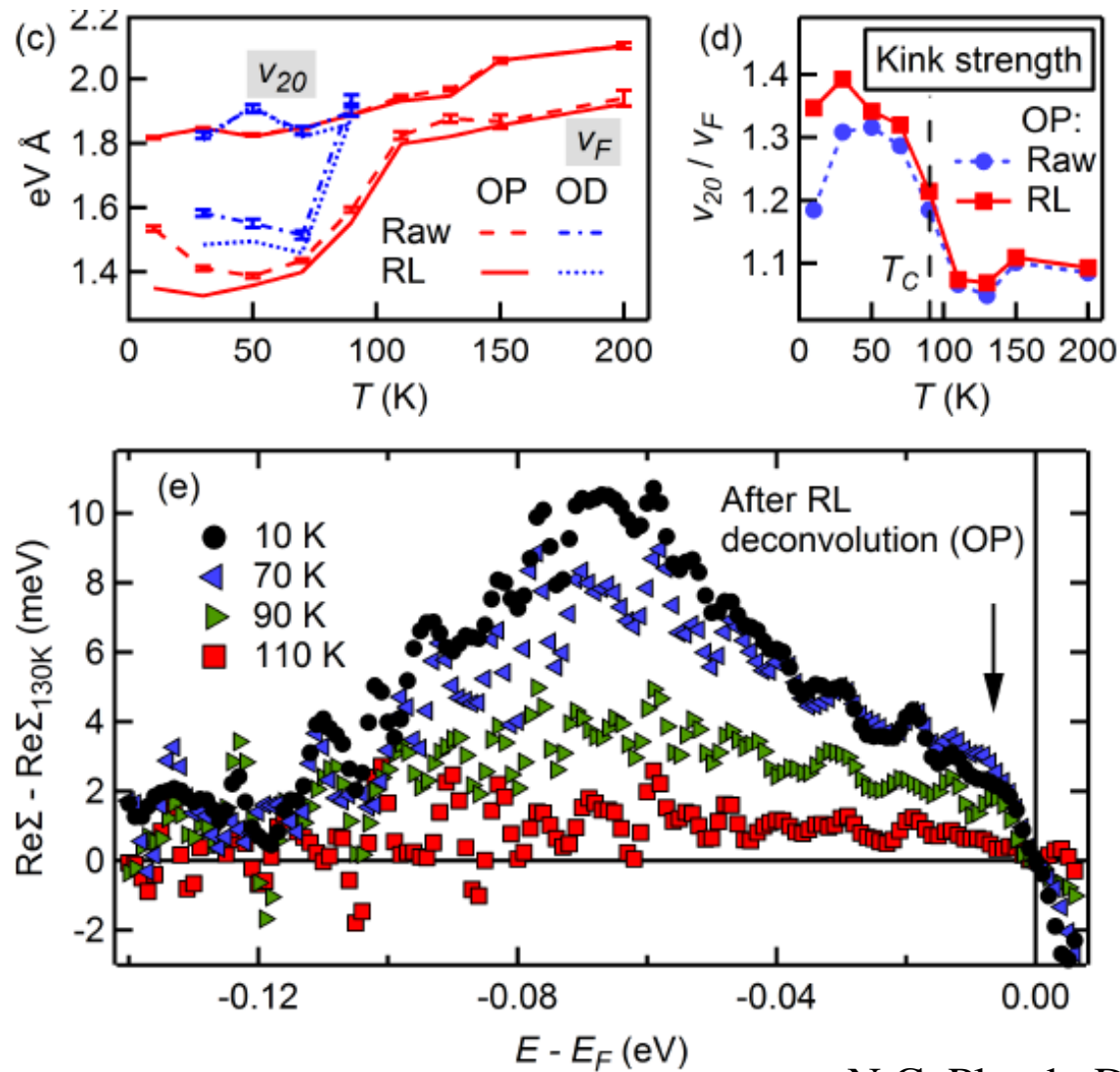
Calculation of  $g^2(k,k')$   
(electron-phonon vertex)



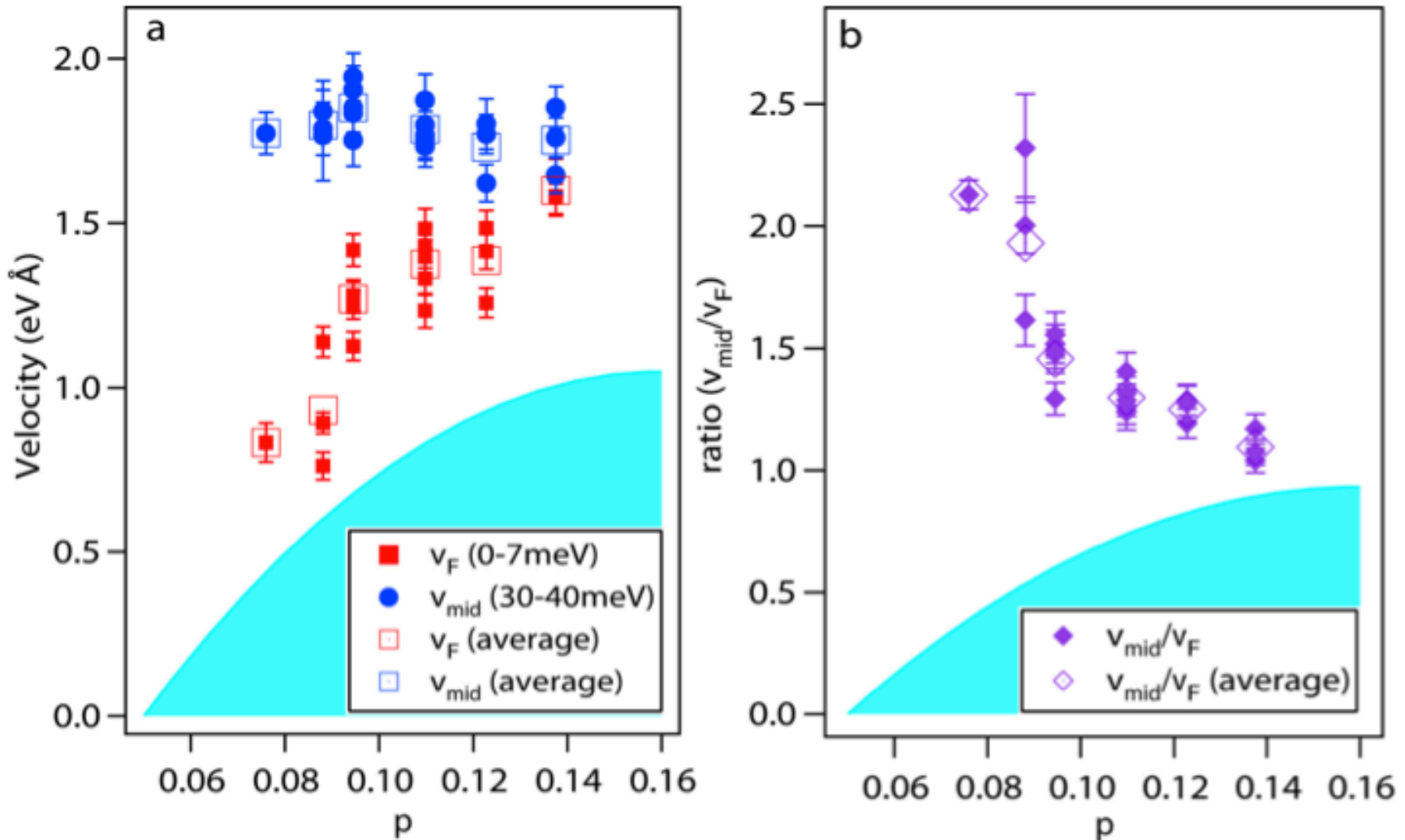
T. Cuk, ZX Shen, T. Devereaux et al, PRL 2004

# 10 meV scale kink at node in Bi2212

## Only visible in SC state



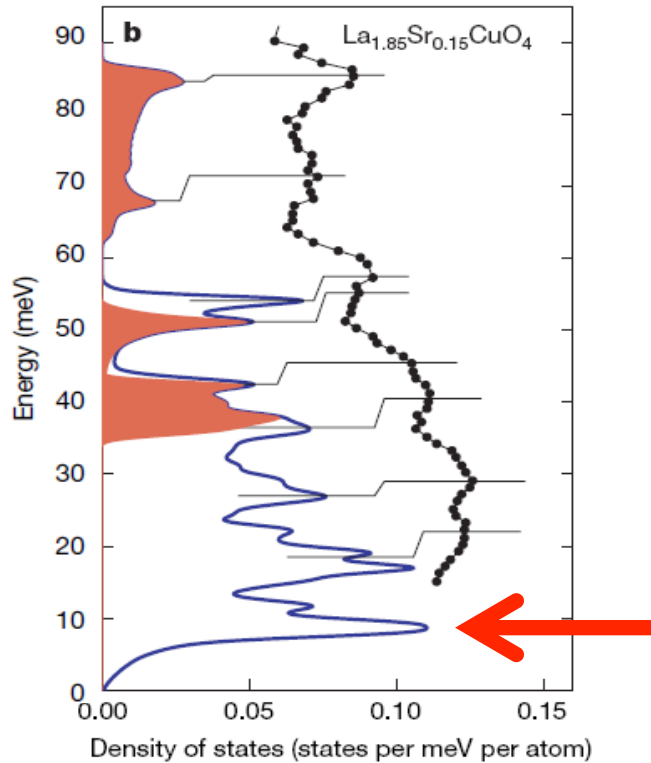
# Doping dependence of the low energy (< 10 meV) kink



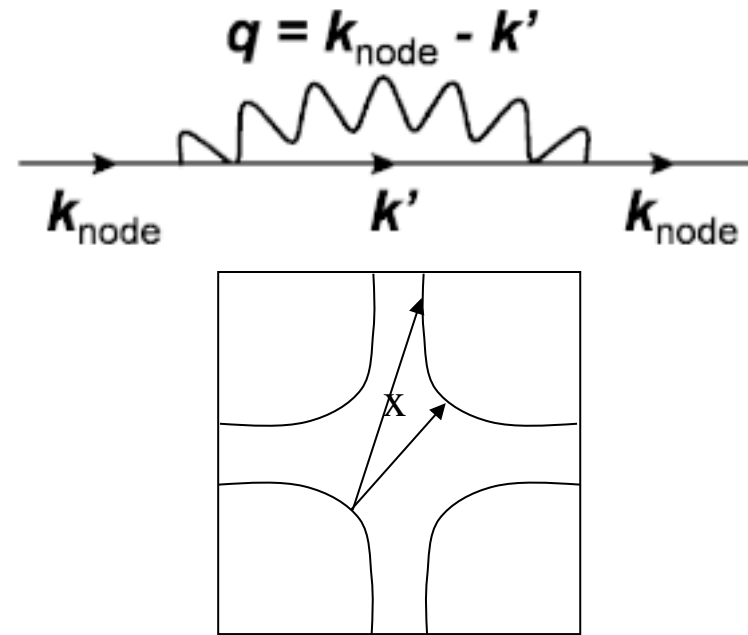
Low E kink stronger for UD samples.



# Possibility of phonons?



Phonon DOS: Giustino, Cohen & Louie, Nature **452**, 975 (2008).

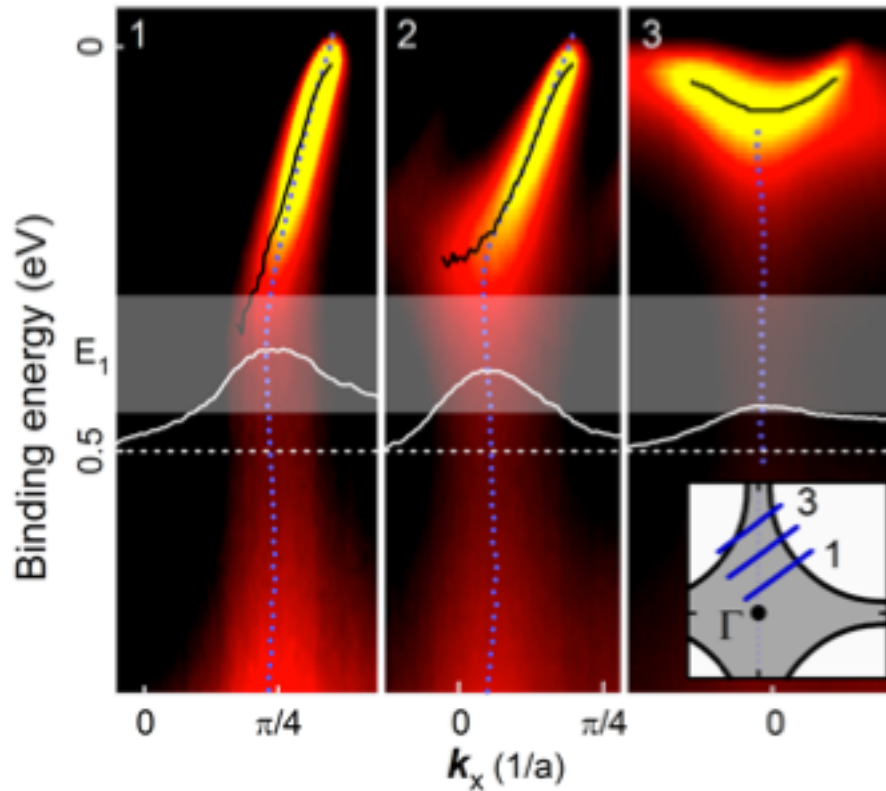


If phonons:

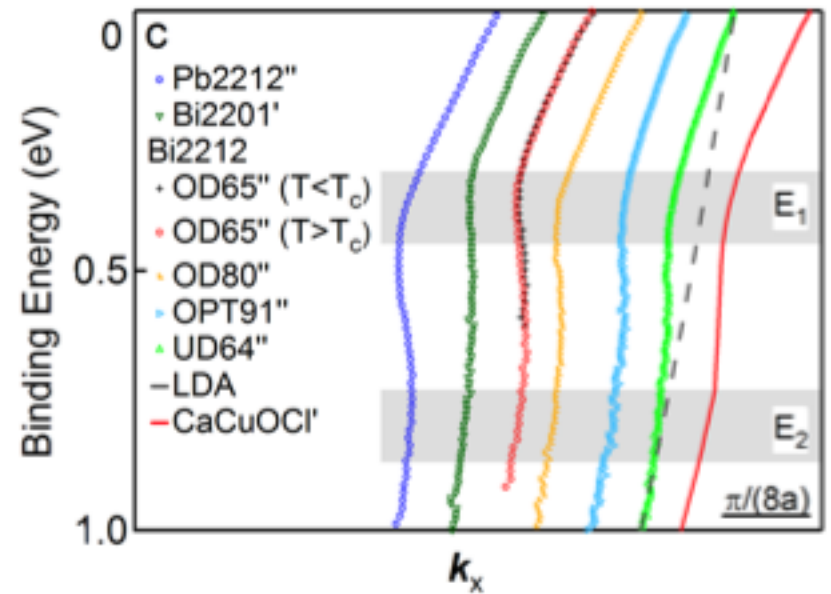
- Extreme forward scattering required.
- Why kink turns on at  $T_c$ ?

Johnston and Devereaux studied this in detail. Unusual case where  $\Omega < \Delta$ . (PRL 2012)

# High energy anomaly or kink

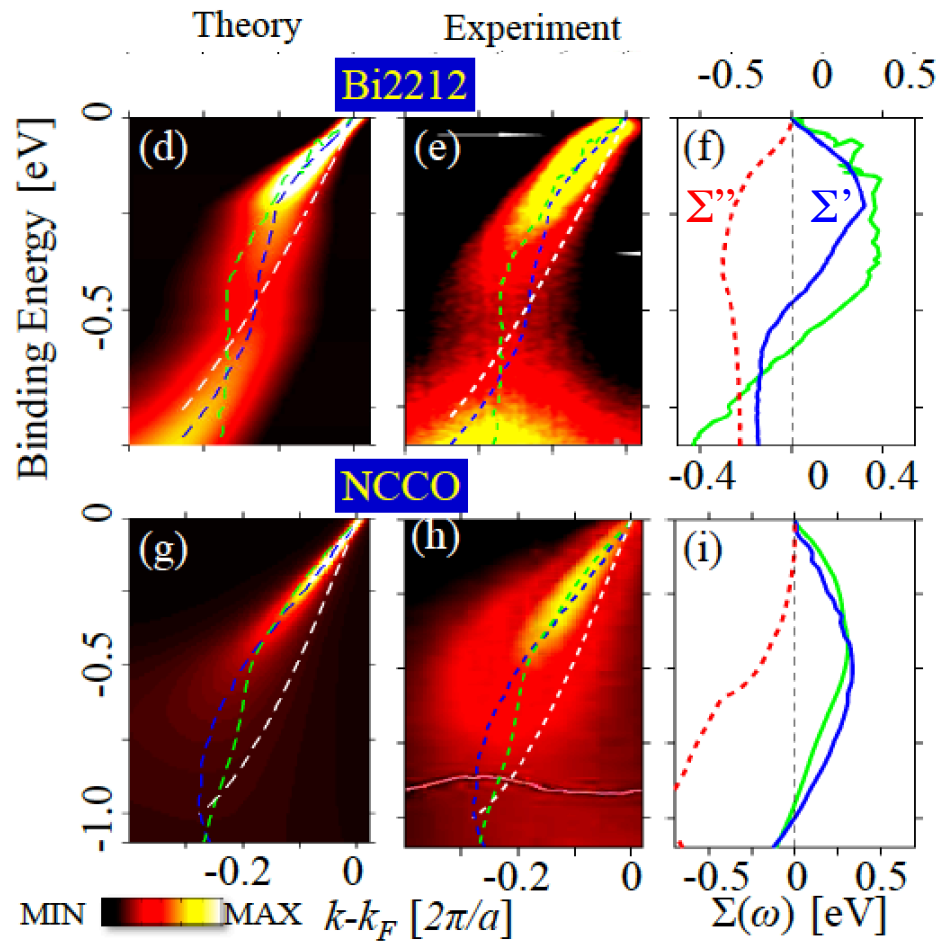


MDC-derived dispersion



Graf, Lanzara 2006

A new energy scale ( $\sim 0.3$  eV)? Interplay of different energy scales?  
 An issue of background/scattered weight/matrix elements?  
 Zero crossing of  $\text{Re}\Sigma$ ?



# Superconducting order parameter symmetry

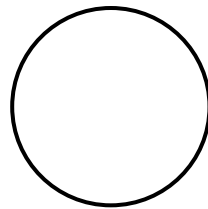
SC gap  $\Delta$  = magnitude of order parameter. Varies as a function of  $k$  in a d-wave SC

$$\Psi(r_1, \sigma_1; r_2, \sigma_2) = \psi(\text{orbital}) \cdot \chi(\text{spin})$$

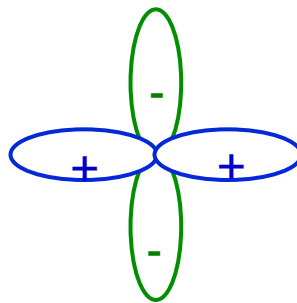
Antisymmetric under exchange

$\chi(\text{spin})$  : known to be a singlet ( $S=0$ )  $\downarrow\uparrow$

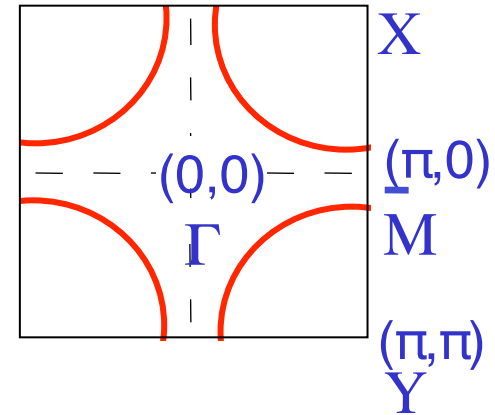
$S = 0, l = 0$   
 -- s-wave superconductor  
 (conventional SC)



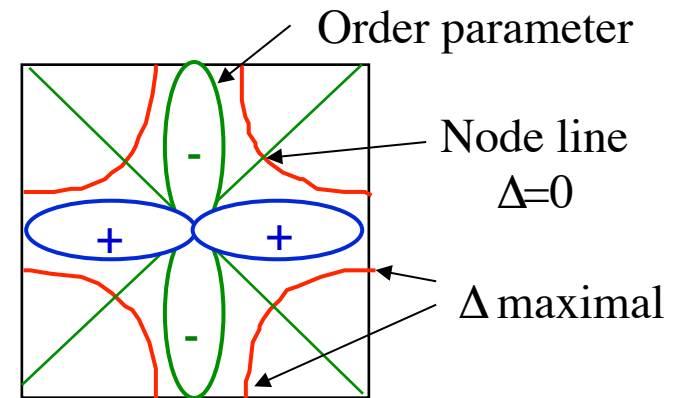
$S = 0, l = 2$   
 -- d-wave superconductor  
 (HTSCs - pretty sure)

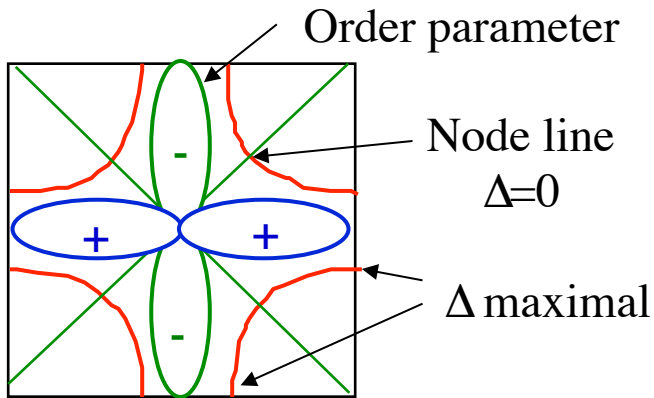


## Hole-like Fermi Surface



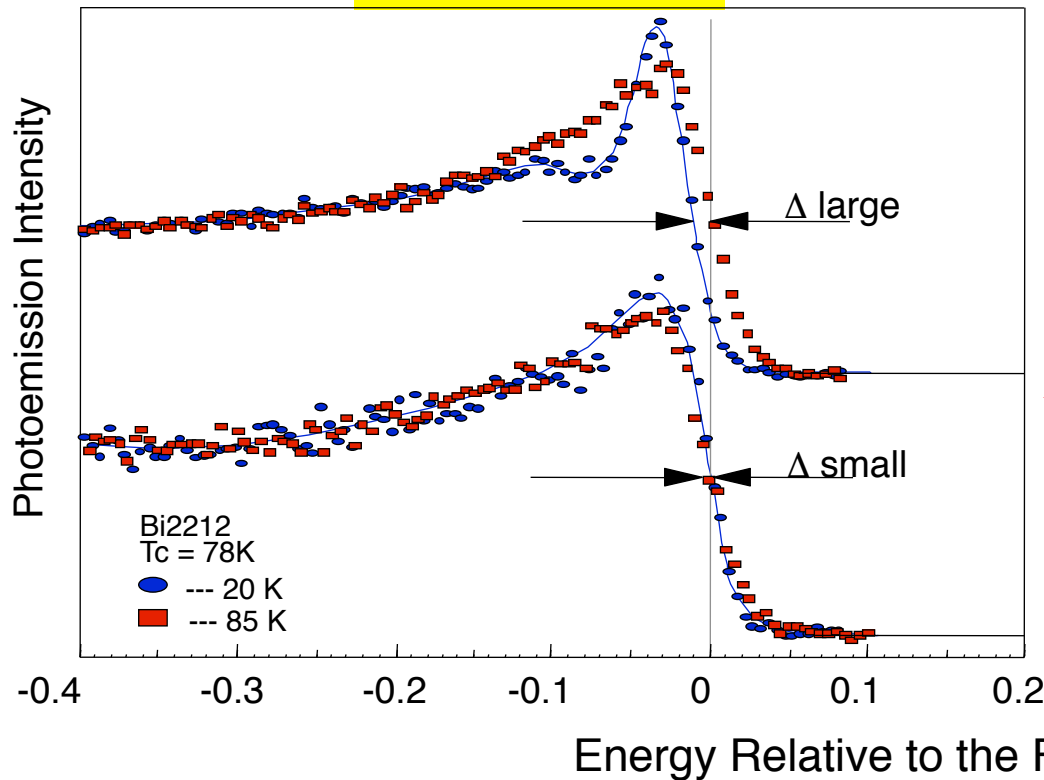
## d-wave SC gap - maximal near $(\pi, 0)$





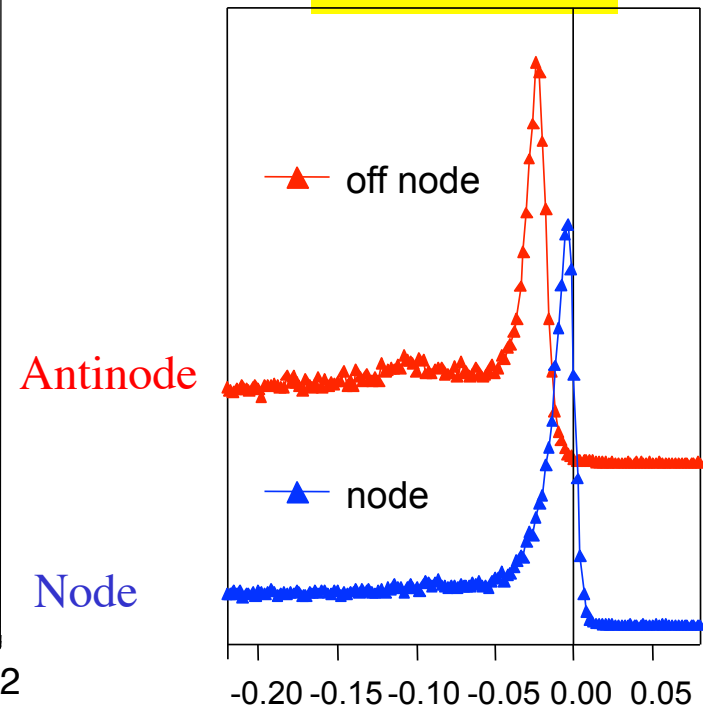
k-space dependence of superconducting energy gap  $\Delta$   
 $\rightarrow$  Symmetry of Cooper pair wavefunction is d-wave ( $l=2$ )

Standard ARPES



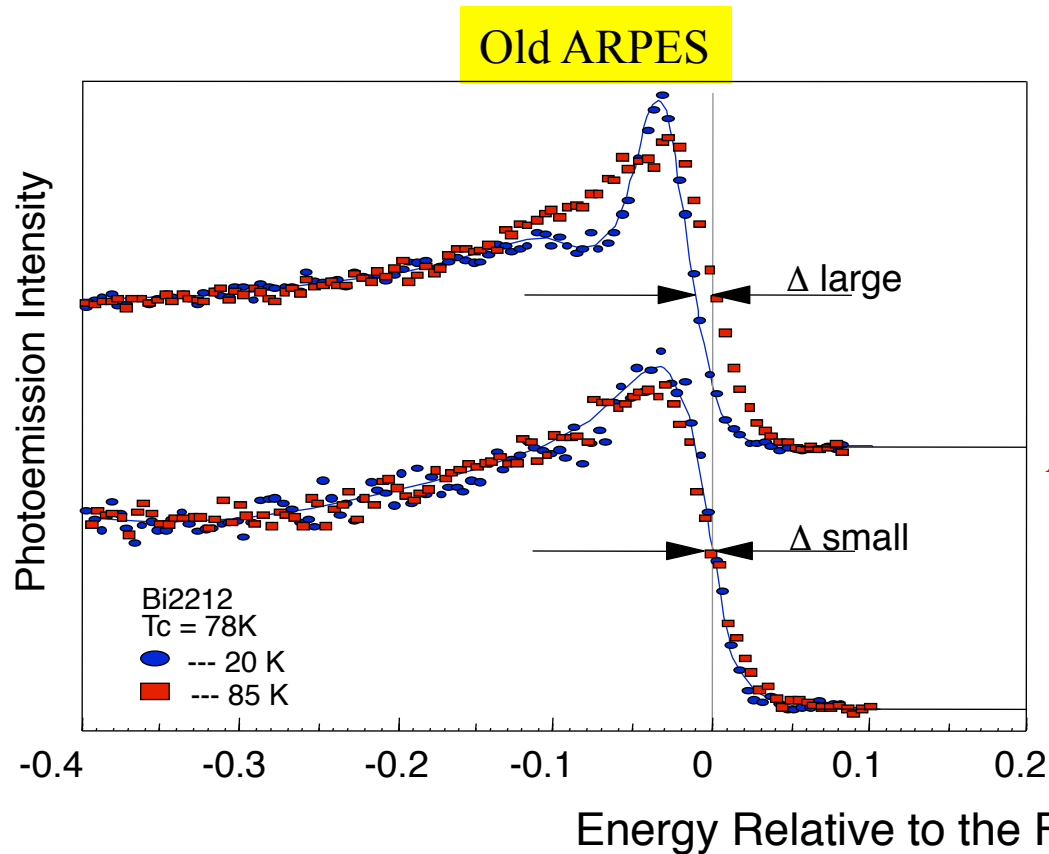
Z.-X. Shen, D.S.D. et al.,  
 Phys. Rev. Lett. **70**, 1553 (1993)

Laser ARPES

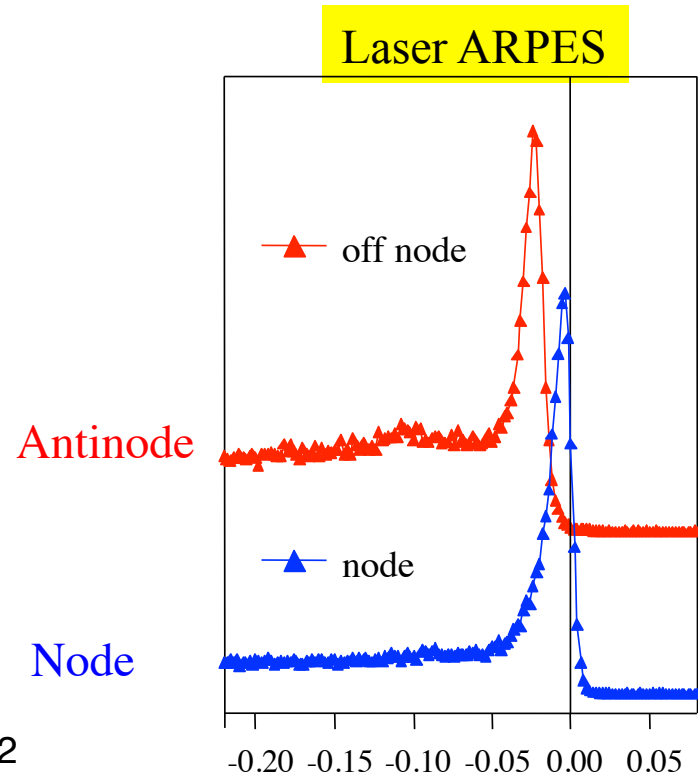


J.D. Koralek, D.S.D. et al.,  
 Phys. Rev. Lett. **96**, 017005 (2006)

# Measurement of the d-wave superconducting gap



Z.-X. Shen, D.S.D. et al.,  
Phys. Rev. Lett. **70**, 1553 (1993)



J.D. Koralek, D.S.D. et al.,  
Phys. Rev. Lett. **96**, 017005 (2006)

How to **quantitatively** determine the gap magnitude?

Midpoint of the leading edge?

Peak separation of symmetrized EDCs?

Fit to model spectral function?

How to understand the self energies or scattering rates (peak broadening)?

**Qualitative** problems when  $\Delta$  is small or T is large.

# Pseudogaps

# Original ARPES pseudogap study in cuprates. Arcs and pockets.

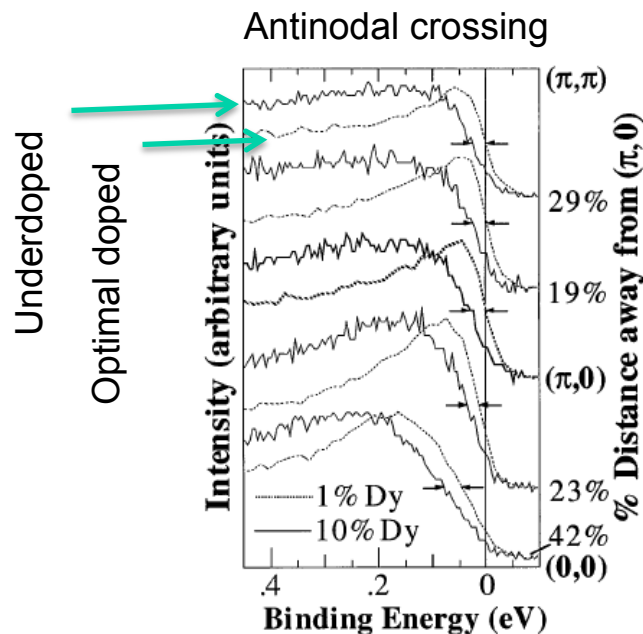
VOLUME 76, NUMBER 25

PHYSICAL REVIEW LETTERS

17 JUNE 1996

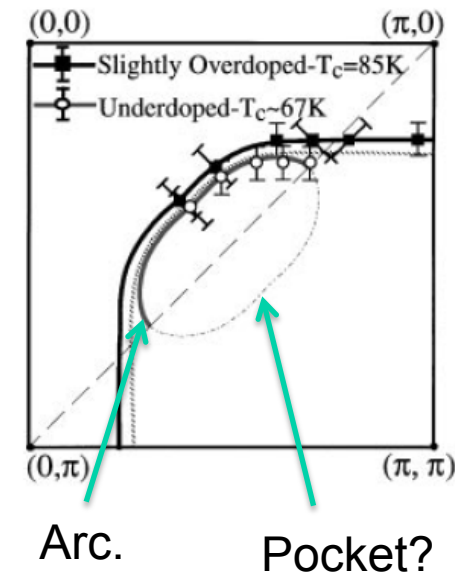
## Unconventional Electronic Structure Evolution with Hole Doping in $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ : Angle-Resolved Photoemission Results

D. S. Marshall,<sup>1</sup> D. S. Dessau,<sup>1,2,5</sup> A. G. Loeser,<sup>1,2</sup> C-H. Park,<sup>1,2</sup> A. Y. Matsuura,<sup>1</sup> J. N. Eckstein,<sup>3</sup> I. Bozovic,<sup>3</sup>  
P. Fournier,<sup>4</sup> A. Kapitulnik,<sup>4</sup> W. E. Spicer,<sup>1</sup> and Z.-X. Shen<sup>1,2,4</sup>



$T=100\text{K}$  (above  $T_c$ )

UD sample has loss of spectral weight at antinodal crossing, but states never reach  $E_F$ .

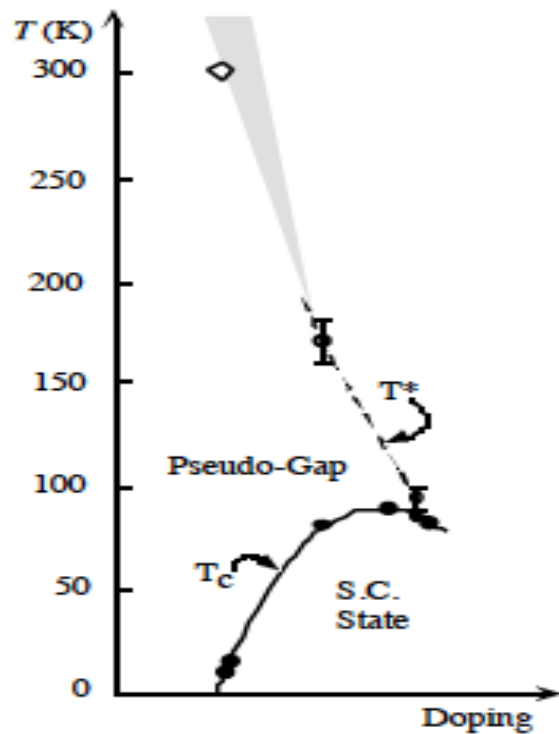


- Pgap is max at  $(\pi, 0)$ , vanishes on diagonal. d-wave like the SC gap. Precursor to SC?
- Pgap persists up to  $T^*$ . Onset of pairing?
- With increasing underdoping, pgap at antinode grows, remaining Fermi arc shrinks.
- Length of arc increases with increasing temperature (as pgap shrinks).
- Issues of band topology. Closed on backside to form pockets?

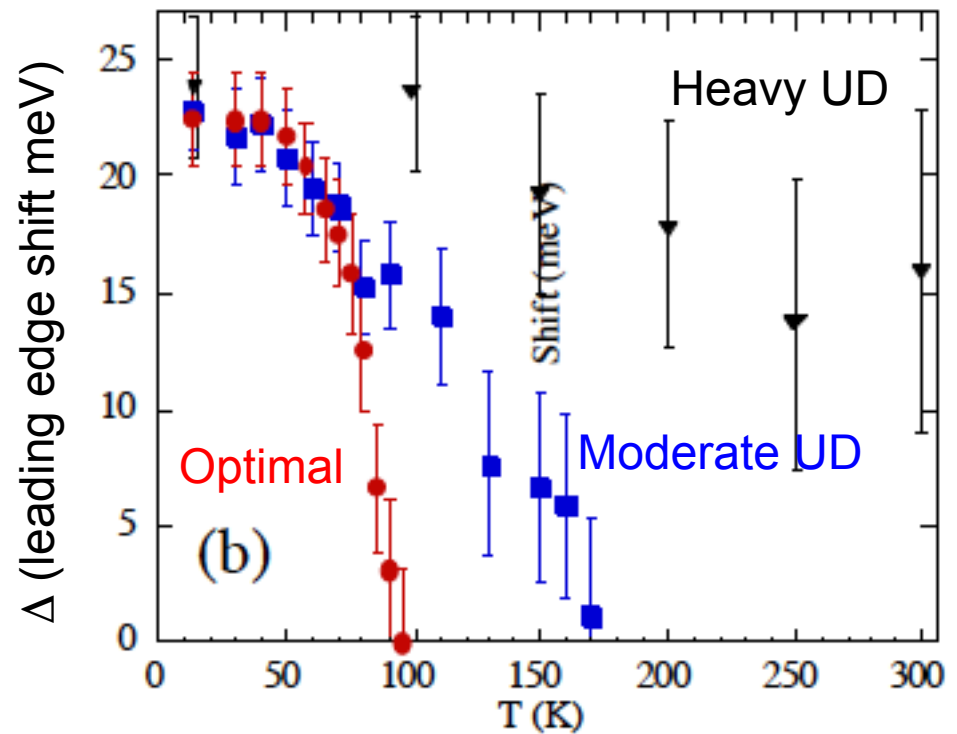


# Spectroscopic evidence for a pseudogap in the normal state of underdoped high $T_c$ superconductors

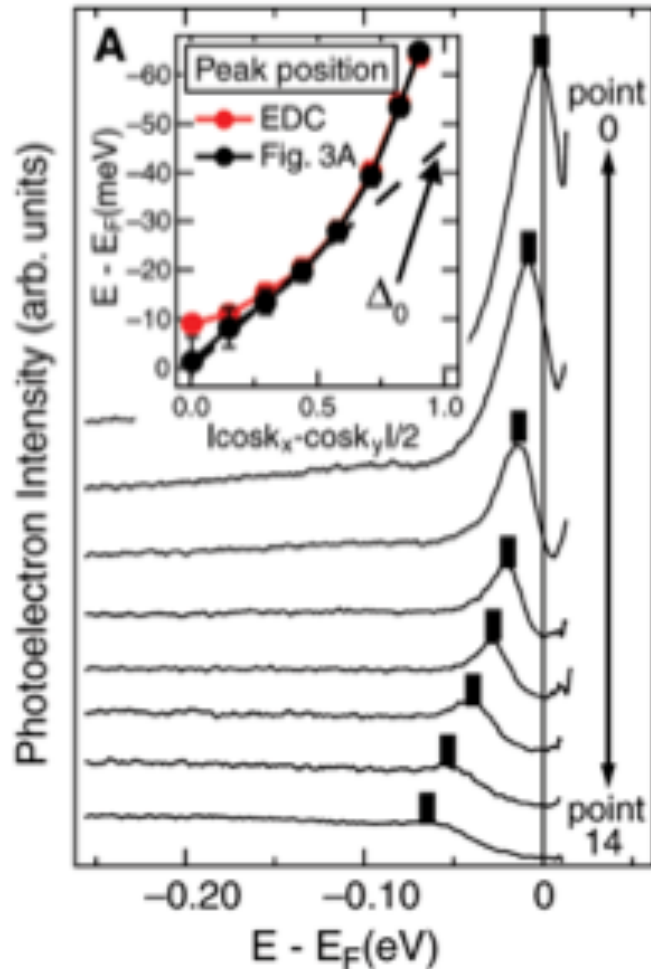
H. Ding<sup>1,2</sup>, T. Yokoya<sup>3</sup>, J.C. Campuzano<sup>1,2</sup>,  
T. Takahashi<sup>3</sup>, M. Randeria<sup>4</sup>, M.R. Norman<sup>2</sup>, T.  
Mochiku<sup>5,6</sup>, K. Kadowaki<sup>5,6</sup>, and J. Giapintzakis<sup>7</sup>



Antinodal gap vs  $T$  for different dopings



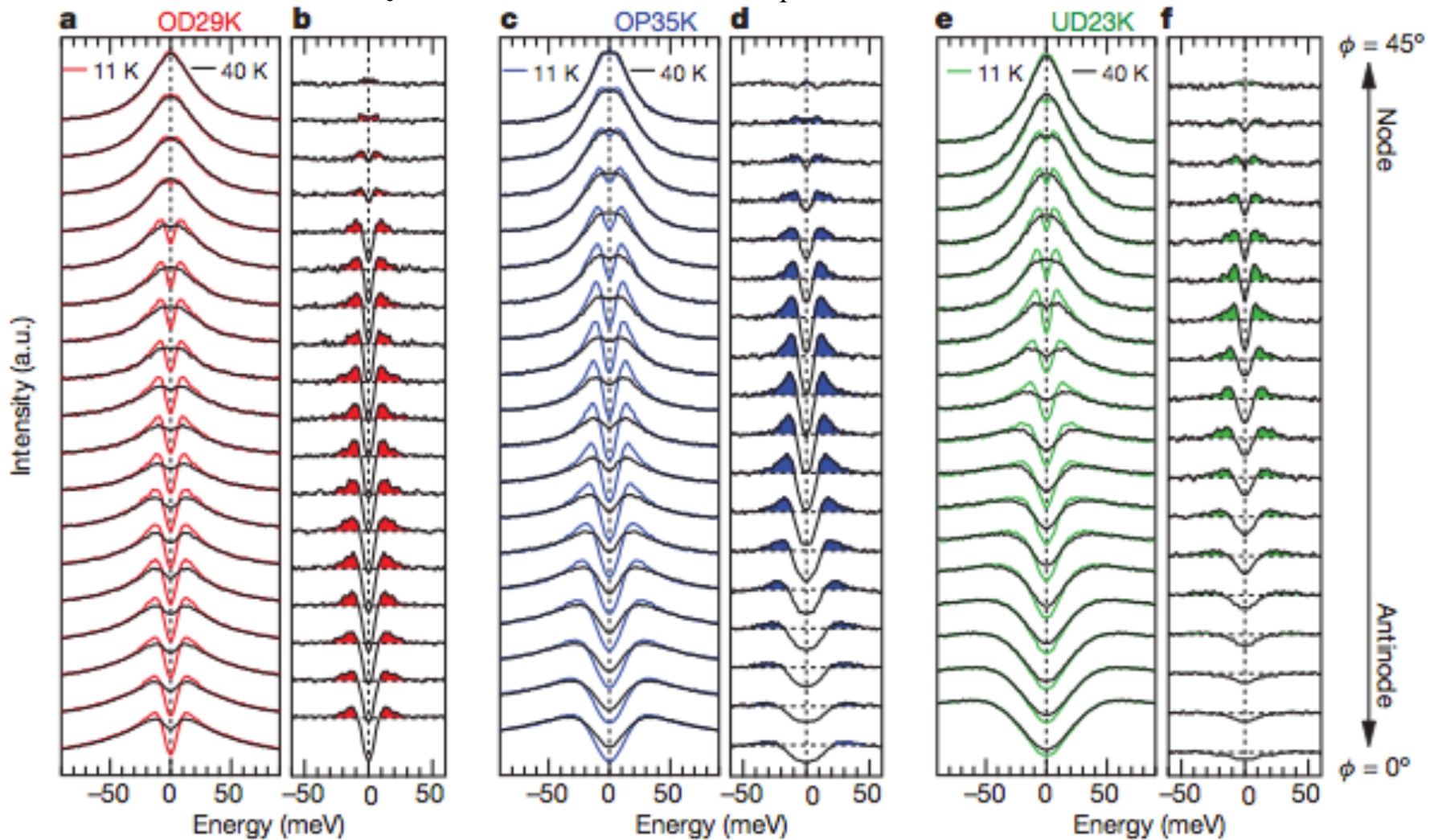
# “Hockey stick” in the gap function $T_c=50\text{K}$ underdoped Bi2212



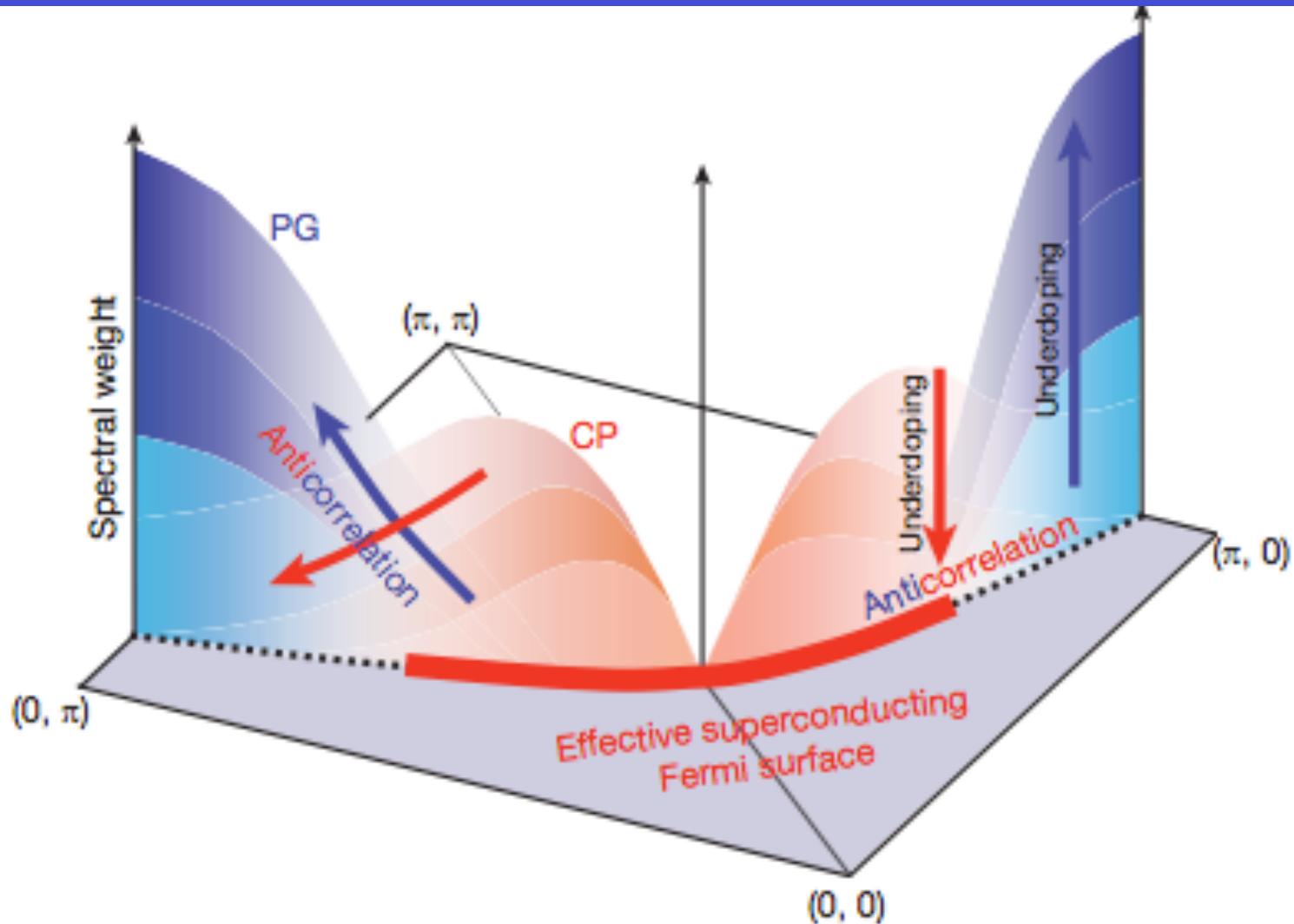
- Peak-position analysis.
- Increase in the gap magnitude in antinodal regime beyond the expectations from the pure SC d-wave form.
- Absent for overdoped samples, strong effect for underdoped samples.
- Is this indicative of a different form for the SC gap, or is it due to a different origin of the gap in the antinodal regime?

# Competition between the antinodal pseudogap and the SC gap (single layer Bi2201)

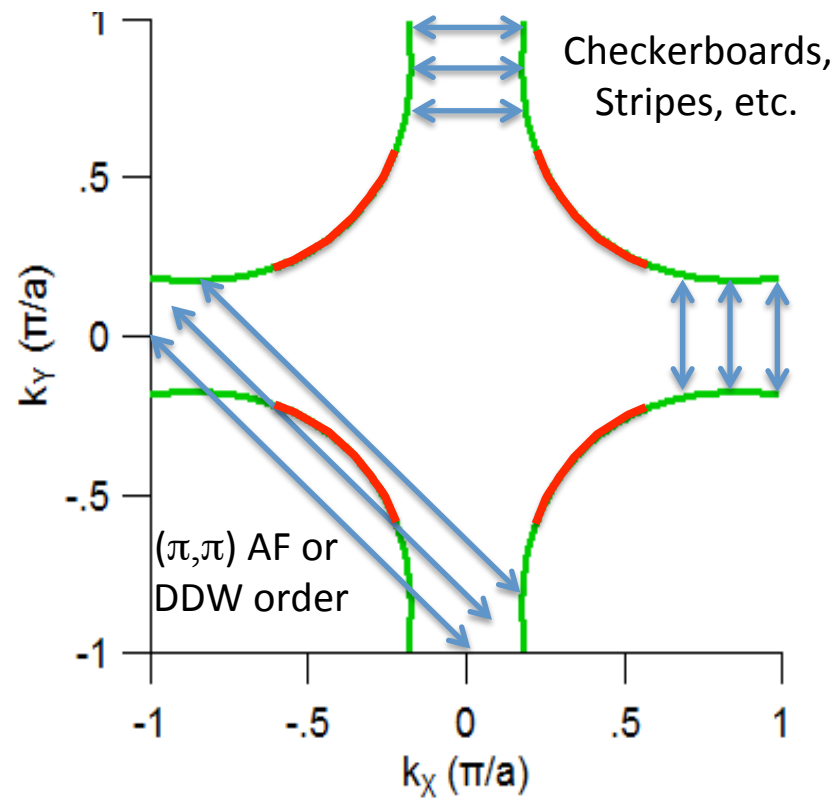
Symmetrized EDCs at  $k=k_F$  around the zone



# Competition between the antinodal p<sub>g</sub>ap and the SC gap (Bi2201)

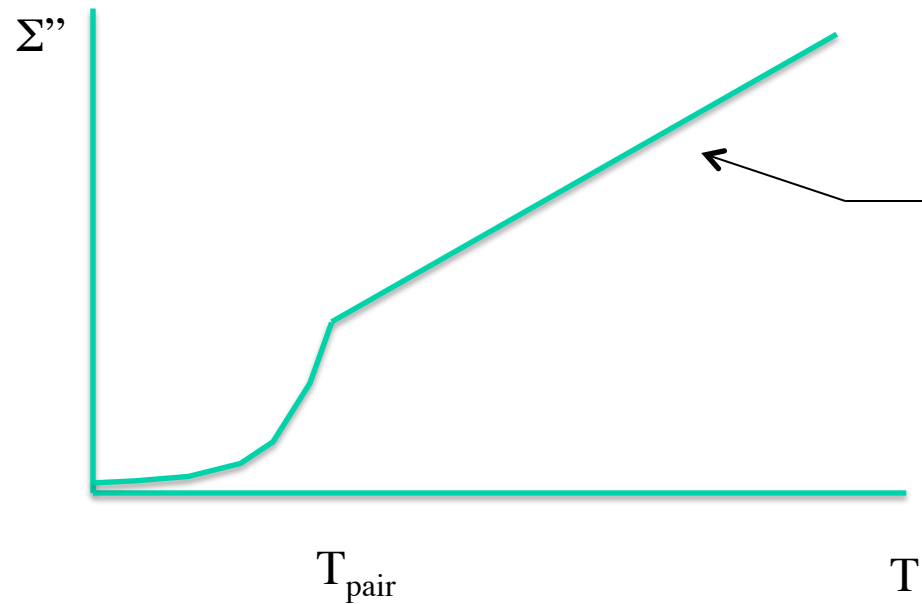


Near-node (away from the pseudogap) is the cleanest place to study the superconductivity



# Self energy effects inside the gap

In addition to the opening of the d-wave SC gaps, there are dramatic drops in the single particle scattering rates (presumably due to the opening of the gaps themselves).

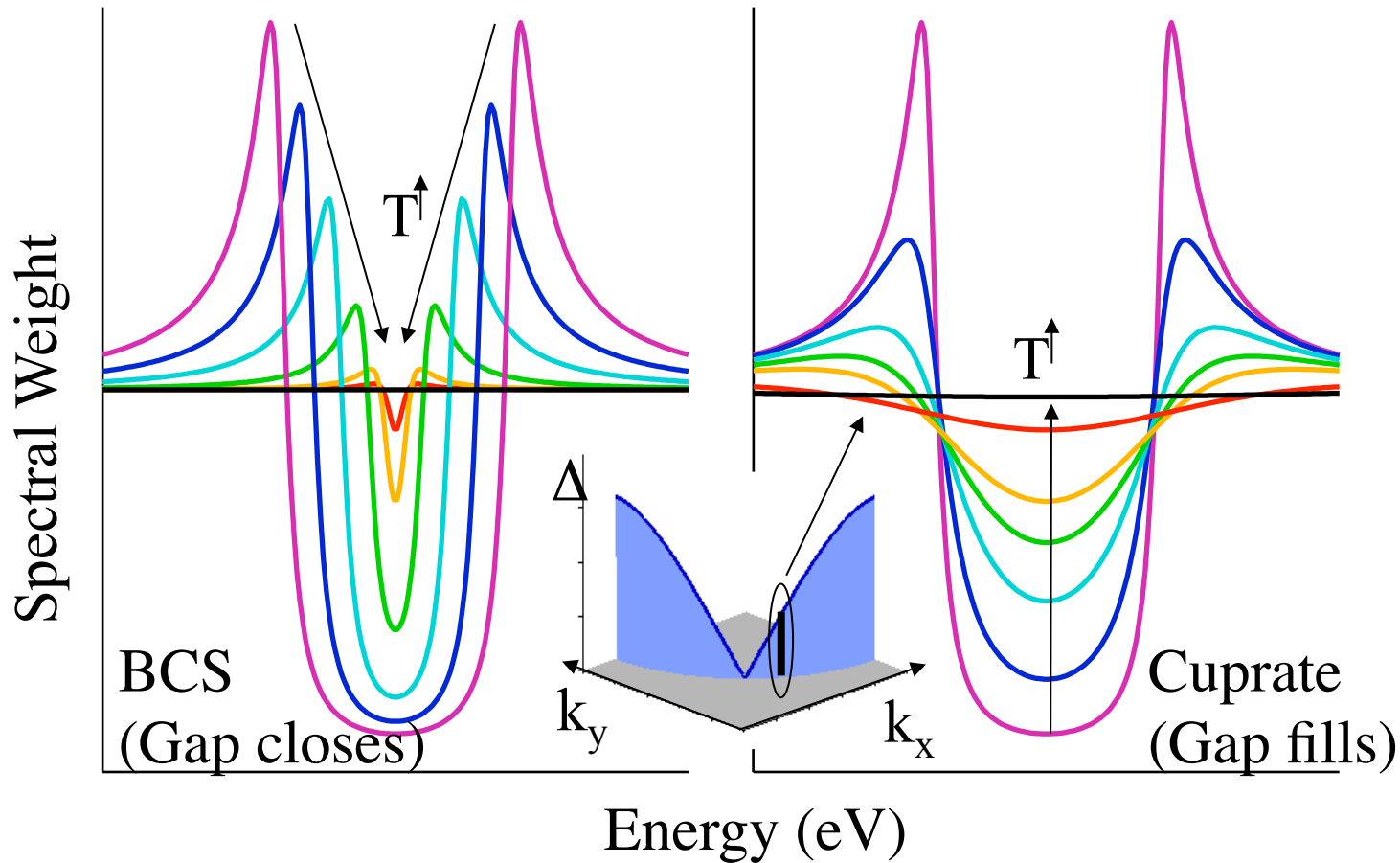


Linear-in-T scattering of the normal “strange metal” state.  
Marginal Fermi Liquid” state, or better the “Power Law Liquid” state.

T. J. Reber, D.S.D. et al.  
arXiv 1509.01611 (2015)

We wish to access these scattering rates at low energy inside the gap. MDC analysis methods fail because there are no MDC peaks inside the gap. EDC lineshapes have never been understood.

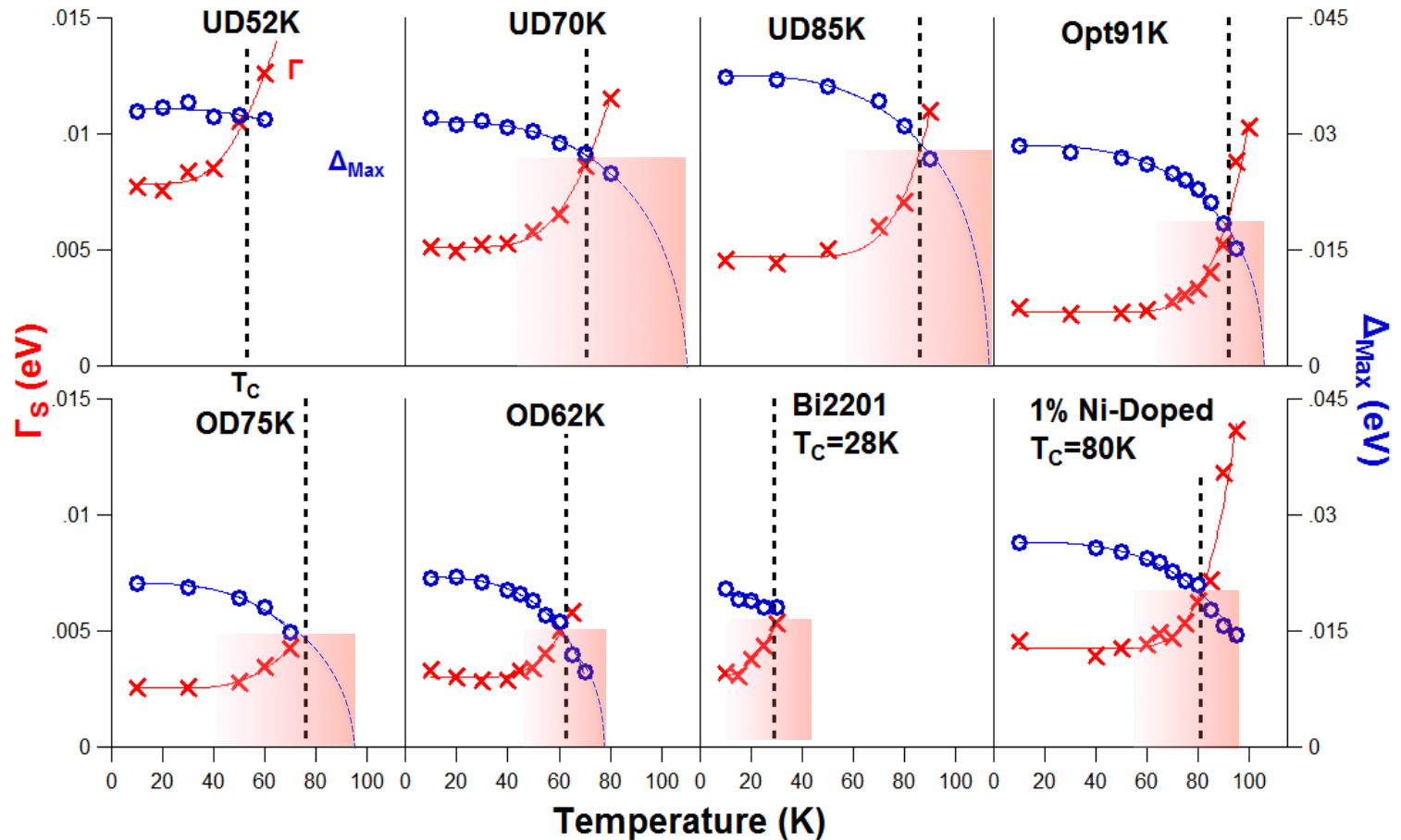
# Closing/Filling of the gaps with temperature



The filling of the gap in cuprates is due to the rapidly rising  $\Gamma$  (scattering rate) with temperature. This is a phenomenology observed in essentially all spectroscopies on cuprates, but has been difficult to quantify.

# Crossover between superconductive pairing ( $\Delta$ ) and a self-energy term ( $\Gamma$ ) occurs at/sets the $T_c$ in cuprates.

Near nodal data uncontaminated by pseudogap effects.

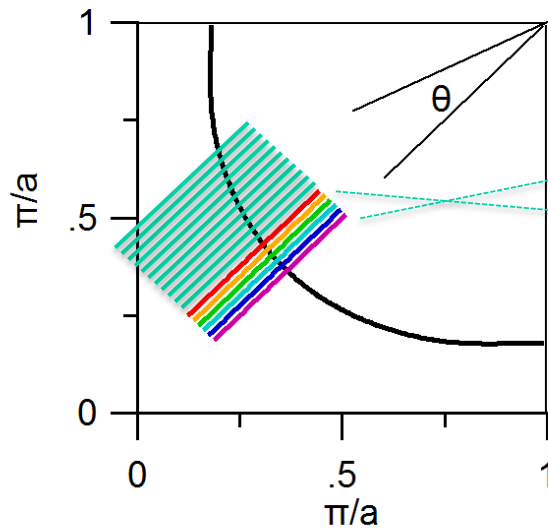


Pairing ( $\Delta$ ) extends well above  $T_c$  in all cases (indicates pre-formed pairs above  $T_c$ , which condense at  $T_c$ ).  $\Gamma$  “fills in” the gap.

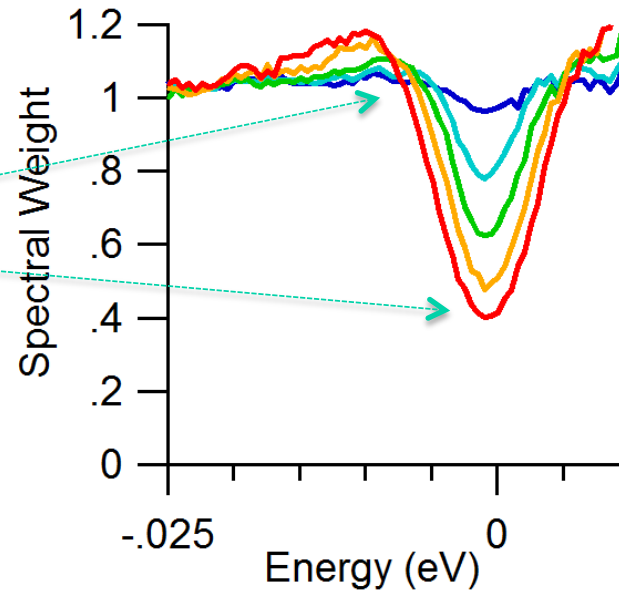


# New method for analyzing gaps and scattering rates. Tomographic Density of States (TDoS)

Tomographic = sliced or sectioned.

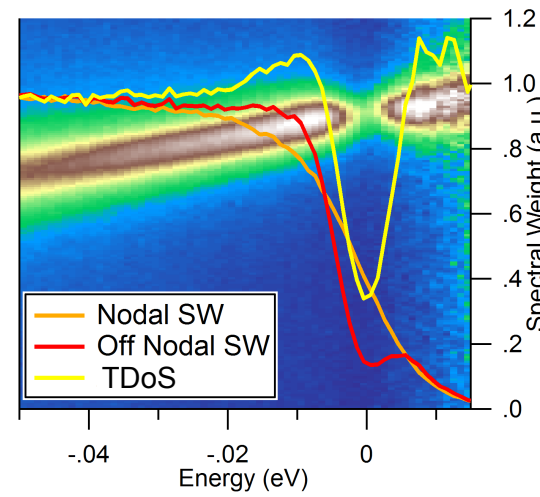
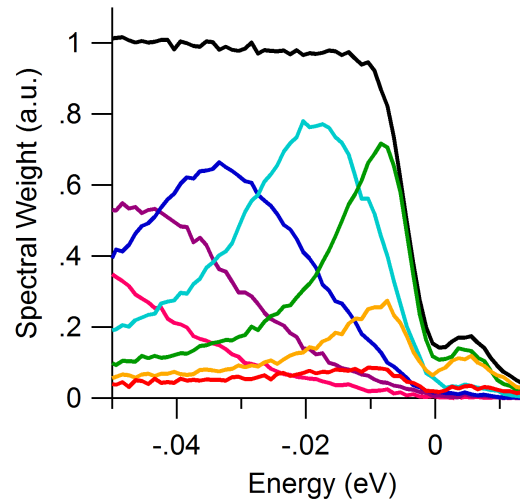
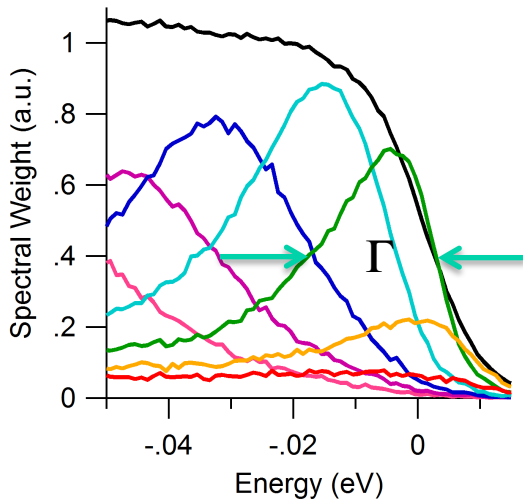
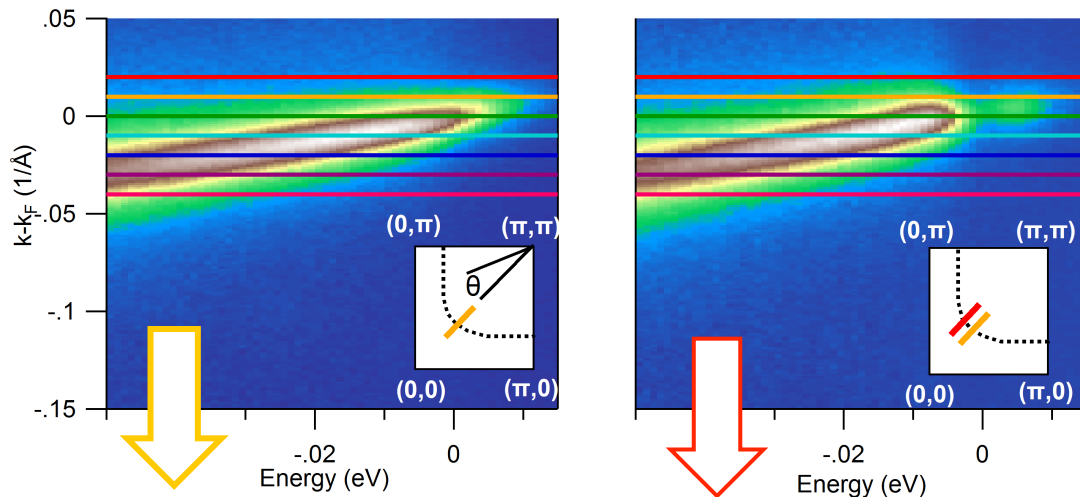


Flat DOS modulated by d-wave SC gap.



**Quantitative** determination of gaps and scattering rates (via Dynes tunneling formula).

# Creating the Tomographic Density of States (TDoS)



Sample: Bi2212  
 T: 50 K  
 $T_C$ : 91 K  
 $h\nu$ : 7 eV

Colored: EDCs along one cut.  
 Black: Sum of  $\sim 170$  EDCs = spectral weight curves.  
 Yellow (above): Normalized spectral weights = TDoS

The weight above  $E_F$  is real (no symmetrization has been done).

EDC peak widths (scatt rates)  $\sim 15$  meV or greater. Full scattering, including heterogeneous contribution.

TDoS scattering rate  $\sim 2-3$  meV – homogeneous contribution?

# Fitting to Dynes's Tunneling Formula (1978)

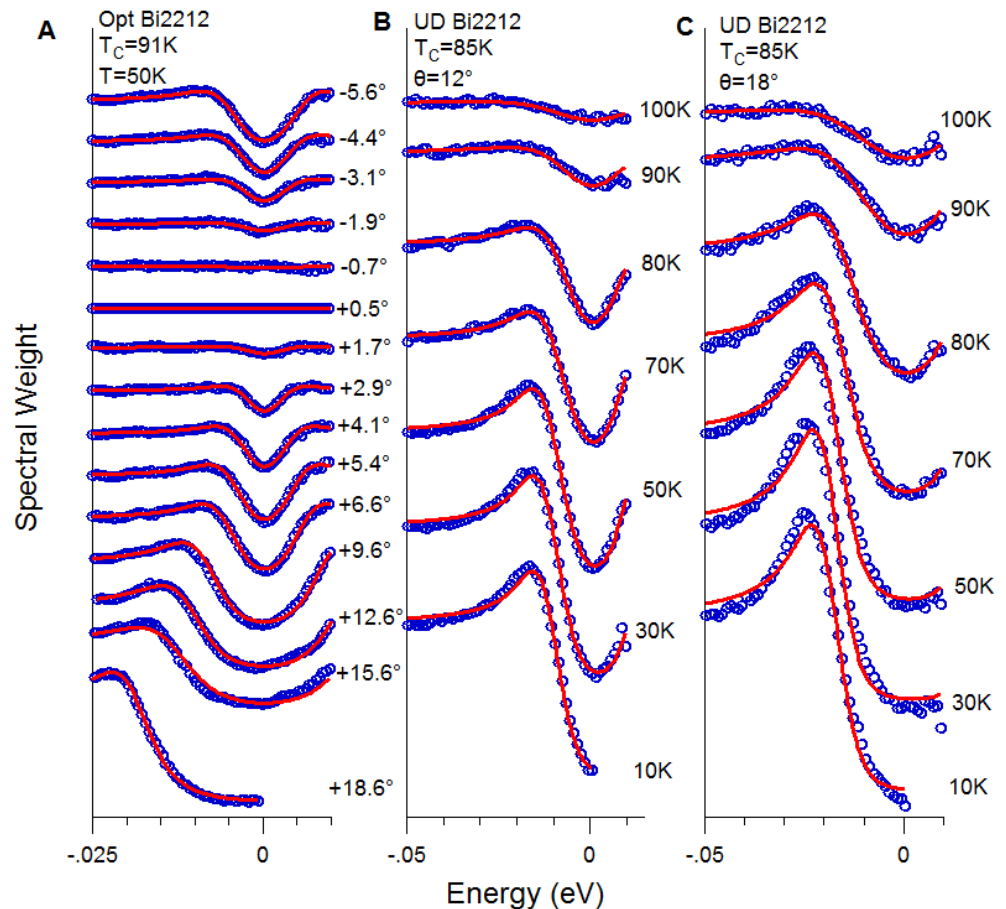
$$I_{TDoS}(\omega) = \rho_{Dynes}(\omega) = \text{Re} \frac{\omega + i\Gamma}{\sqrt{(\omega + i\Gamma)^2 - \Delta^2}}$$

Represents a broadened BCS DOS.

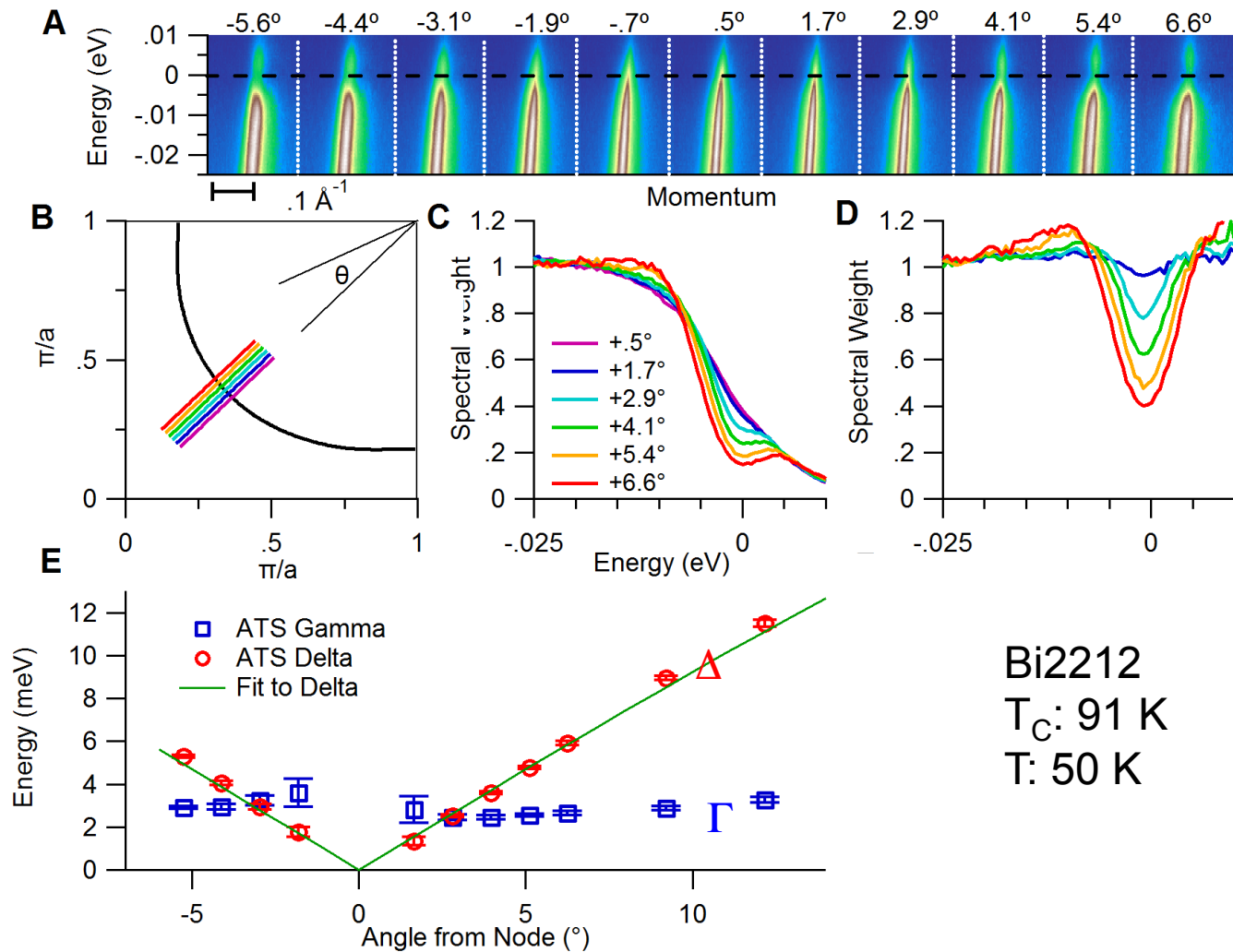
The TDoS are well fit by the Dynes formula over the full range of accessible angles and temperatures.

Each fit gives: pairing strength  $\Delta$ , and pair-breaking rate  $\Gamma$ .

Similar fits of actual tunneling in cuprates are not nearly as successful because of the d-wave nature of  $\Delta$ , the van-Hove in the DOS, etc.

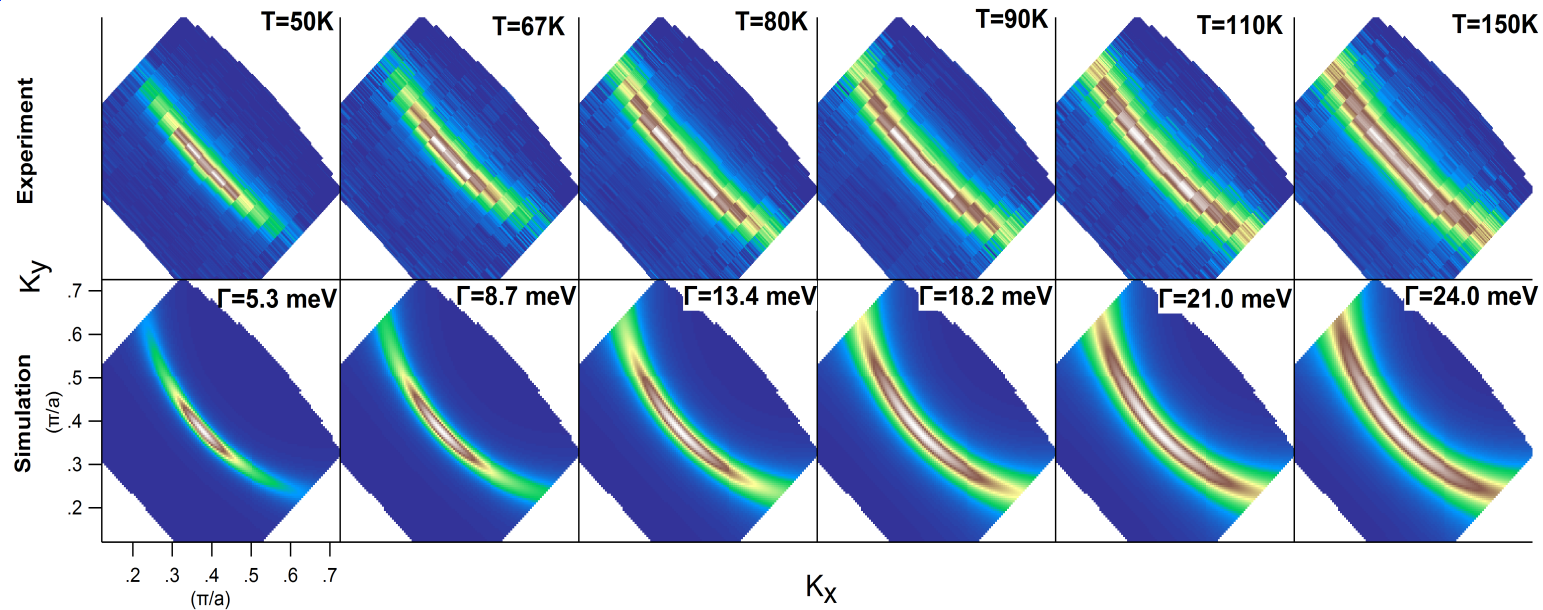


# Near-Nodal Angular Evolution of TDoS

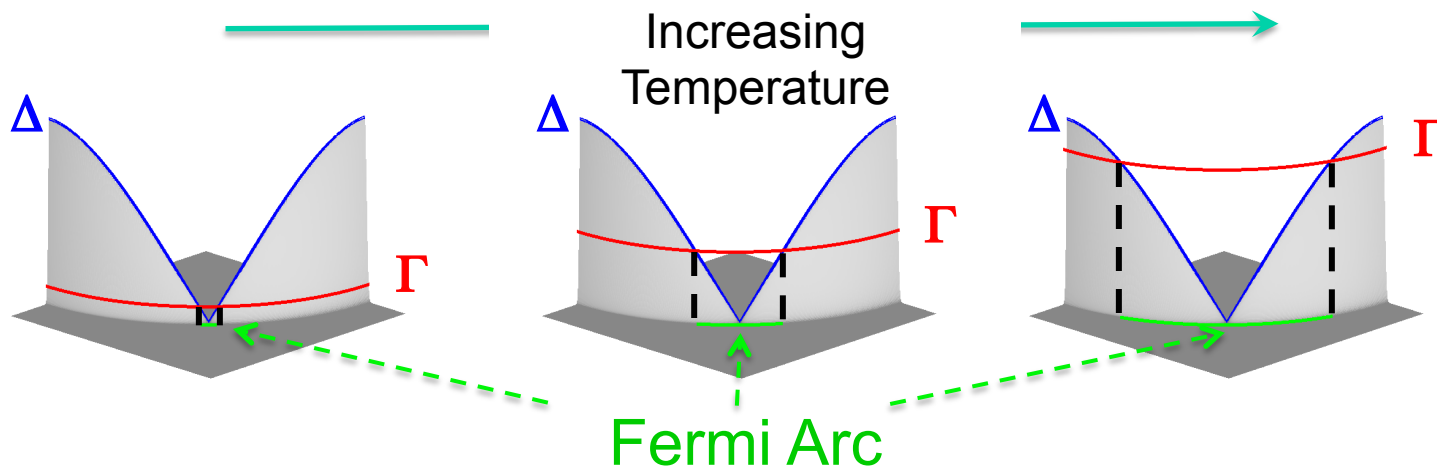


The TDoS extracts a d-wave  $\Delta$  with a nearly isotropic  $\Gamma$  in the near nodal region. Improved accuracy and precision over previous techniques for determining  $\Delta$  or  $\Gamma$ .

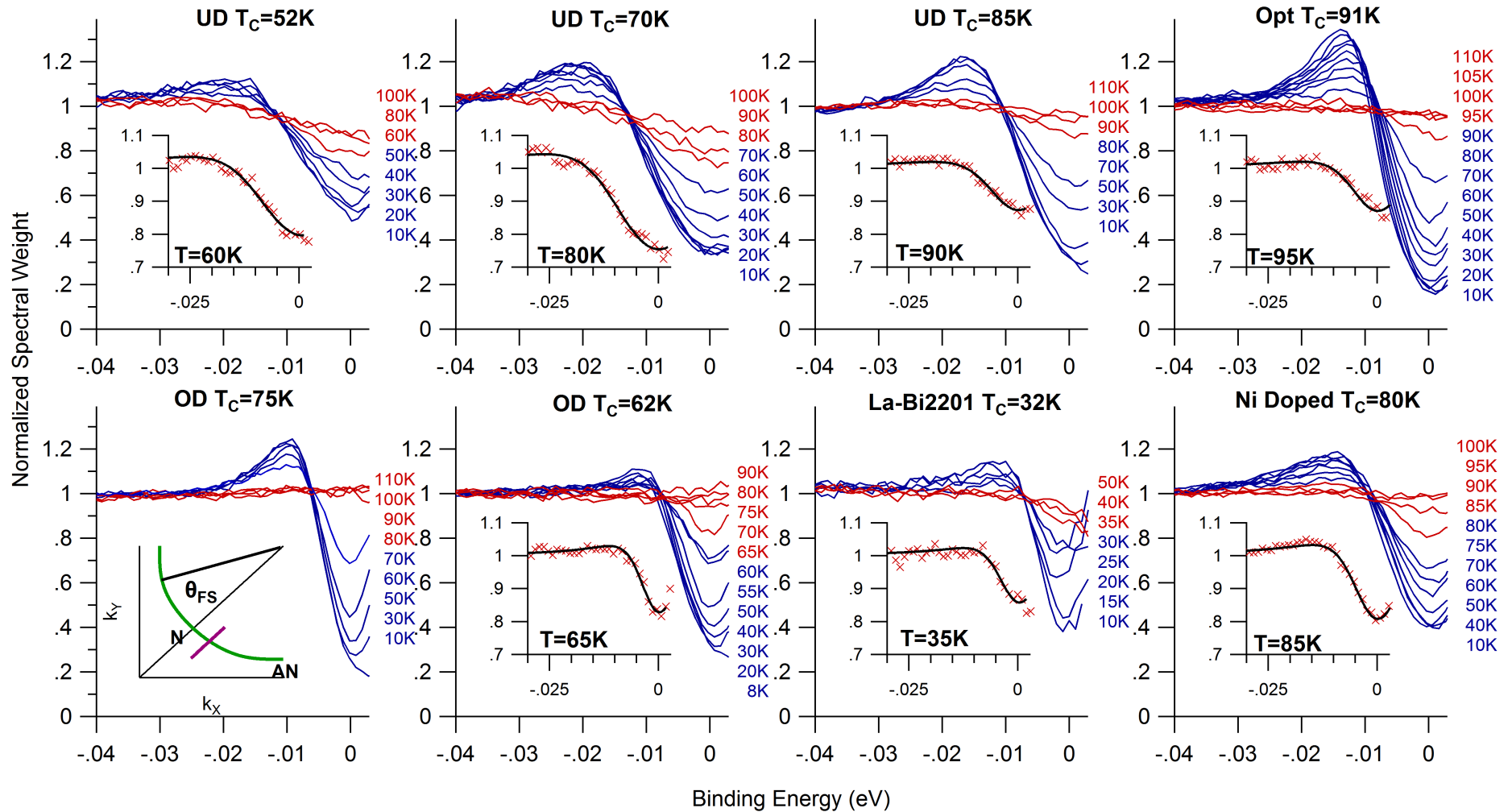
# Temperature dependence of Fermi Arc Measured (top) and simulated (bottom)



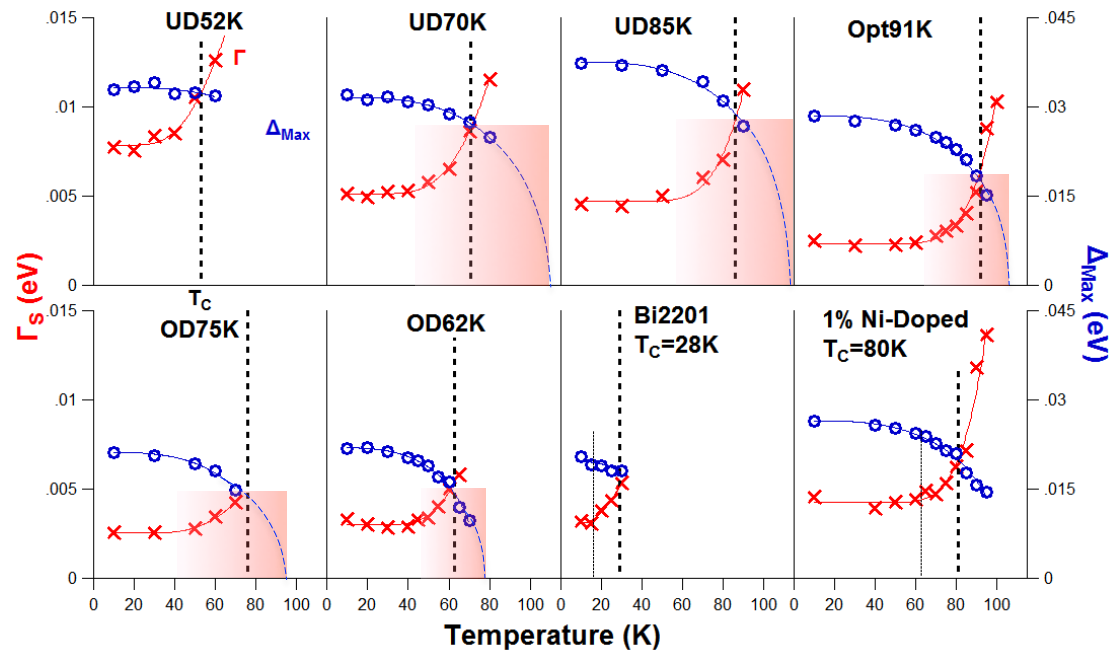
Sample:  
UD  
Bi2212  
 $T_C$ : 67 K  
hv:7 eV



# Near-nodal TDoS's for many doping levels, and in the SC state and non-superconducting (pre-pairing) state



# Why does the crossover seem to set $T_C$ ?

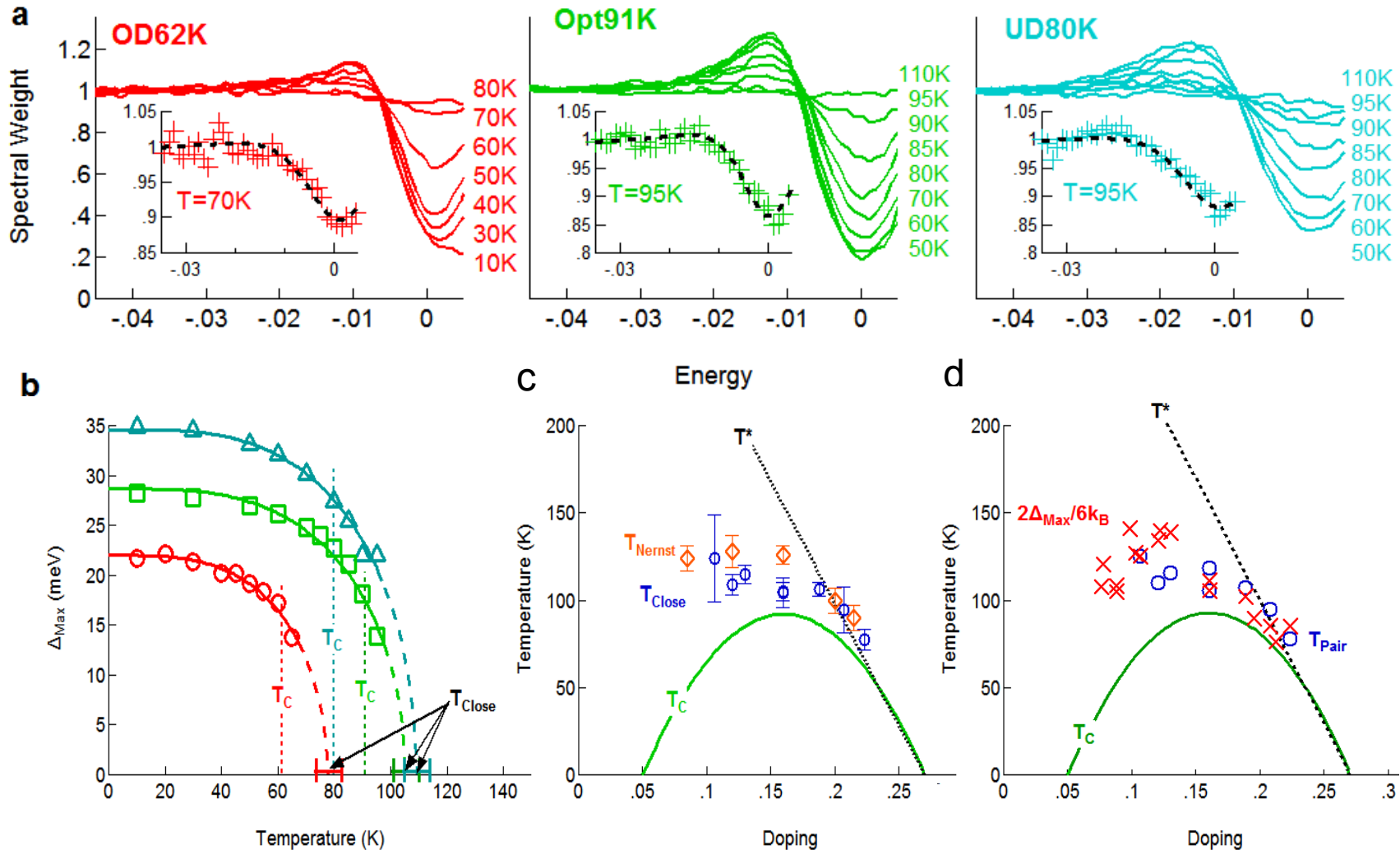


Pairs are broken at the same rate that they are created.  
- pair density low while gap still large.

Pairs need to be dense enough and long-lived enough for phase coherence to form (at  $T_C$ ).

Similar physics observed in granular aluminum, where localization becomes very important –  $\Gamma$  is tuned by varying grain size. SC disappears when  $\Gamma$  crosses  $\Delta$  (static effect – in contrast to the dynamic effect observed here).

# Doping Dependence of $T_{\text{Close}}$

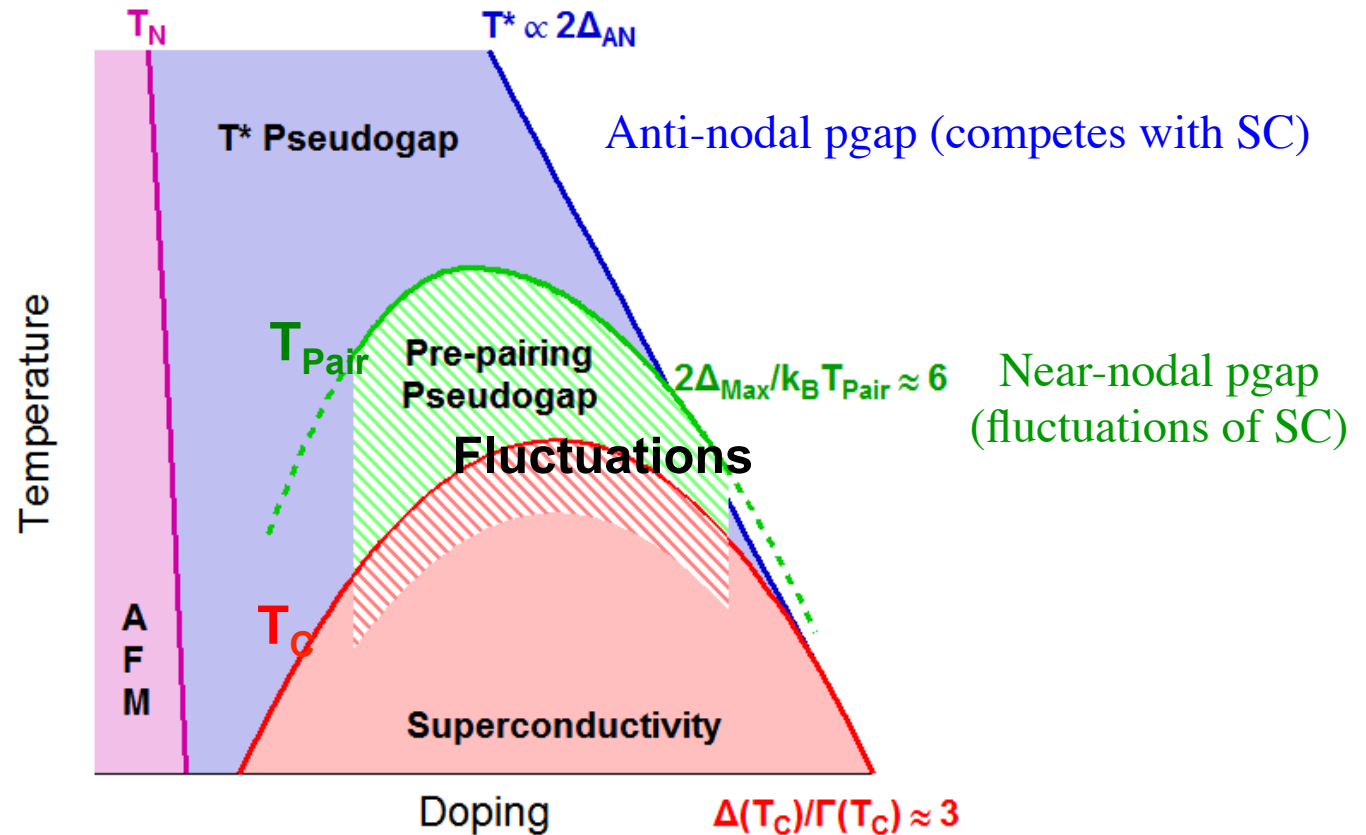


Pre-pairing observed at all dopings studied.  
 $T_{\text{Close}}$  matches  $T_{\text{Onset}}$  as found in Nernst expts.  
 Wang/Ong et al. *PRL* (2005)

Qualitative match to Josephson Plasma  
 Resonance expts on UD YBCO.  
 Bubroka/Bernhard et al. *PRL* (2011)



# Doping phase diagram from gap measurements



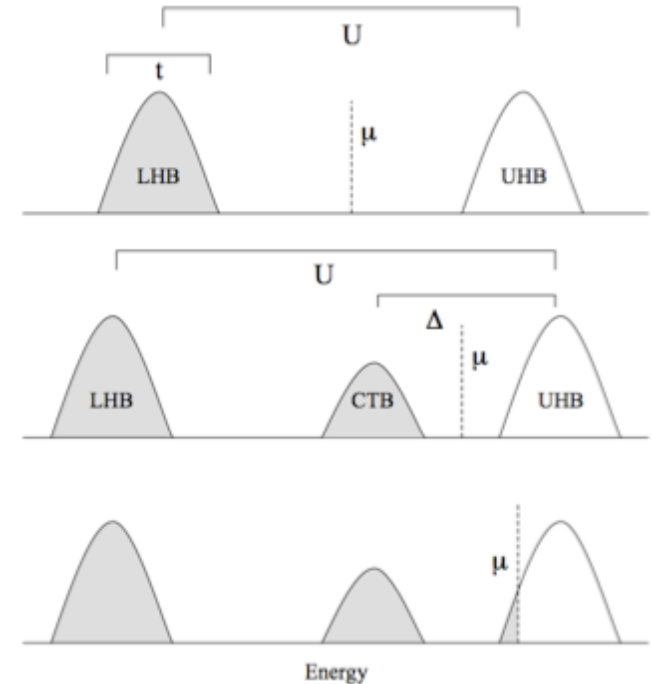
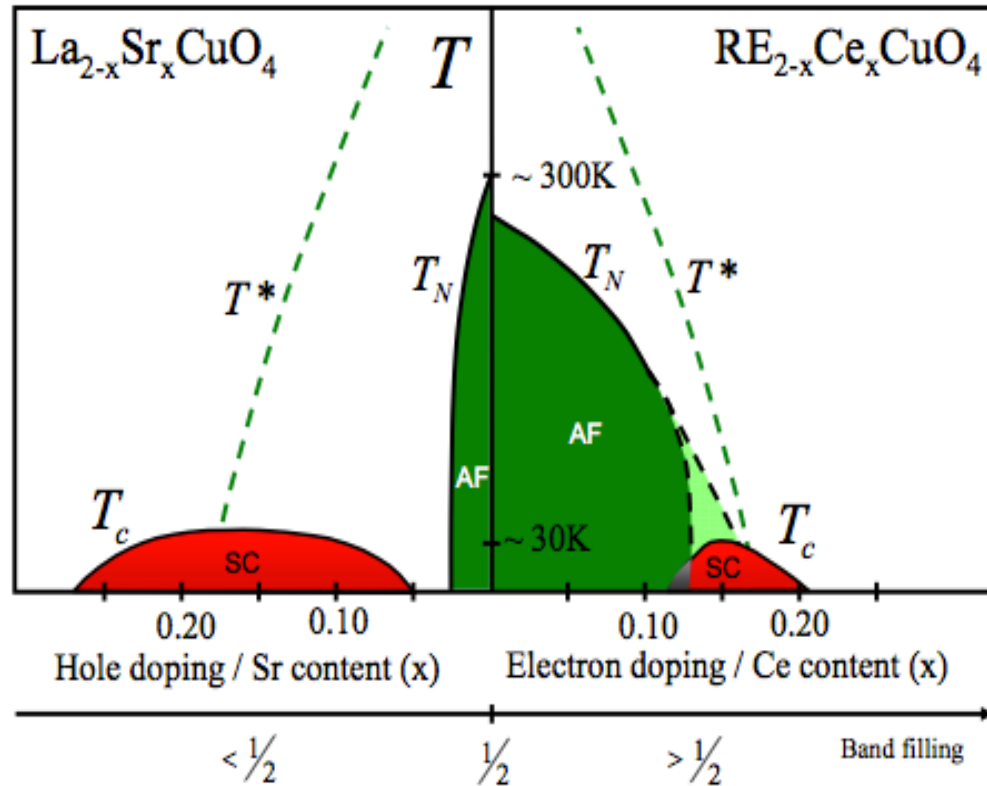
Superconductivity (from near-nodal measurements):

- $2\Delta_{NN}$  and  $T_{close}$  (not  $T_c$ ) are proportional with a ratio of  $\sim 6$ .
- strong coupling both in UD and OD regimes.

$T^*/$ pseudogap (from antinodal measurements):

- Distinct from superconductivity.

# n-type cuprates

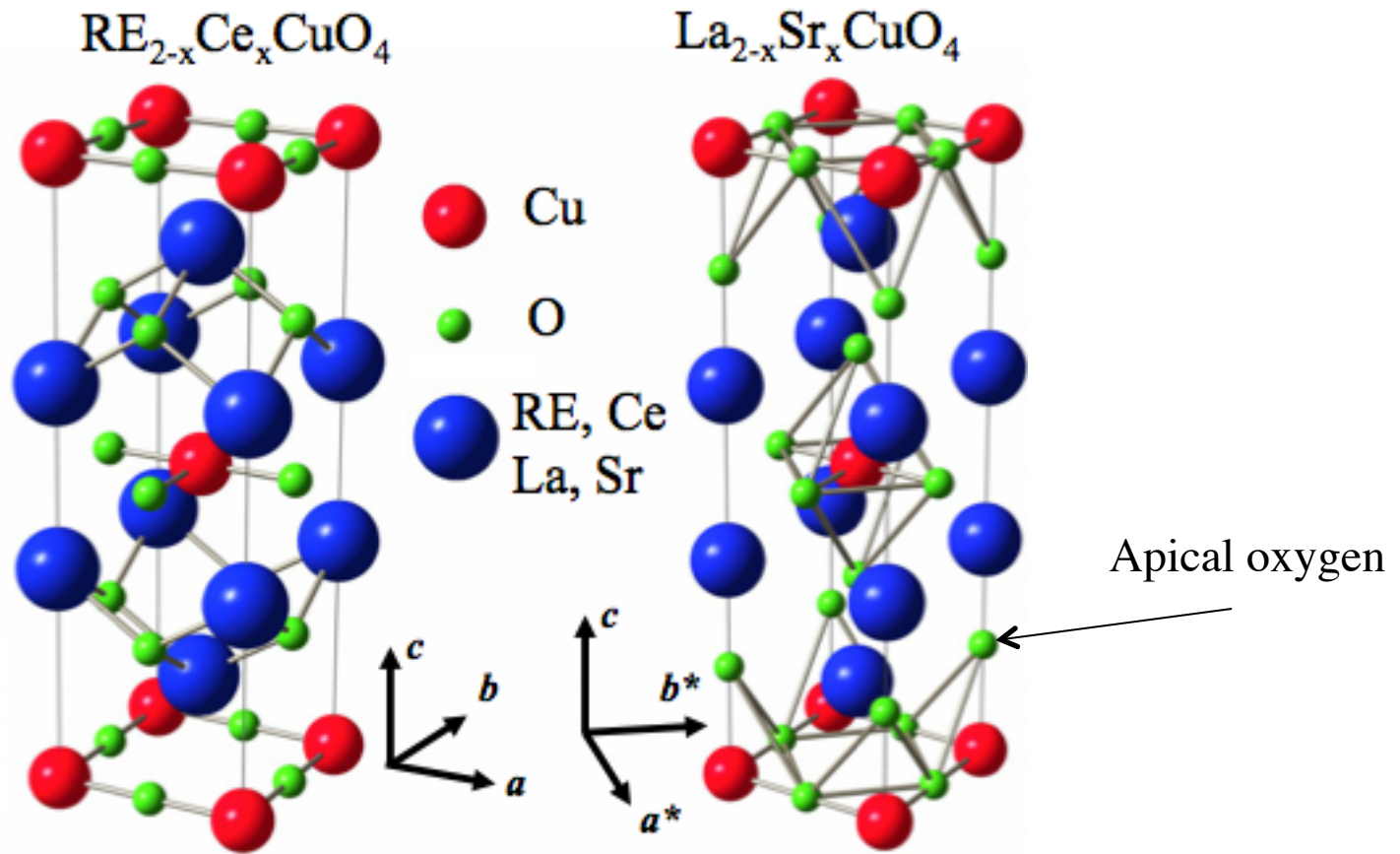


Armitage et al., Rev. Mod. Phys. 82, 2421-2487 (2010)

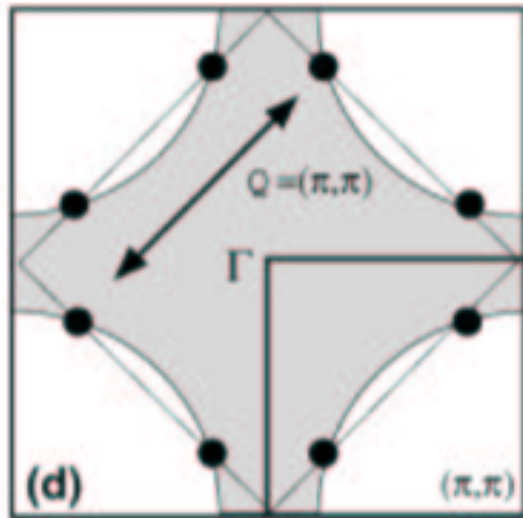
In the n-types:

- Long range AF order extends much farther, out to the SC doping levels.
- SC dome covers a smaller doping range.
- Possible coexistence of SC and AF order.
- Slightly different crystal structure (lack of apical oxygen atom).

# Crystal structure of n-and p-type cuprates



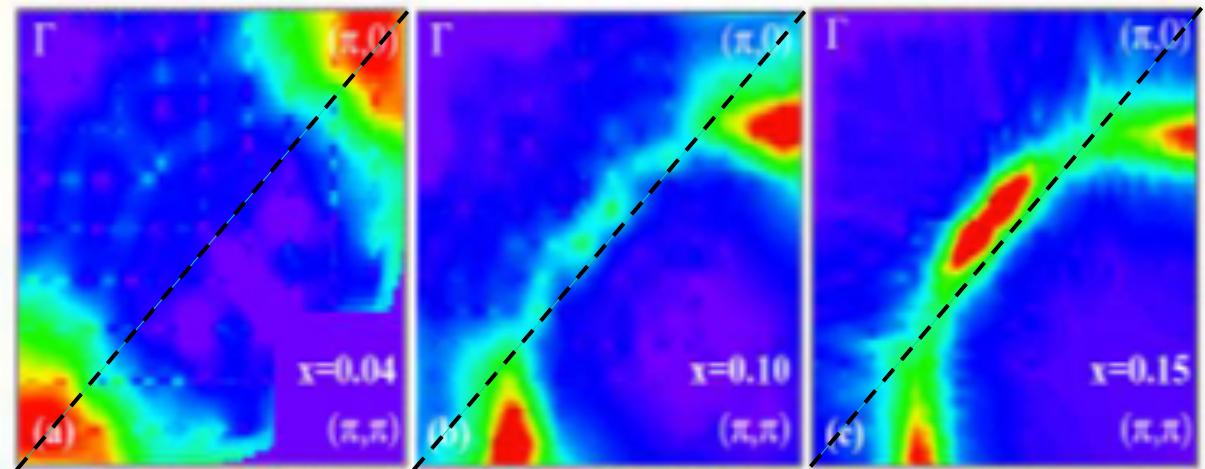
# “hot spots” and FS arcs



$x=0.04$

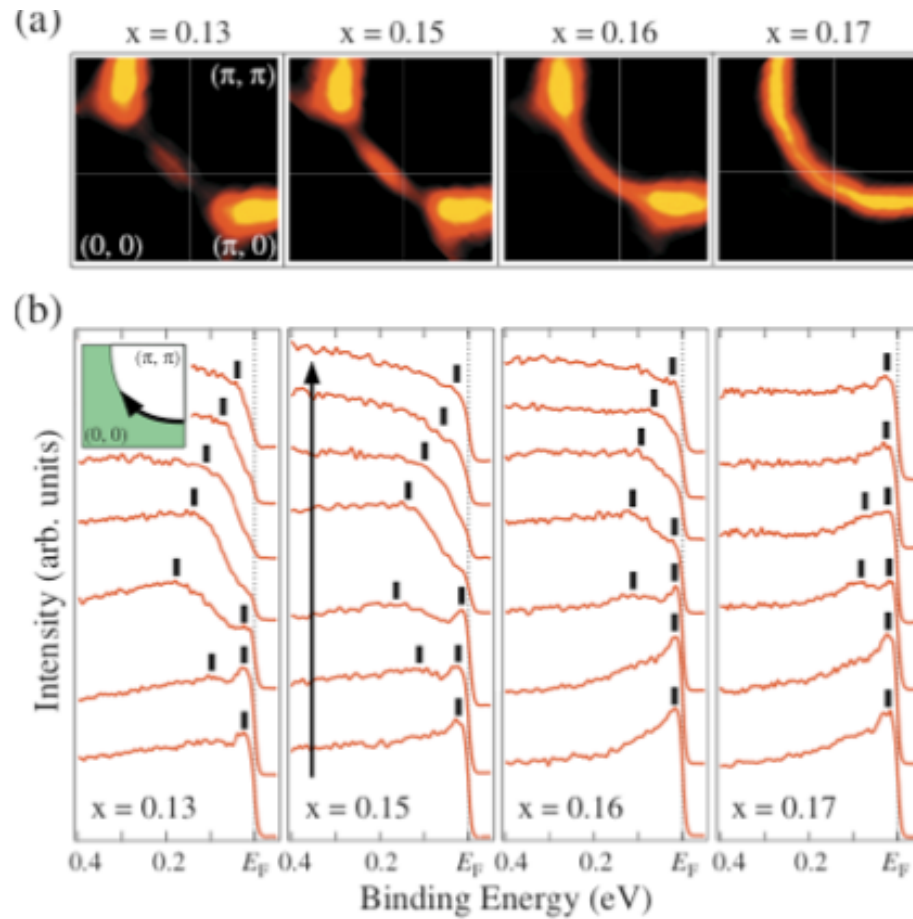
$x=0.10$

$x=0.15$



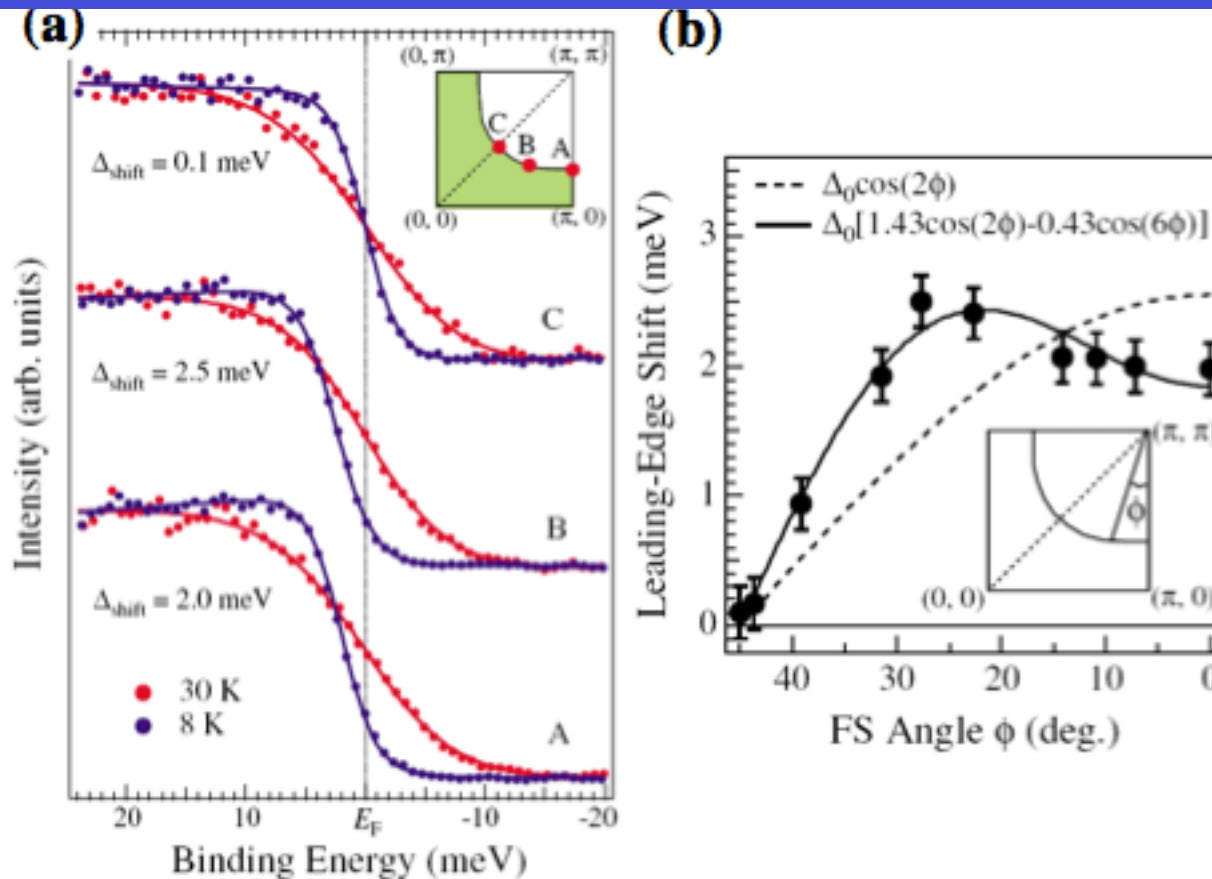
Armitage et al., 2002

# $\text{Nd}_{2-x}\text{Ce}_x\text{CuO}_4$



Hot spots go away at large doping levels.

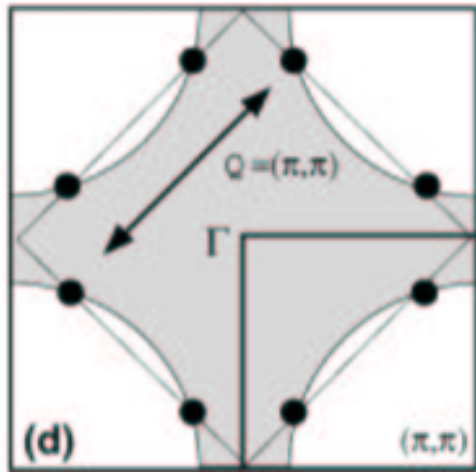
# Non-monotonic gap as a function of $k$



Matsui 2005

Effect originally seen in polarized Raman spectroscopy (Blumberg 2002).  
Maximum gap appears roughly at the locations of the hot spots.  
→  $(\pi, \pi)$  AF fluctuations driving the d-wave superconductivity

## “hot spots” in p-type cuprates



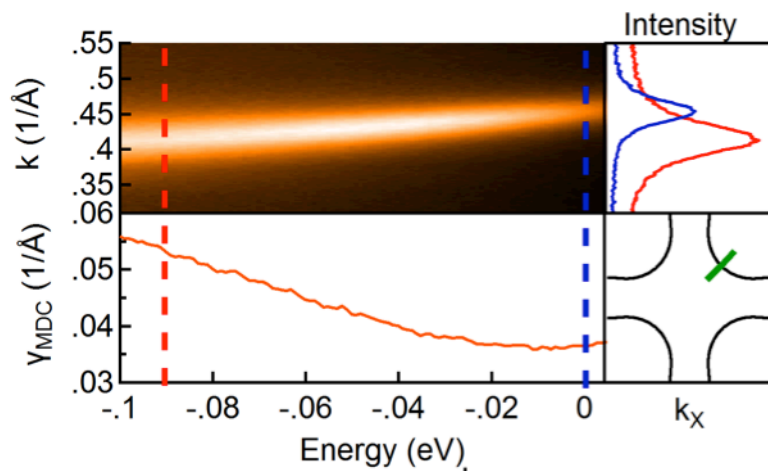
Many aspects of the data in p-type cuprates are consistent with hot spot physics, but it is not as incontrovertible as in the n-type cuprates.

N-state scattering rates (peak broadening) are stronger as one goes from the node to the antinode. In p-types there is no evidence that the scattering gets “colder” past the hot spots.

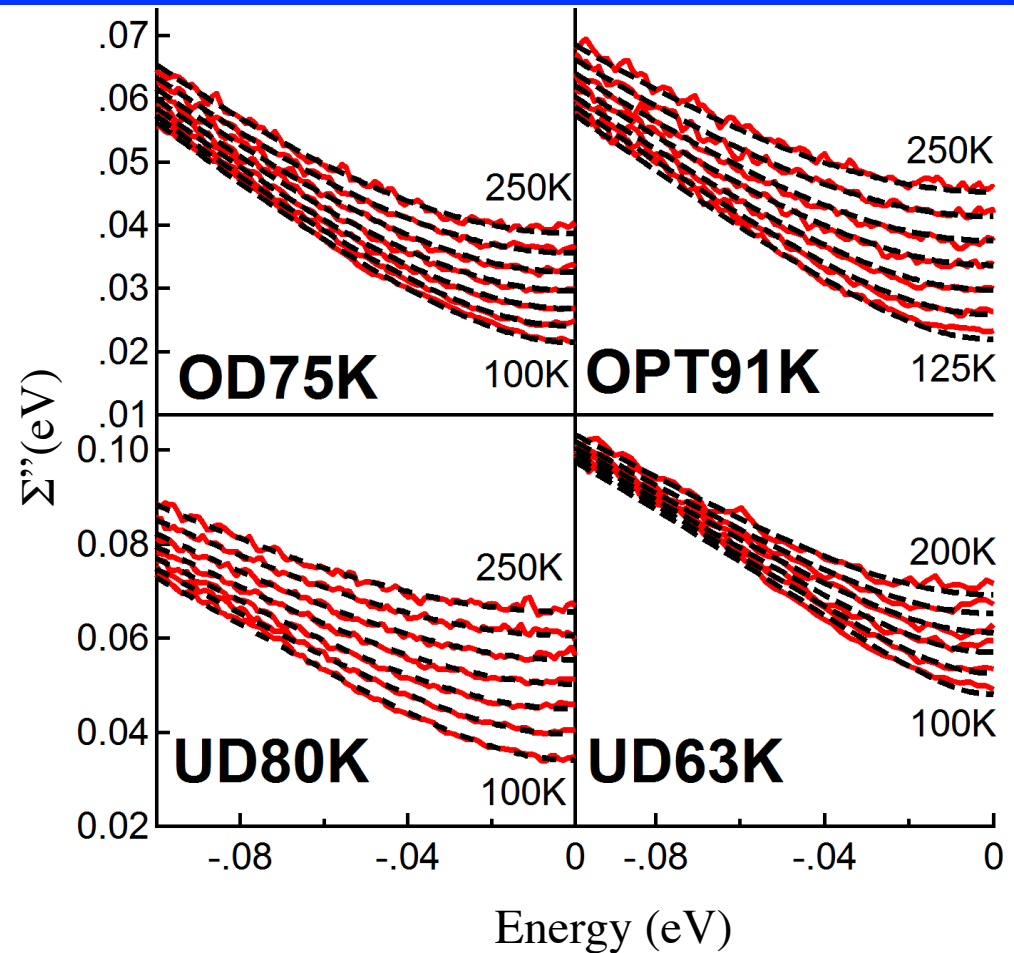
This is not inconsistent with broadly peaked AF scattering due to very short-ranged AF fluctuations. But then these would be hot regions and not hot spots.

Edges of the Fermi arcs (which are also not at all sharp in  $k$ -space) sometimes associated with the hot spots.

# Normal-state nodal ARPES scattering rates ( $\Sigma''$ ) of Bi2212 as a function of $\omega, T$ , doping.



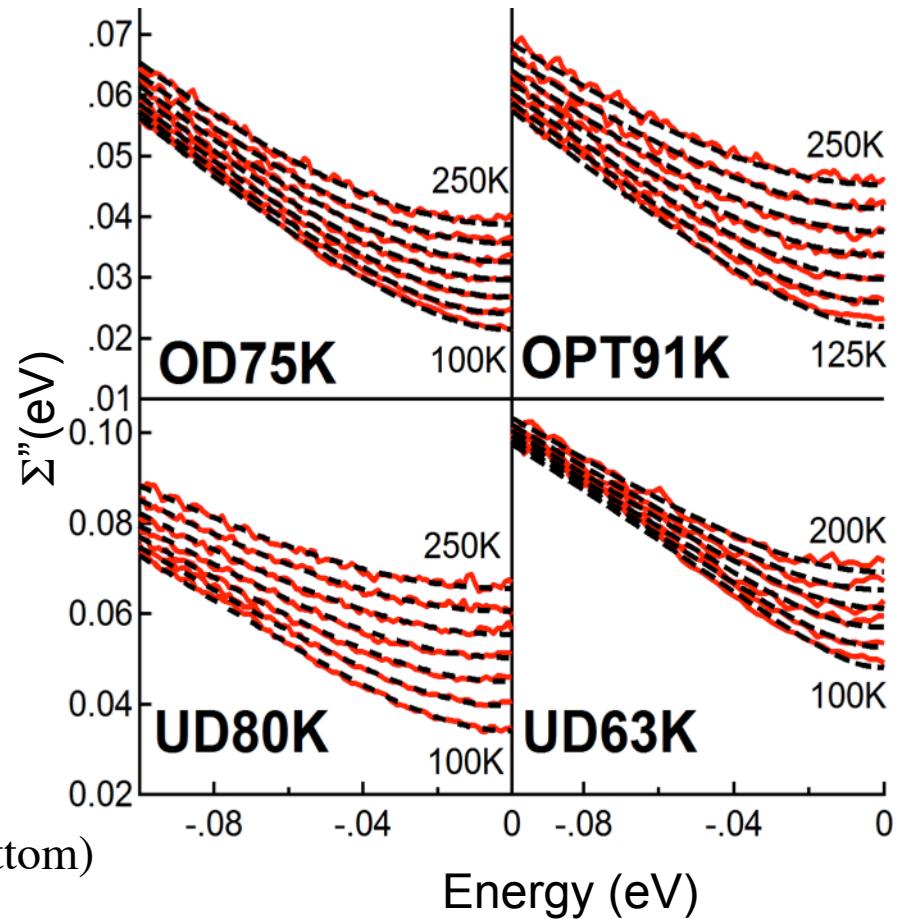
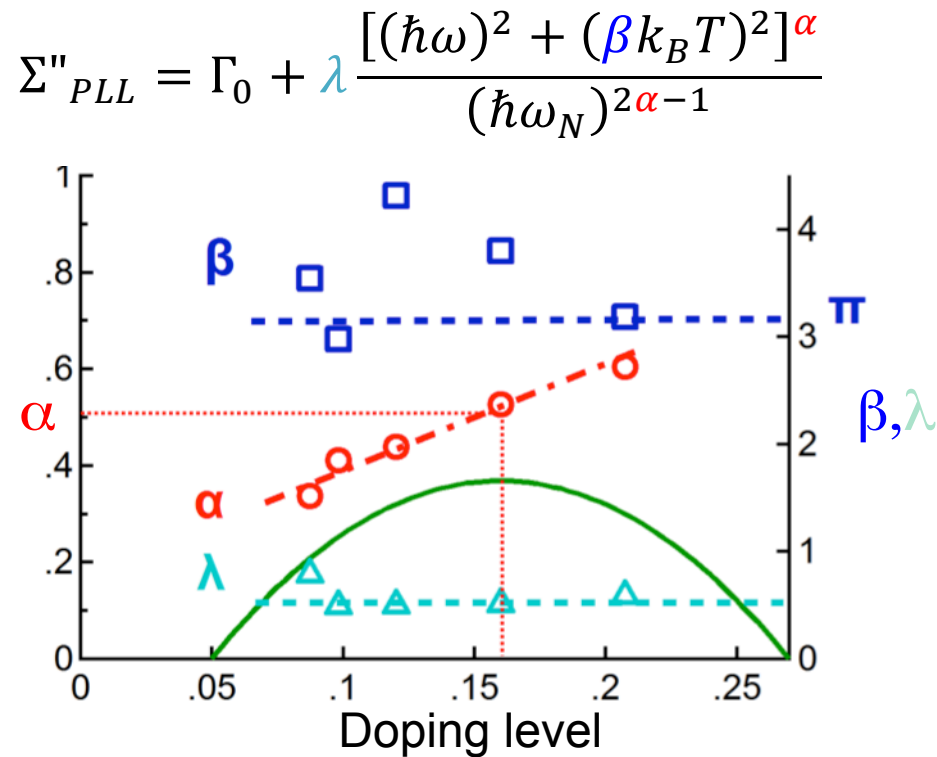
$$\Sigma''(\omega) = v_{\text{bare}} * \Gamma_{\text{MDC}}(\omega) / 2$$



All data looks quadratic at low  $\omega$  (FL-like), linear at high  $\omega$  (MFL-like).



# A new experiment-motivated ansatz for normal state $\Sigma''$ The Power Law Liquid (PLL)



$\omega_N$  (unit normalization) fixed at 0.5 eV ( $\sim$  band bottom)

$\Gamma_0$ =impurities+disorder (discussed later)

$\beta \sim \pi$ . Expected from Matsubara and Fermi Liquid (not previously proven).

$\lambda$  = coupling strength  $\sim$  constant=0.5.

$\alpha = 0.5$  :  $\omega, T$  linear (Marginal Fermi Liquid).

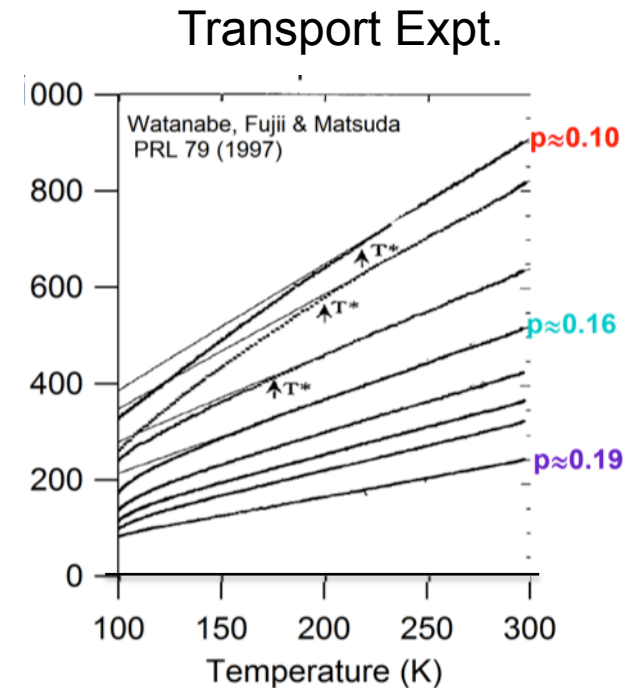
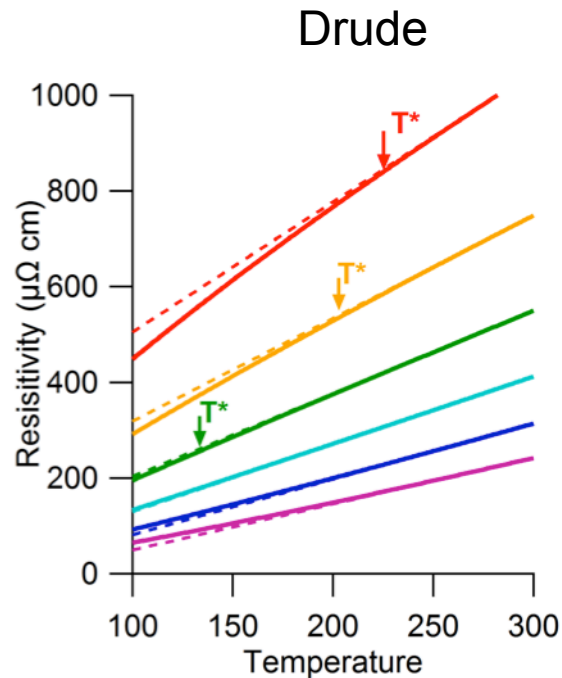
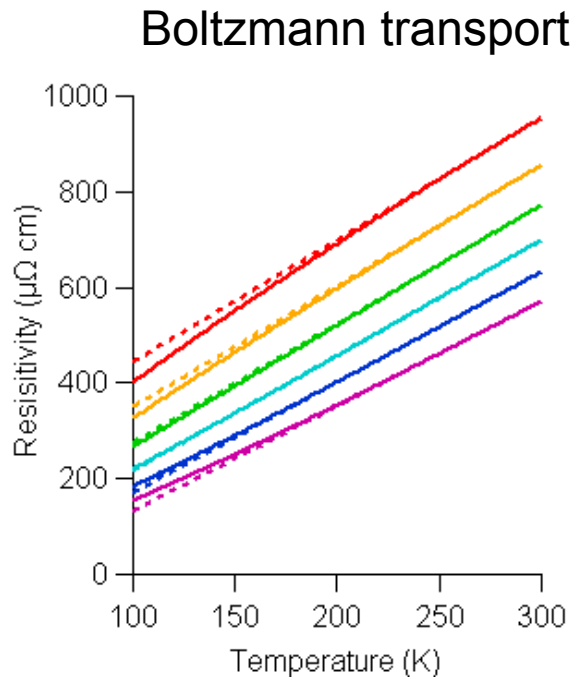
$\alpha = 1$  :  $\omega, T$  quadratic (True Fermi Liquid)

**Entire evolution essentially controlled by the one parameter  $\alpha$ .**

T.J. Reber, D.S. Dessau arXiv (2015)

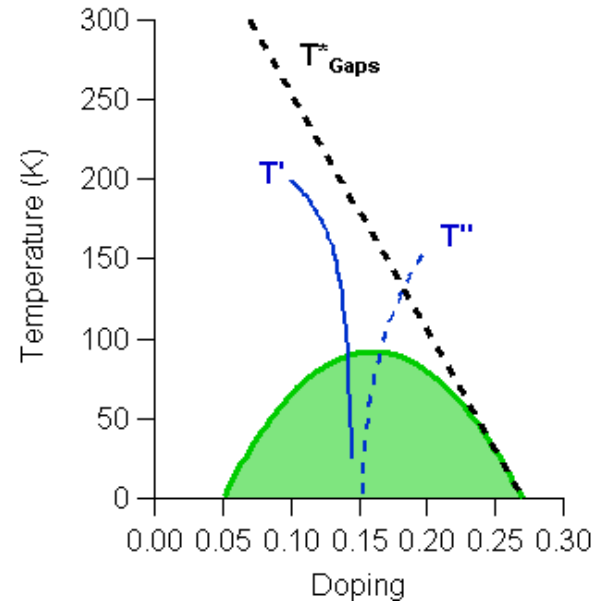
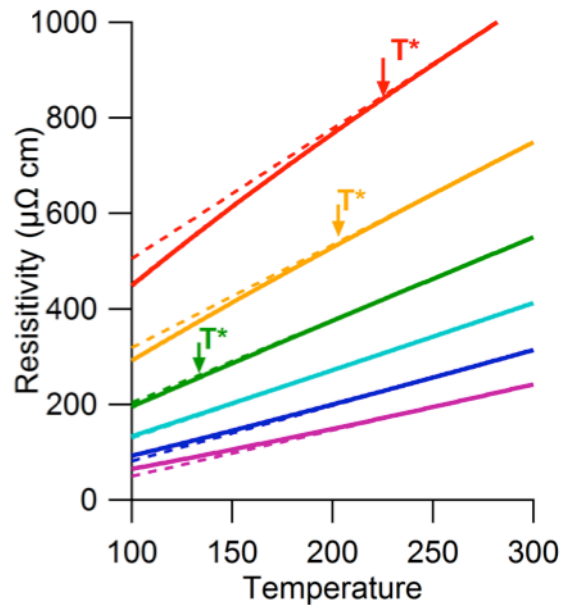
# Resistivity vs T from Power Law Liquid $\Sigma''$

The most detailed connection/best agreement between ARPES and transport from any material.



- Simplest assumption of a large tight-binding Fermi surface with fully isotropic PLL scattering rates over the full Fermi surface, with no spectral weight pseudogaps (i.e. no arcs or pockets). PLL offset  $\Gamma_0=0$ .
- “T\*” curvature change closely mimics the experimental transport data.

# $T^*$ from the calculated (Power Law Liquid-based) resistivity



- Mimics a quantum critical point near optimal doping.
- PLL is actually scaleless and doesn't have the  $T^*$  scale explicitly included in it.

# Origin of the PLL self energy?

## Other precedents for power law scattering rates?

Luttinger liquid physics in 1D. PLL spectra (and ARPES data) don't have the power law spectral weight that the LL physics has. Extend these ideas to 2D? RVB?

Doped Hubbard model? Si, Kotliar 1993

Quantum critical phases?

Quantum gravity-based ideas (ADS/CFT)? Others?

The superconductivity is born out of these states. How is all this connected?