Angle Resolved Photoemission Spectroscopy

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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

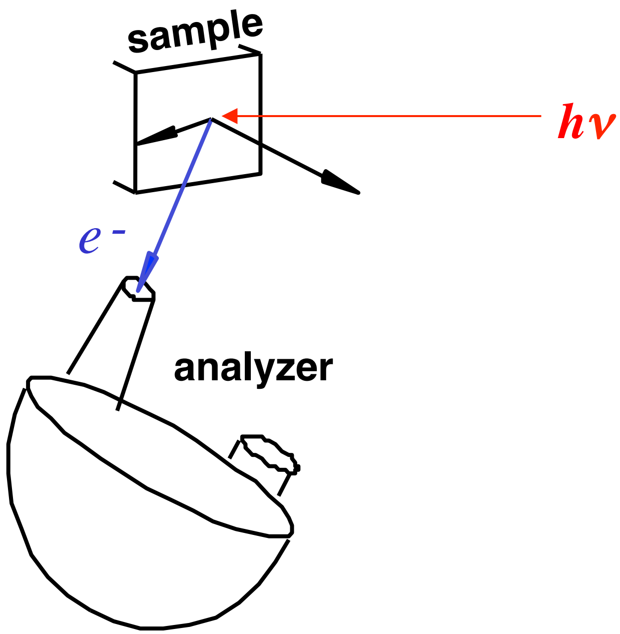
Compared to other spectroscopies:
- The k resolution is unique. Arguably the most direct of all spectroscopies.
- Surface sensitive. Requires high quality surfaces for studies of "bulk" physical effects. Laser-ARPES has improved this somewhat.
- Energy resolution (~ 1-20 meV scale) and base temperatures (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.
- Still developing rapidly.

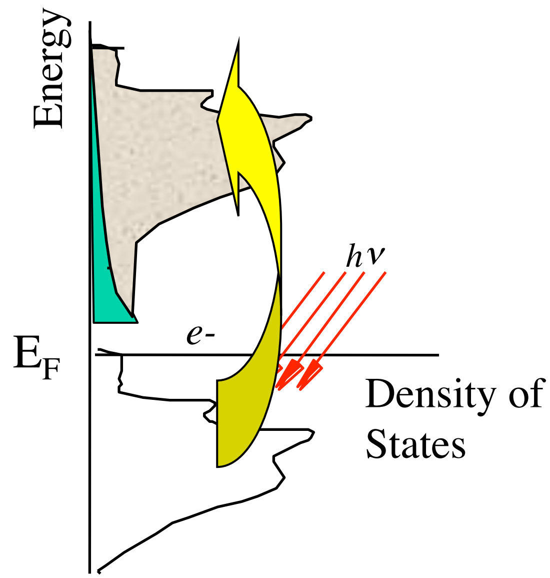
Plan

- 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
  - Some discussion of n-type cuprates, and pnictides 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.

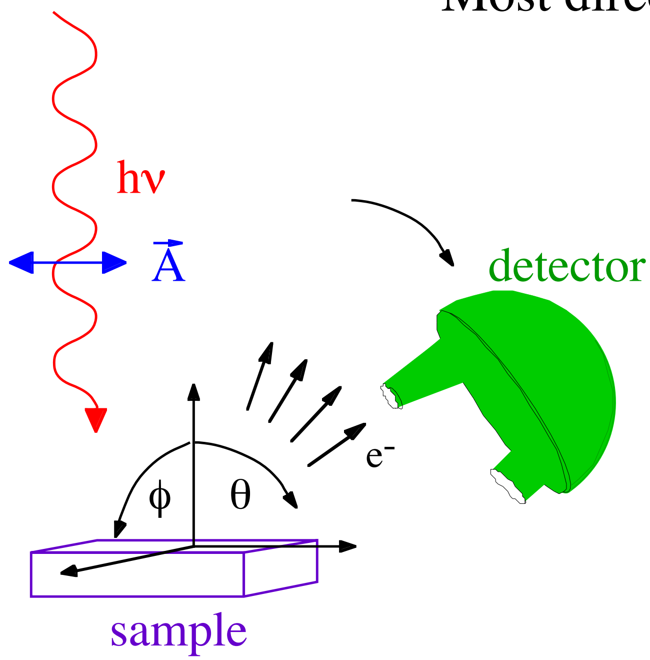
Primary electrons – no scattering events. Contain information of the electron spectral function

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

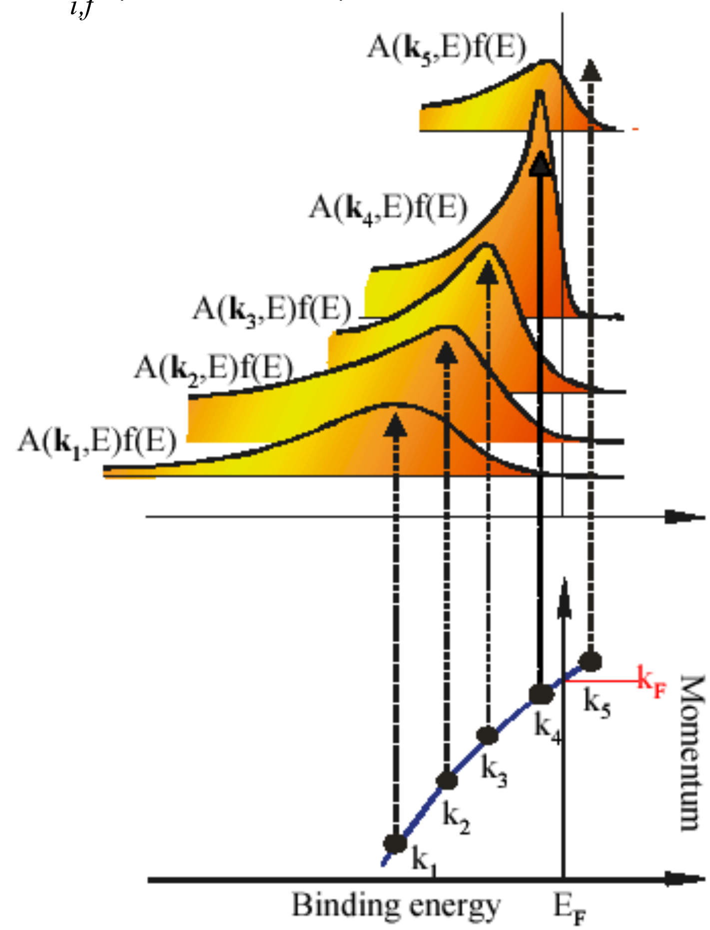
$$E_{kin} = \hbar\omega - \Phi - |E_B|$$

Angle Resolved Photoemission (ARPES)
A momentum resolved spectroscopy

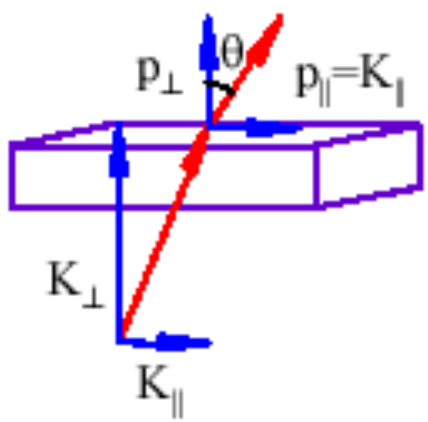
Most direct way to measure E vs. k of a solid.



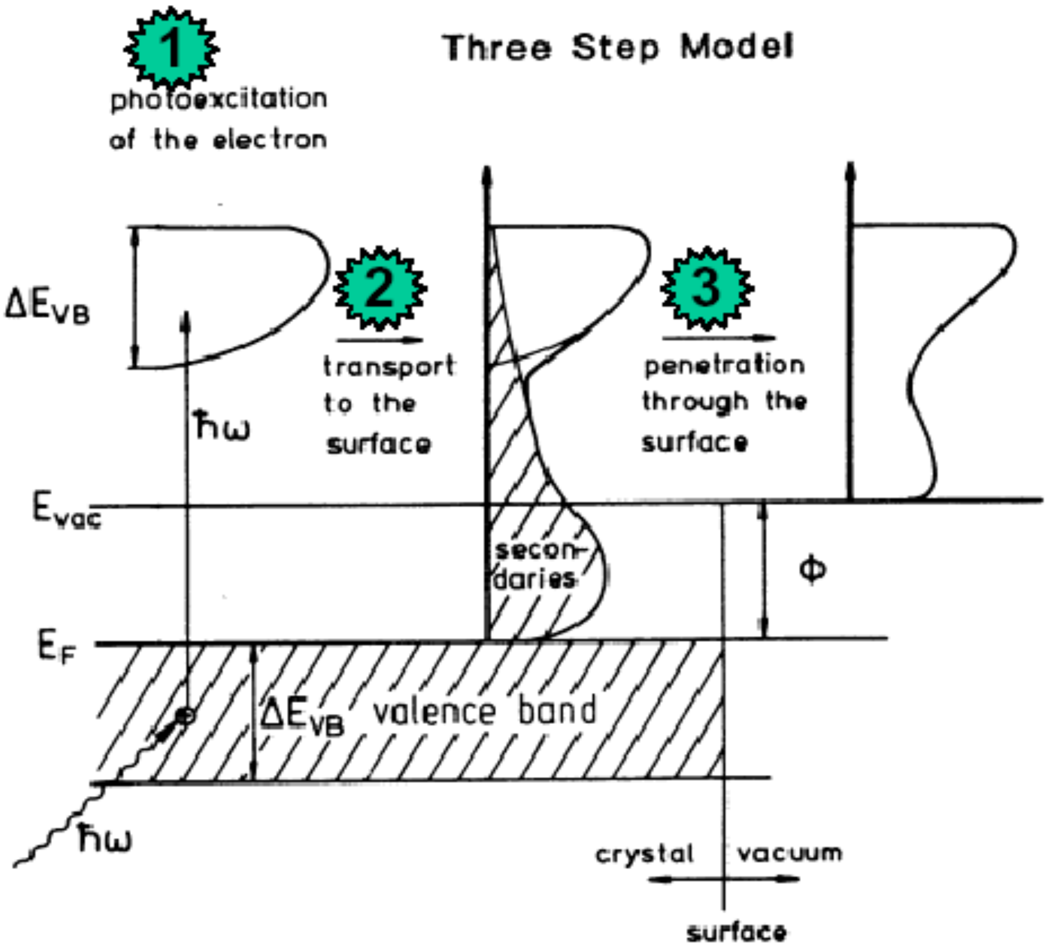
$$\text{Intensity} \propto \sum_{i,f} \left| \left\langle f \middle| \vec{\mathbf{p}} \bullet \vec{\mathbf{A}} \middle| i \right\rangle \right|^2 A(\vec{\mathbf{k}}, E)\, f(E)$$



Electron momentum
Parallel to the surface is
conserved



Three Step Model
W.E. Spicer

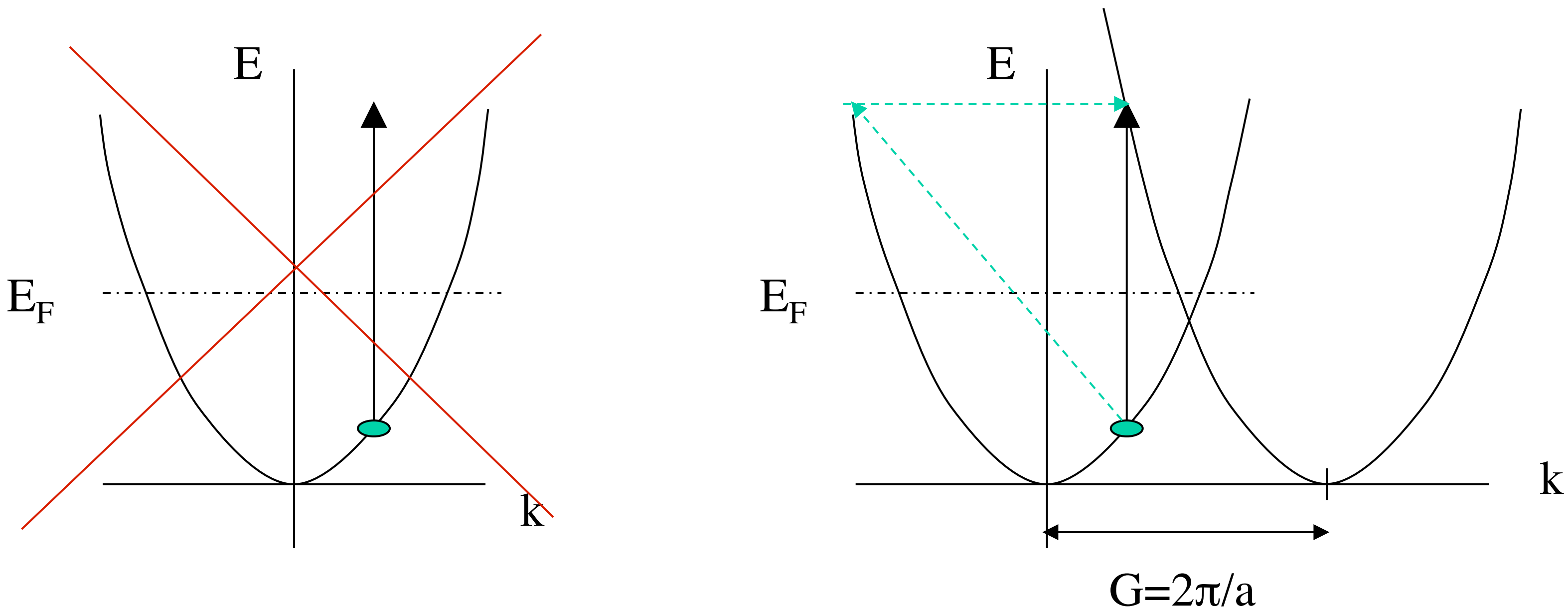


"One-step" models in which the photoemission process is considered as a single quantum mechanical event are more accurate, but not as illuminating.

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).

PHYSICAL REVIEW B VOLUME 21, NUMBER 8 15 APRIL 1980

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)

$$E_f(\vec{k}) = \hbar^2 |\vec{k}|^2/2m + E_0 = \hbar^2(k_\parallel^2 + k_\perp^2)/2m + E_0$$

Final Bloch states. E_o = "bottom of Muffin tin" – starting point for parabolic band dispersions = -9.34 eV for GaAs.

$$E_f(\vec{k}) = E_i(\vec{k}) + h\nu$$

Direct or k-conserving transitions.

$$E_f = E_k + e\Phi$$

$e\phi$ = work function of sample, E_k=kinetic energy

$$\hbar k_\parallel = (2mE_k)^{1/2}\sin\theta = [2m(E_i + h\nu - e\Phi)]^{1/2}\sin\theta$$

Projection to parallel component of momentum

$$\hbar k_\perp = [2m(E_k\cos^2\theta - V_0)]^{1/2} = \{2m[(E_i + h\nu - e\Phi)\cos^2\theta - V_0]\}^{1/2}$$

V_o=E_o- $e\phi$ ="Inner potential". Usually just a fitting parameter.

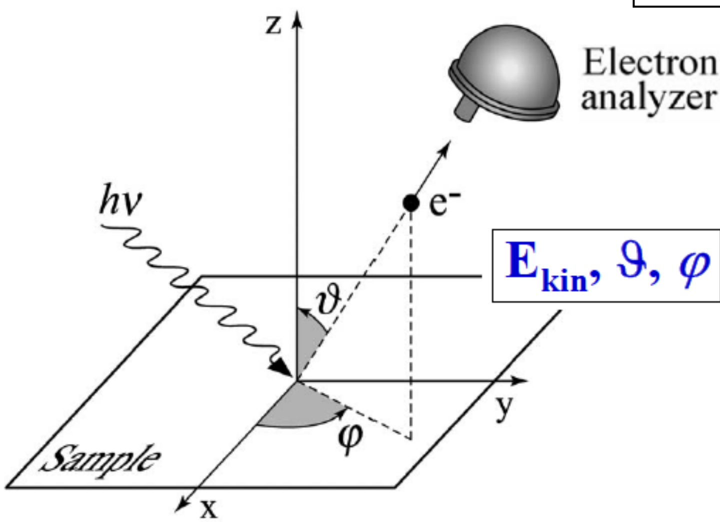
Normal emission: theta=0 $\hbar k_\parallel = 0$ $\hbar k_\perp = [2m(E_i + e\Phi - E_0)]^{1/2}$

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

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



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

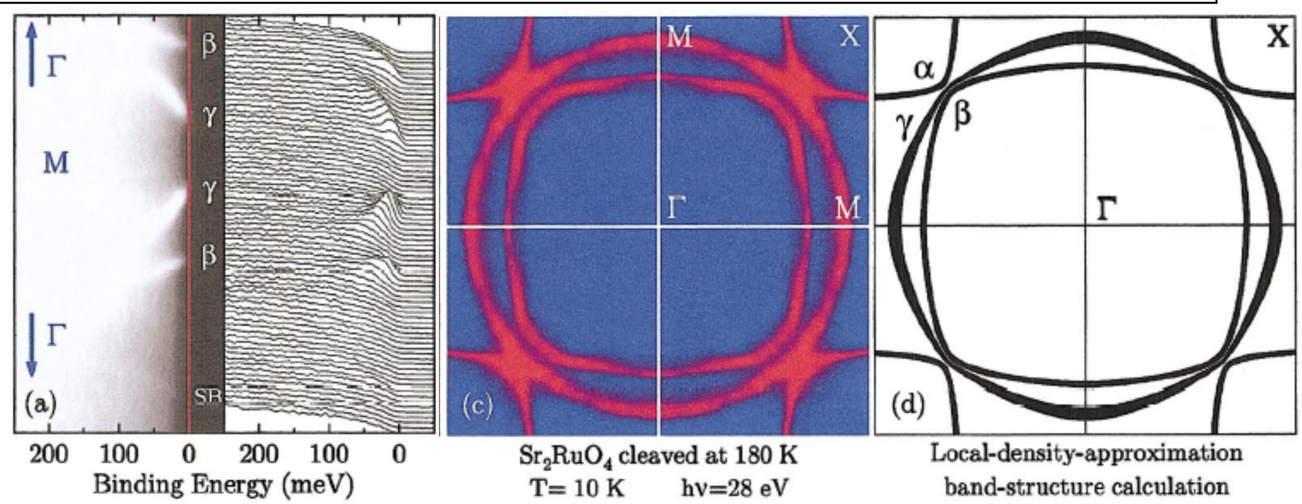
$$K_x = \frac{1}{\hbar}\sqrt{2mE_{kin}}\sin\vartheta\cos\varphi$$

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

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

Example 2D compound

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



Sr_2RuO_4 Fermi Surface
Damascelli and Shen
PRL 2000

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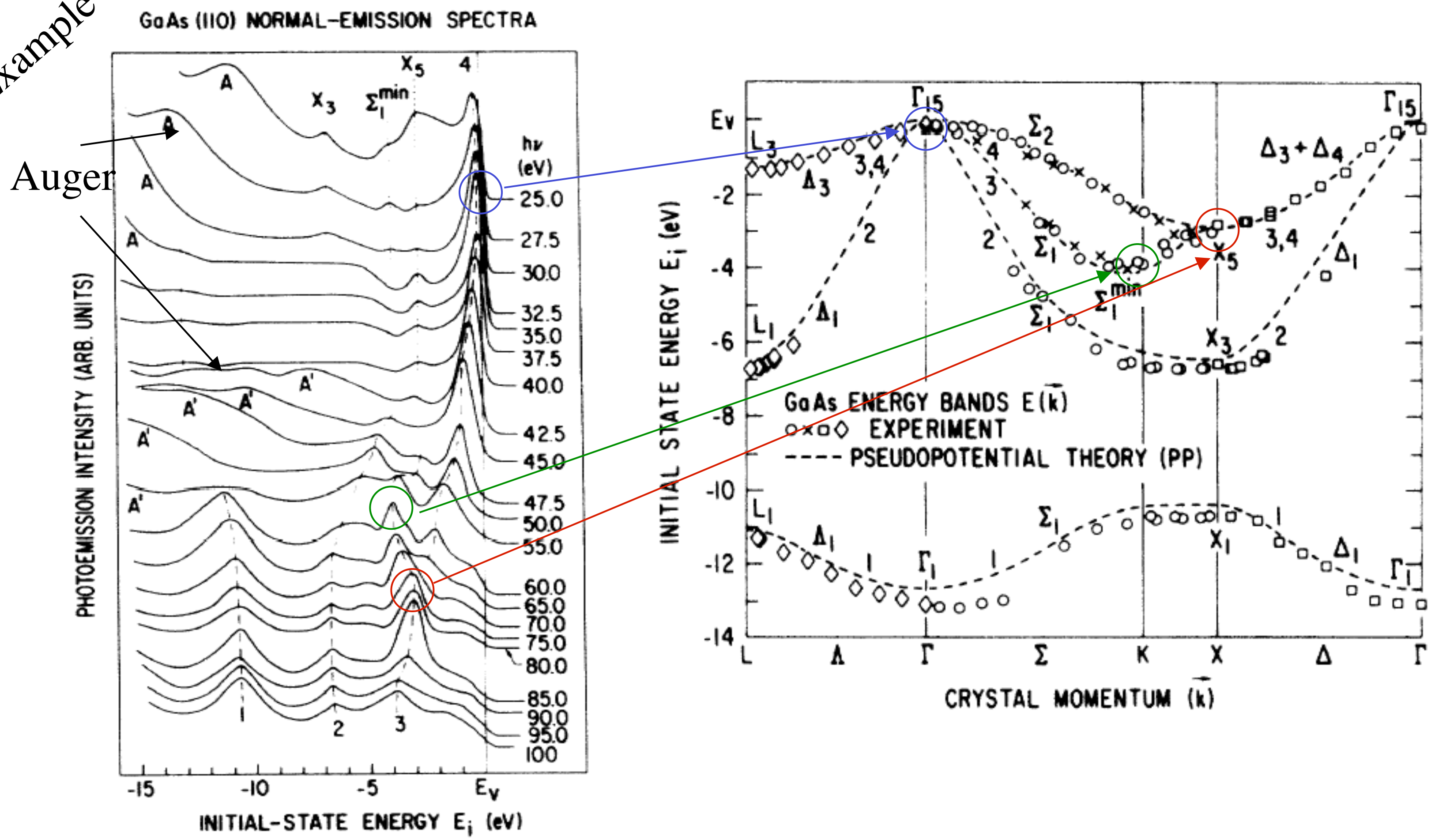
Example 3D compound



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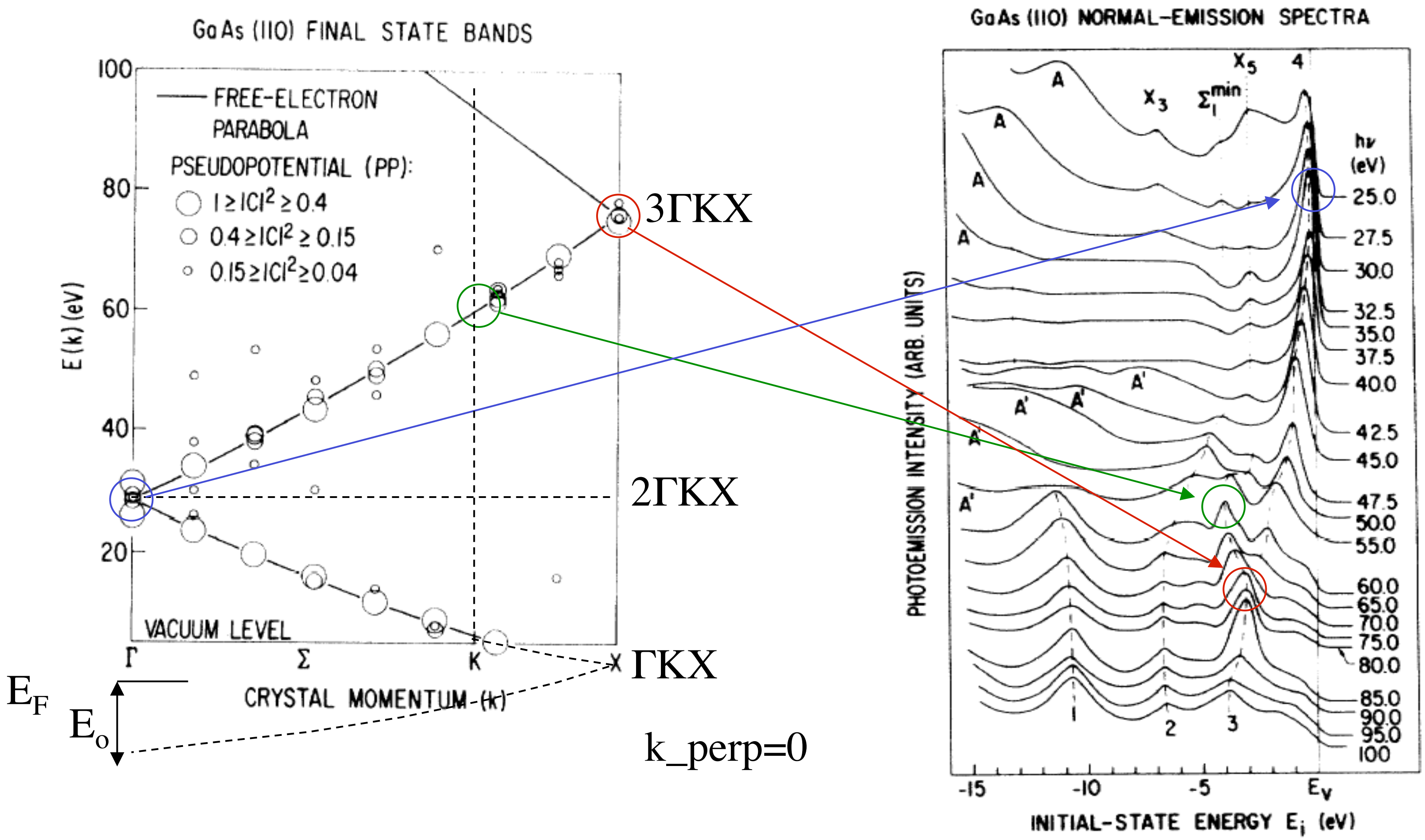
Example 3D compound

Normal emission: theta=0

$$\hbar k_{\parallel} = 0 \qquad \hbar k_{\perp} = [2m(E_i + e\Phi - E_0)]^{1/2}$$



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,

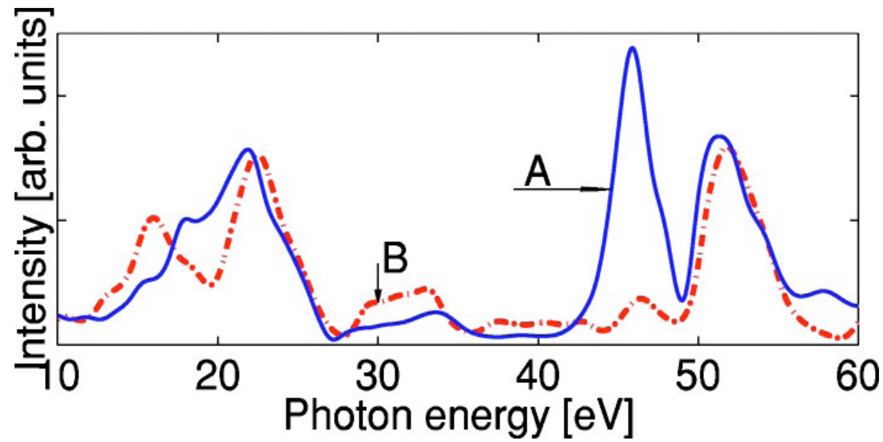
$$H_{\text{int}} = \frac{e}{mc} \mathbf{A} \cdot \mathbf{p}$$

PHYSICAL REVIEW B **69**, 094515 (2004)

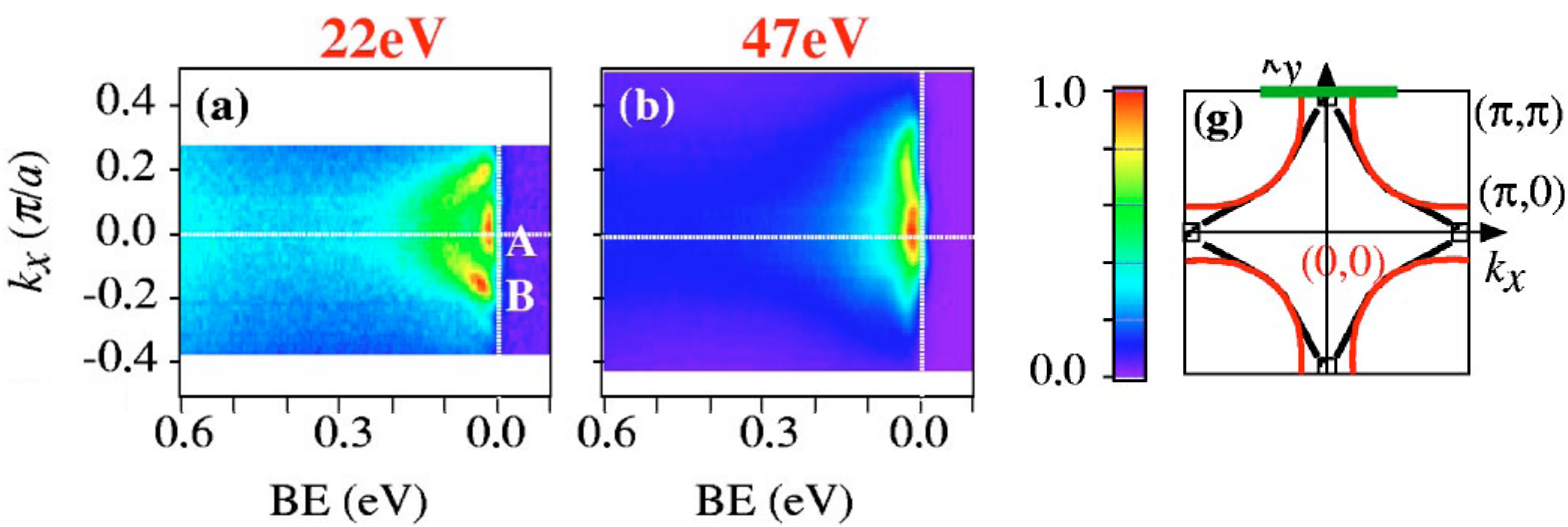
Bilayer splitting and coherence effects in optimal and underdoped $Bi_2Sr_2CaCu_2O_{8+\delta}$

Y.-D. Chuang,[1,2] A. D. Gromko,[1] A. V. Fedorov,[1,2] Y. Aiura,[3] K. Oka,[3] Yoichi Ando,[4] M. Lindroos,[5,6]
R. S. Markiewicz,[5] A. Bansil,[5] and D. S. Dessau[1]

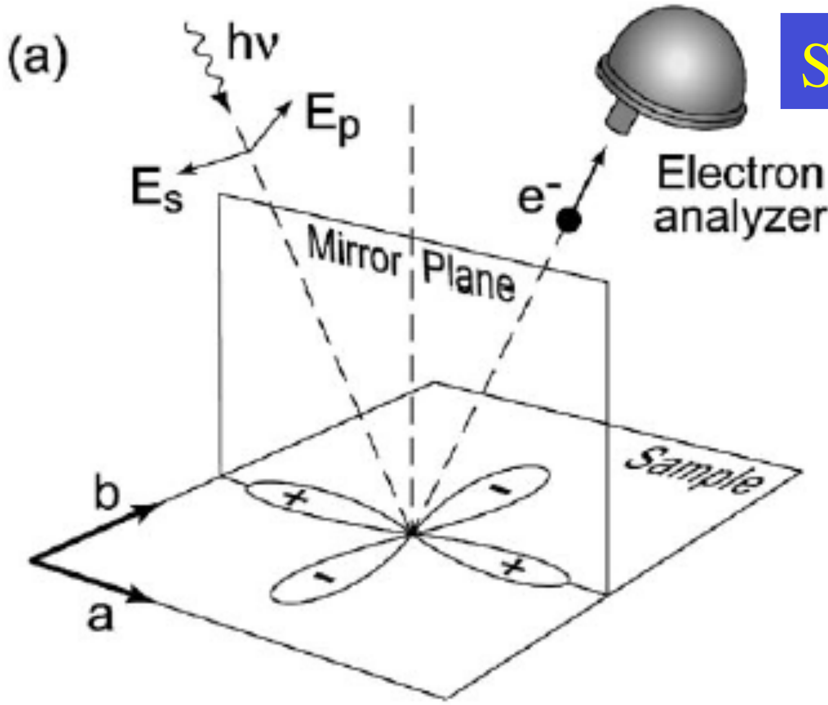
One-step-model matrix element calculations.
Antibonding (A) vs. Bonding (B) bands.



Experiment.



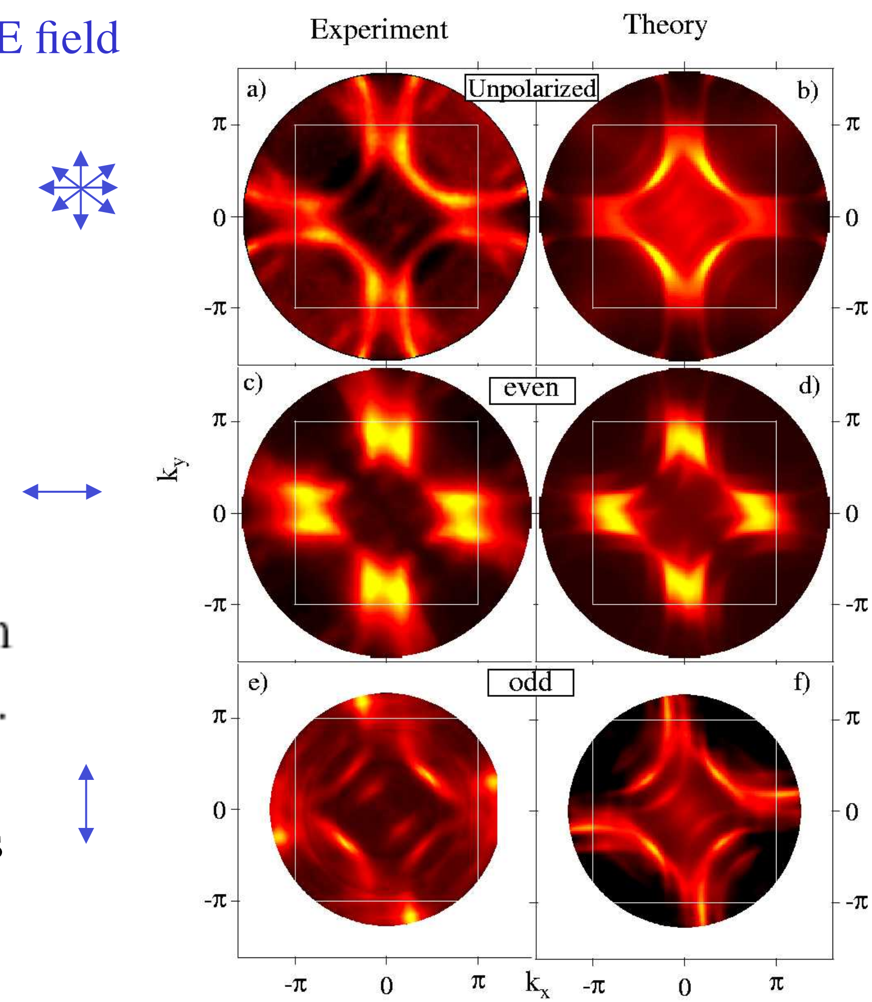
Symmetry Analysis



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

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.

E field

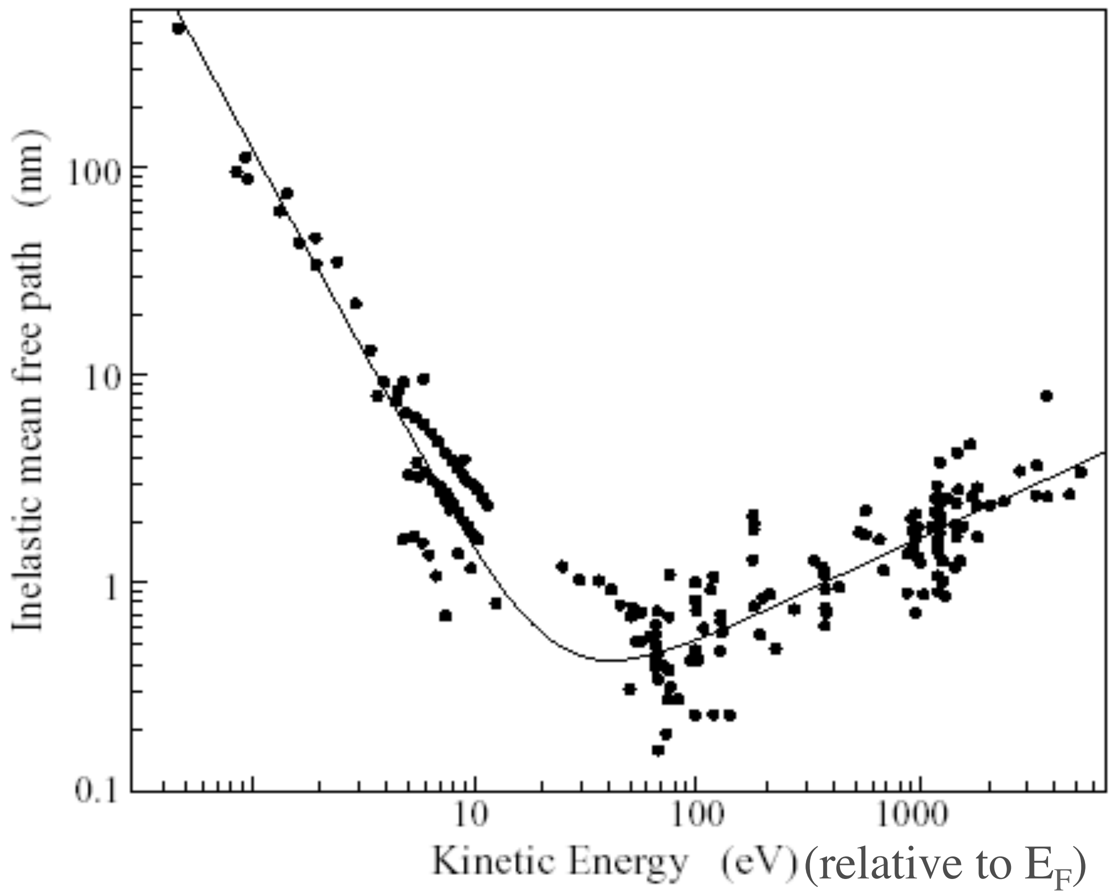


Bansil group.

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!

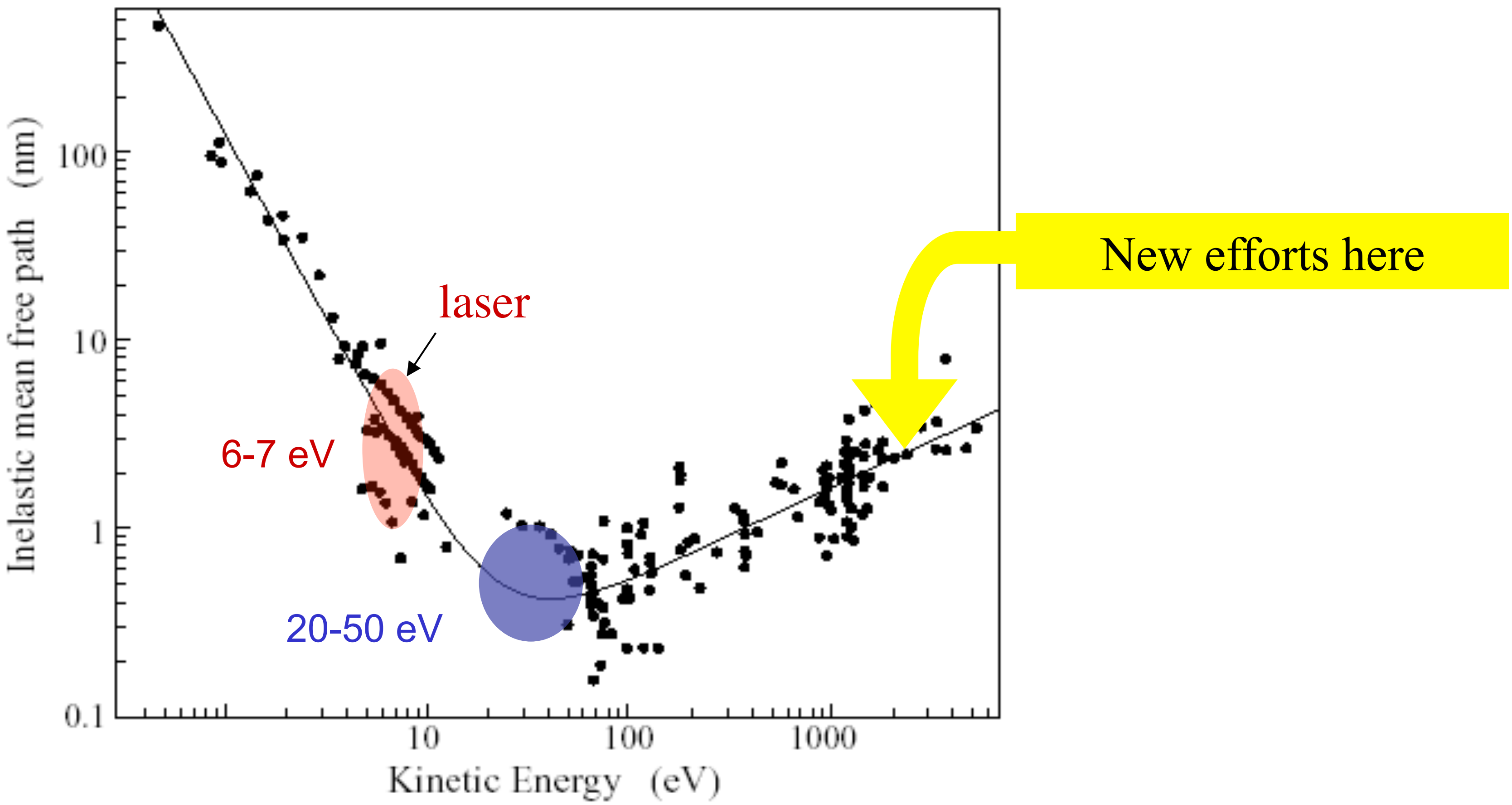


M. P. Seah and W. A. Dench, *Surf. Interface Anal.* **1**, 2 (1979).

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

→ Decreasing interaction times.

Surface sensitivity – electron kinetic energy

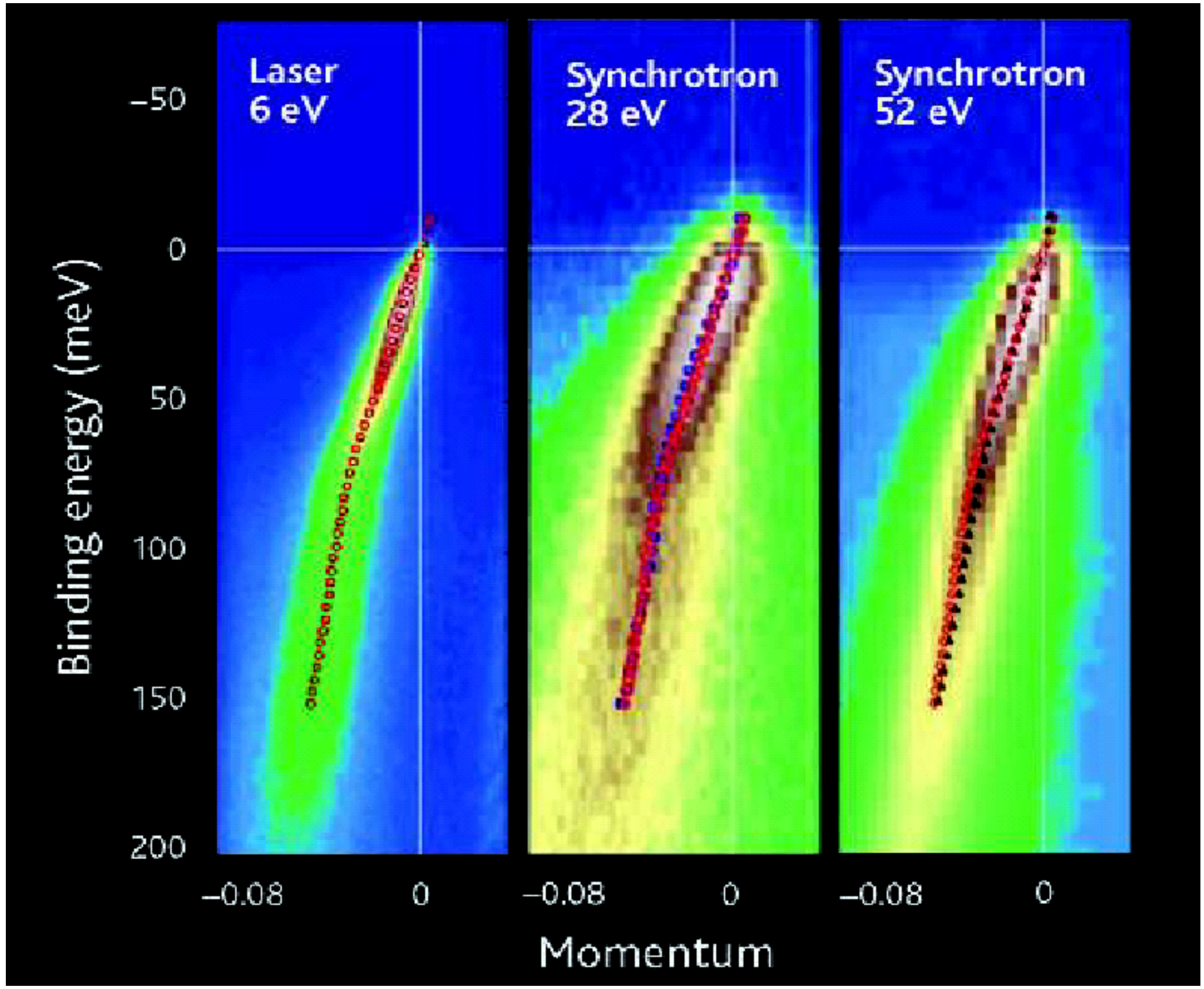


→Laser-ARPES is 3-10 times more bulk sensitive than standard ARPES
Very helpful for studies of "bulk" physics.

M. P. Seah and W. A. Dench, *Surf. Interface Anal*. **1**, 2 (1979).

ARPES dispersion along the nodal line of $Bi_2Sr_2CaCu_2O_8$

T ~ 20K

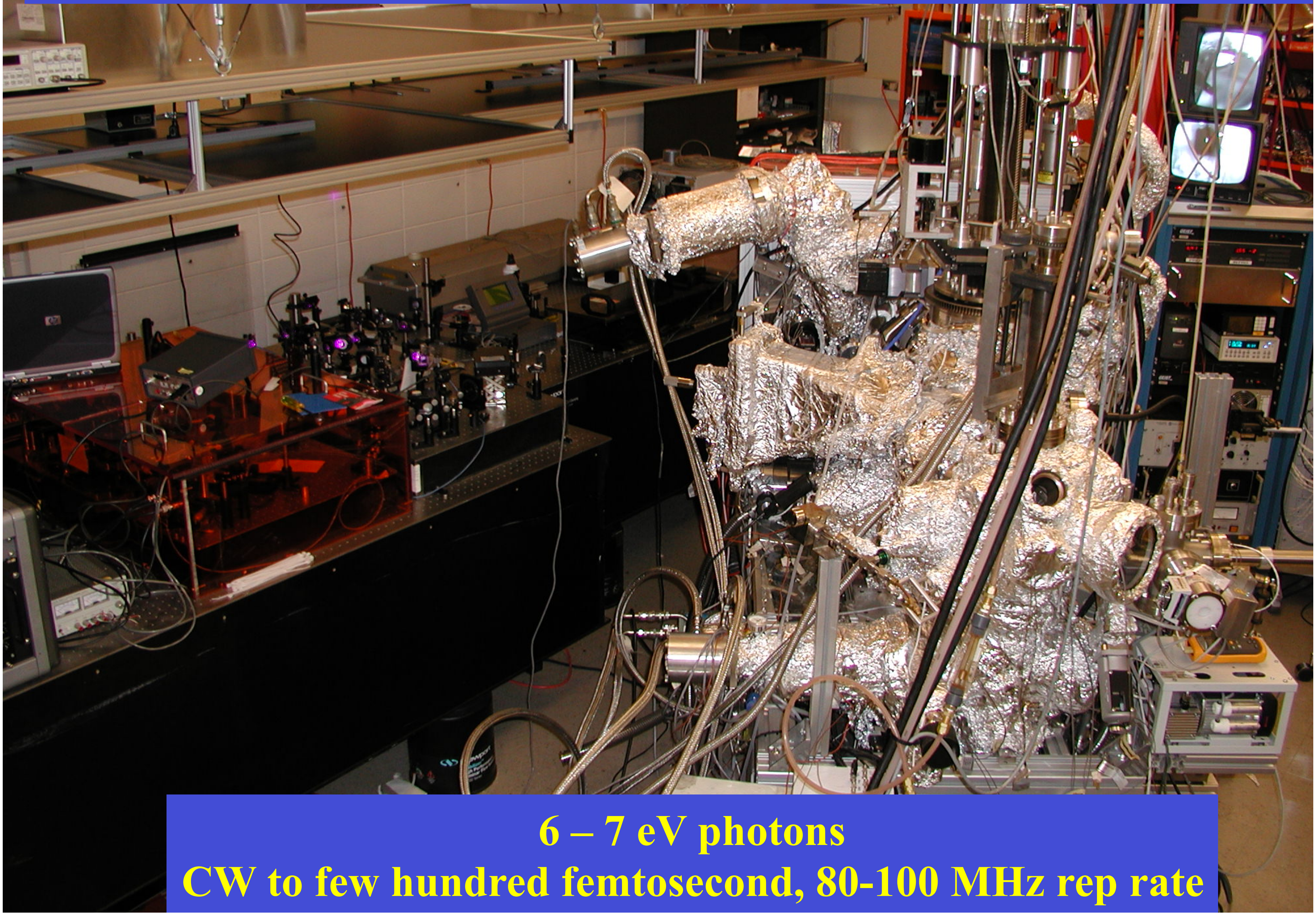


www.sciencemag.org SCIENCE VOL 310 25 NOVEMBER 2005 1271

Published by AAAS

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

Laser-ARPES lab, University of Colorado, room G235



6 – 7 eV photons

CW to few hundred femtosecond, 80-100 MHz rep rate

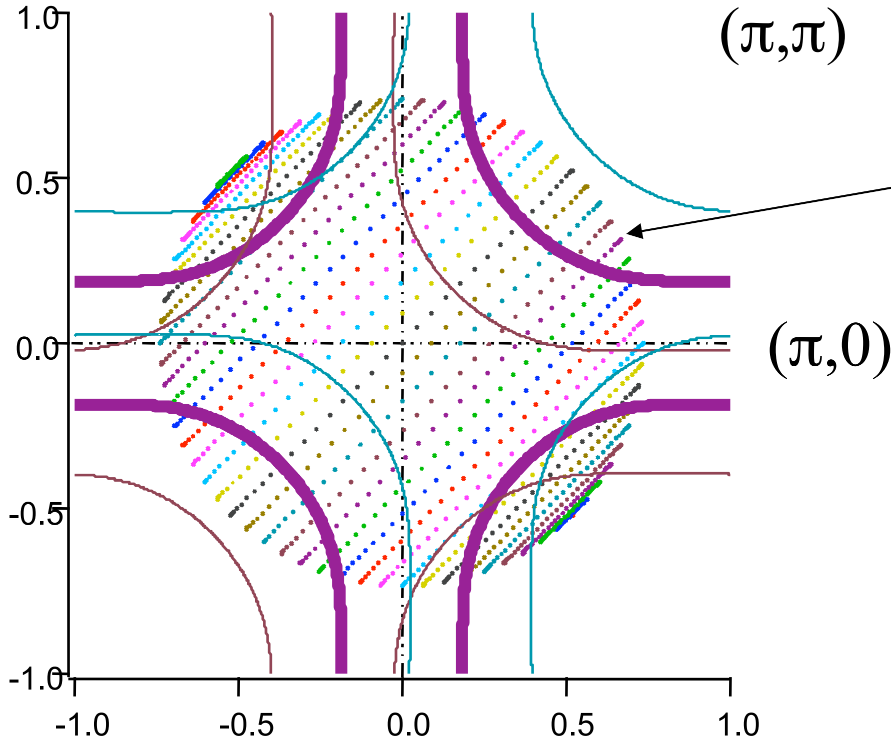
Low photon energy or laser-ARPES

- Improved **k** and E resolution
- Improved bulk sensitivity
- Reduced background
- Decreased space-charge effect
- Increased final state lifetimes (less k_perp broadening)

Disadvantages of low-energy ARPES

- Potential issues with breakdown of the sudden-approximation (but data indicates that this is OK here)
- Technically more challenging (Electron analyzers don’t like low kinetic energy)
- Often a lack of matrix element/photon energy control
- Not many synchrotron beamlines.

Resolution and k-space effect



Range of k-space accessible in Bi2212 at hv= 6 eV

$$\hbar k_{//} = \sqrt{2mE_k}\,\sin\theta$$

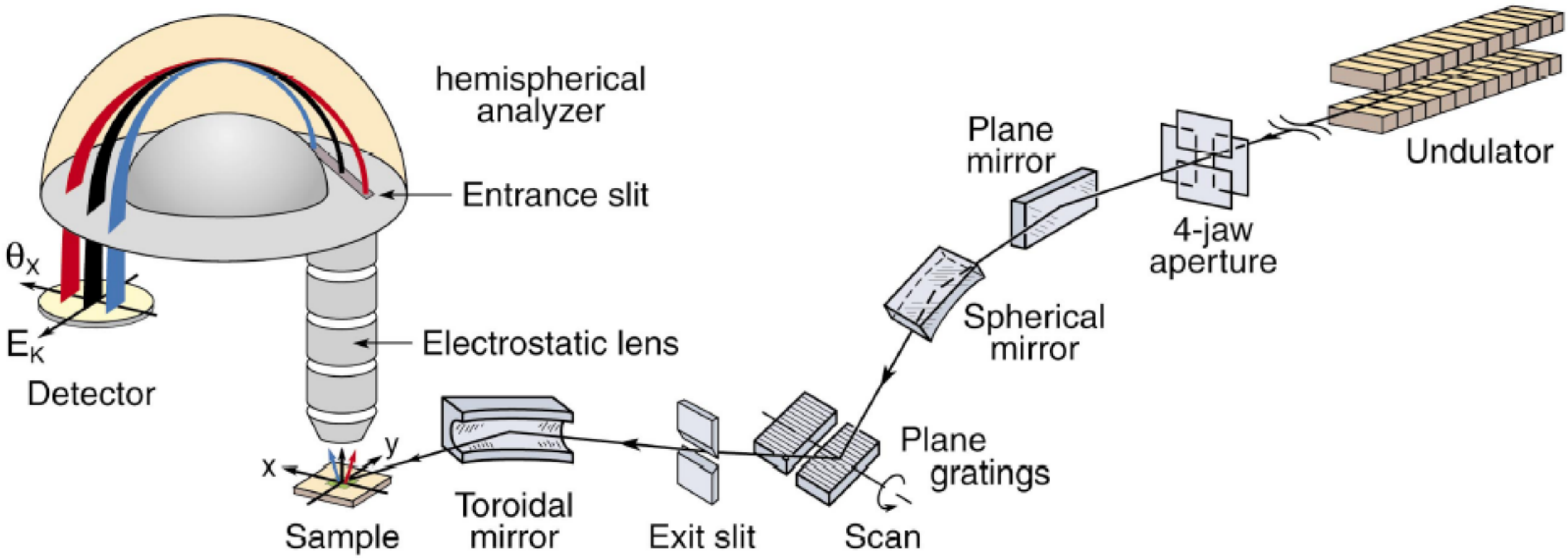
- For the same angular resolution, the k resolution at low E is superior.
- k resolution translates to E widths if the peak is dispersive.

For nodal states & $\pm$ .15 degree angular resolution,

5 meV broadening for hv=6eV, 38 meV for hv=52 eV.

- However – relatively small range of k-space accessible.

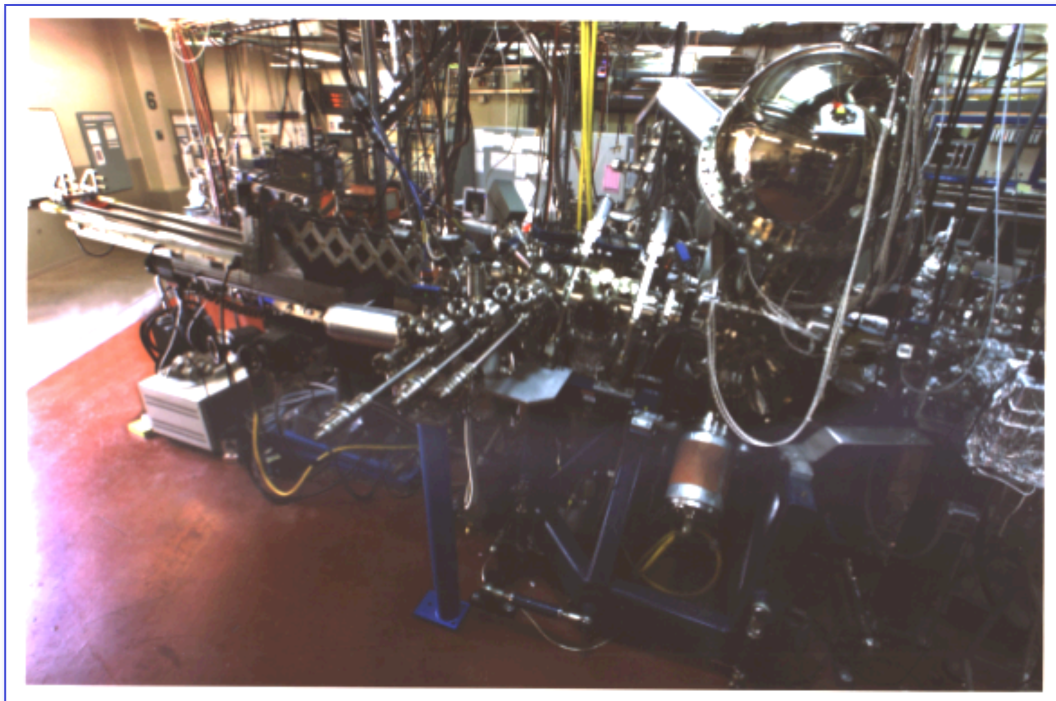
Typical synchrotron beamline for ARPES

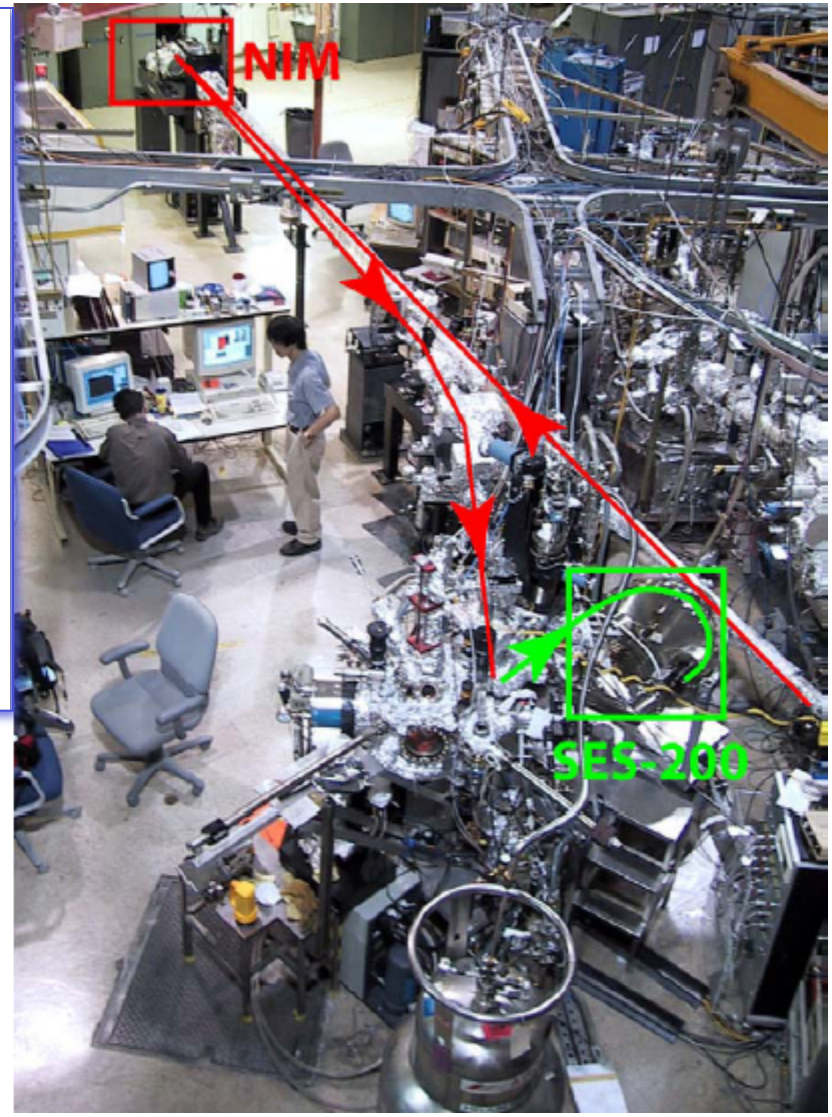


Berkeley Lab

Stanford Synchrotron Radiation Laboratory

SSRL



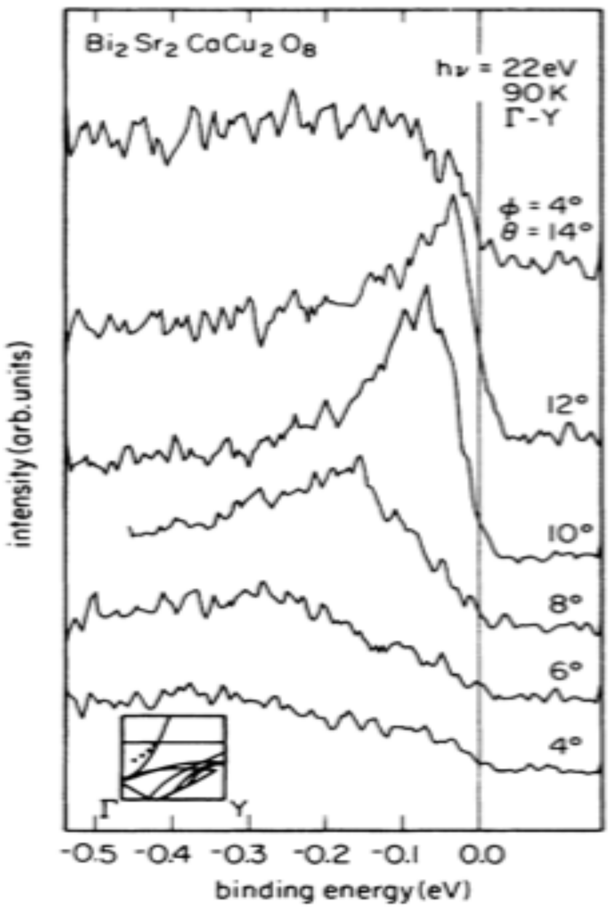


- UHV analysis chamber (10^{-11} Torr)
- 5 or 6 axis, He cooled sample manipulators
- Load-Lock transfer system
- Samples may be cleaved in UHV

Band dispersions, Fermi surfaces, etc.

ARPES compared to LDA band structure.

Normal state near-optimal Bi2212 along the nodal line.

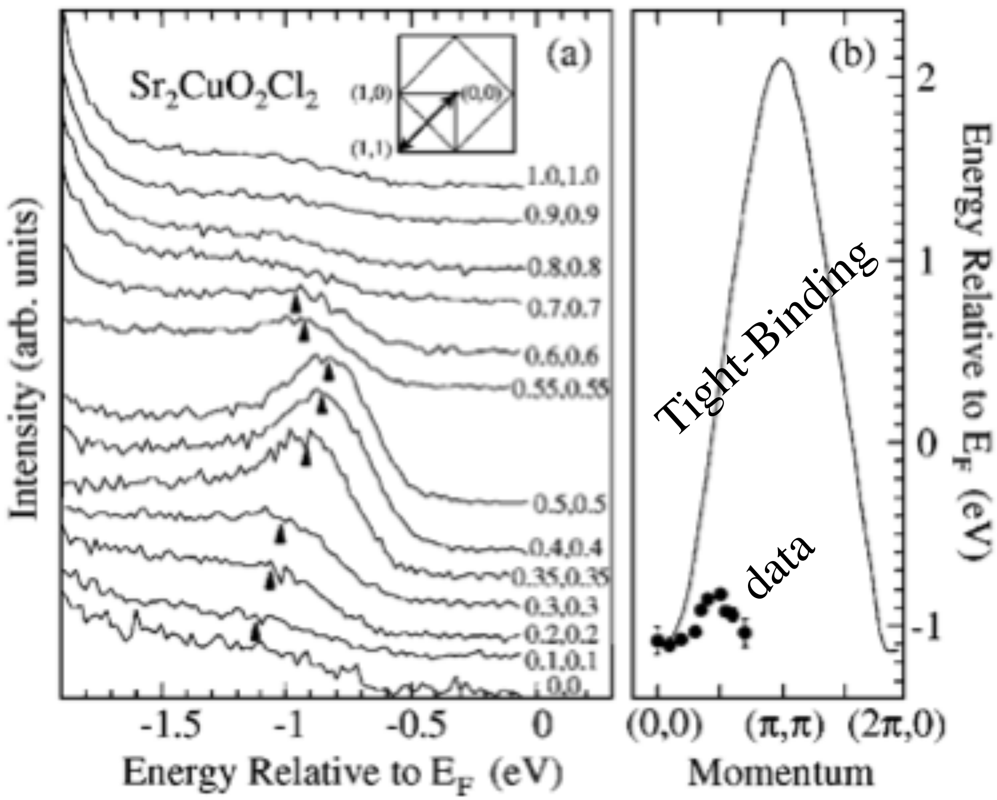


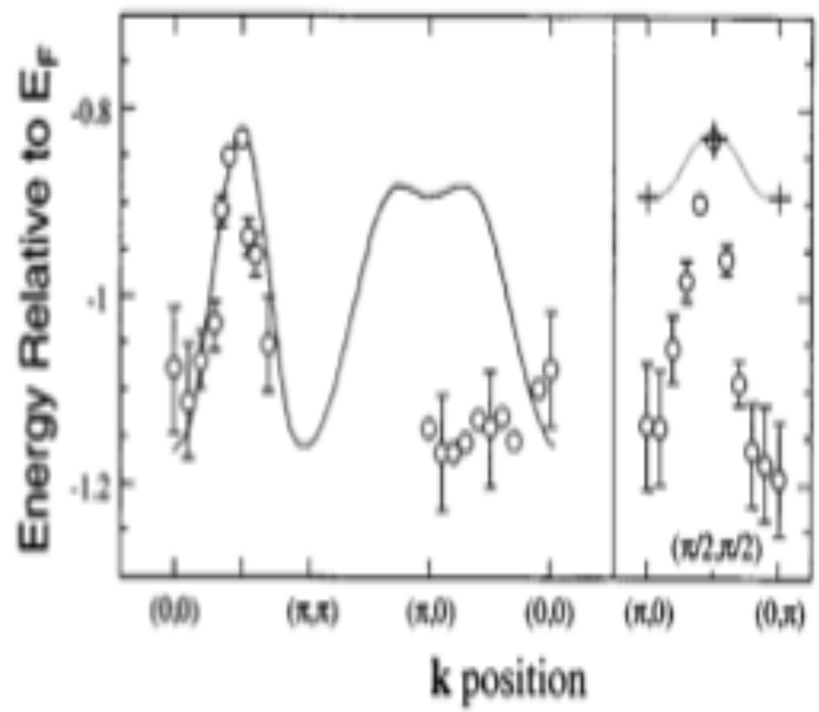
C.G. Olson et al., PRB 1990

~ a factor of two mass enhancement compared to LDA.

E versus k Relations and Many Body Effects in the Model Insulating Copper Oxide $Sr_2CuO_2Cl_2$

Wells et al. 1994, 1995

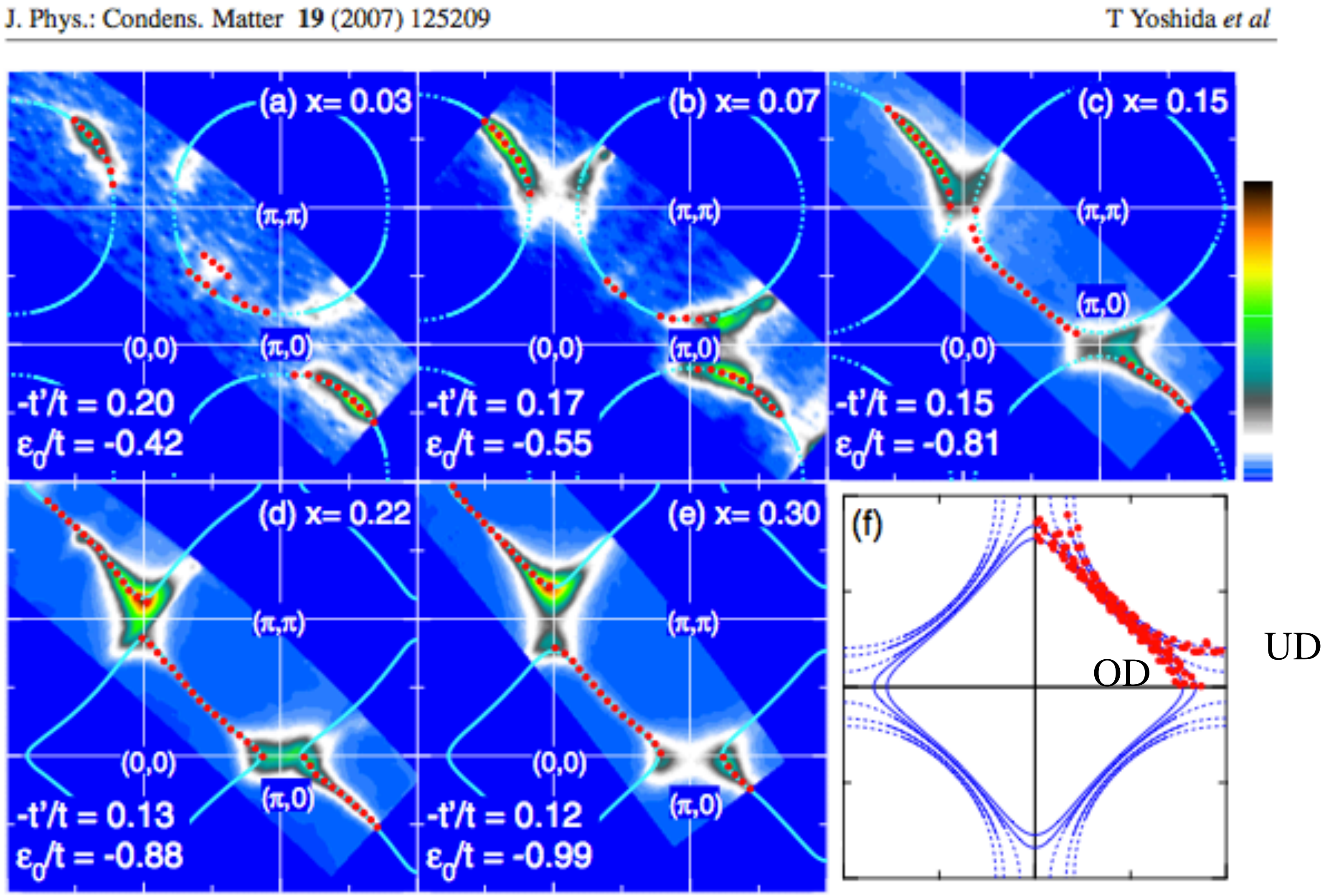




t-J model calculation (solid line) predicts a bandwidth W~2.2J.

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

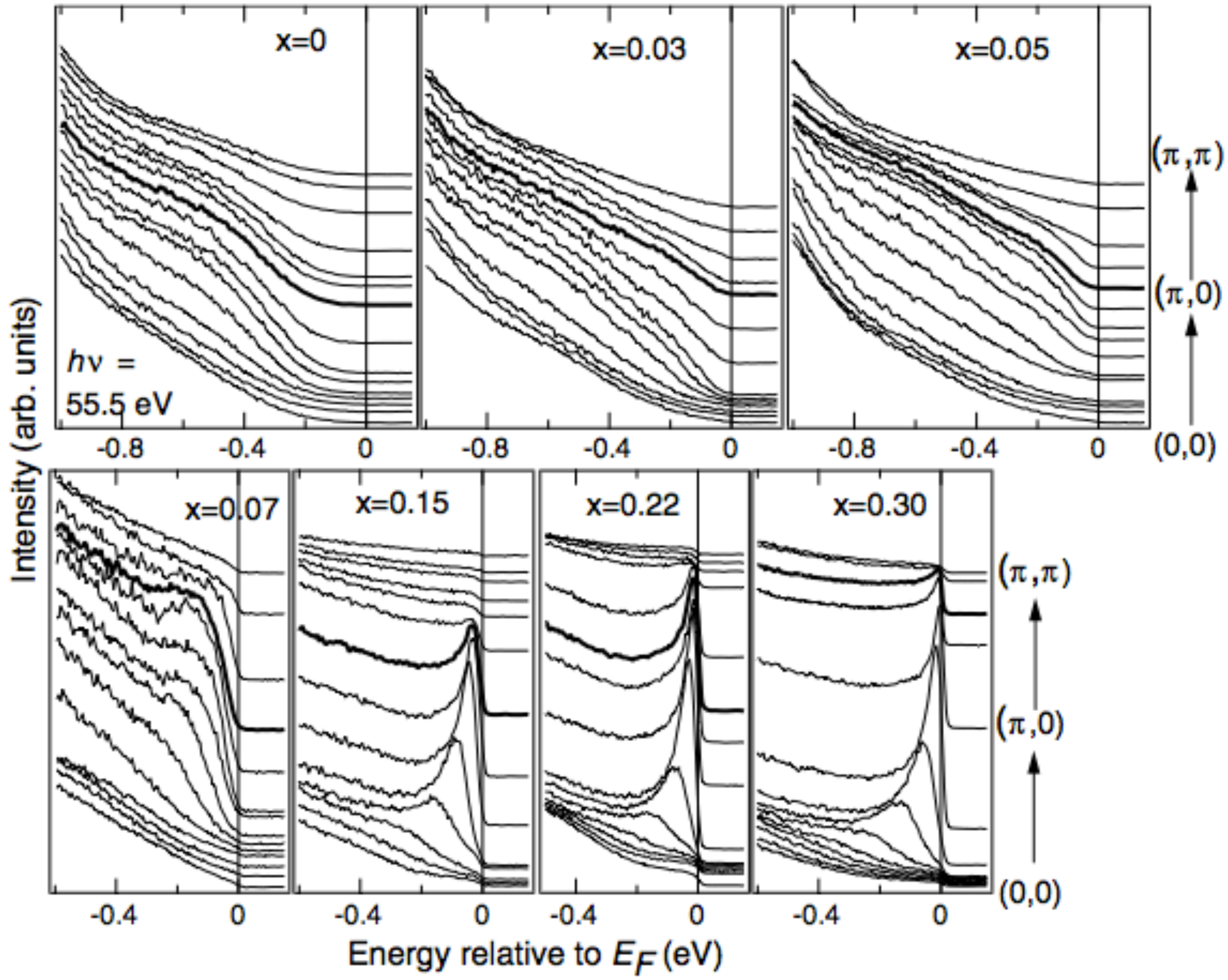
Fermi surface mapping vs hole doping level in $La_{2-x}Sr_xCuO_4$



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

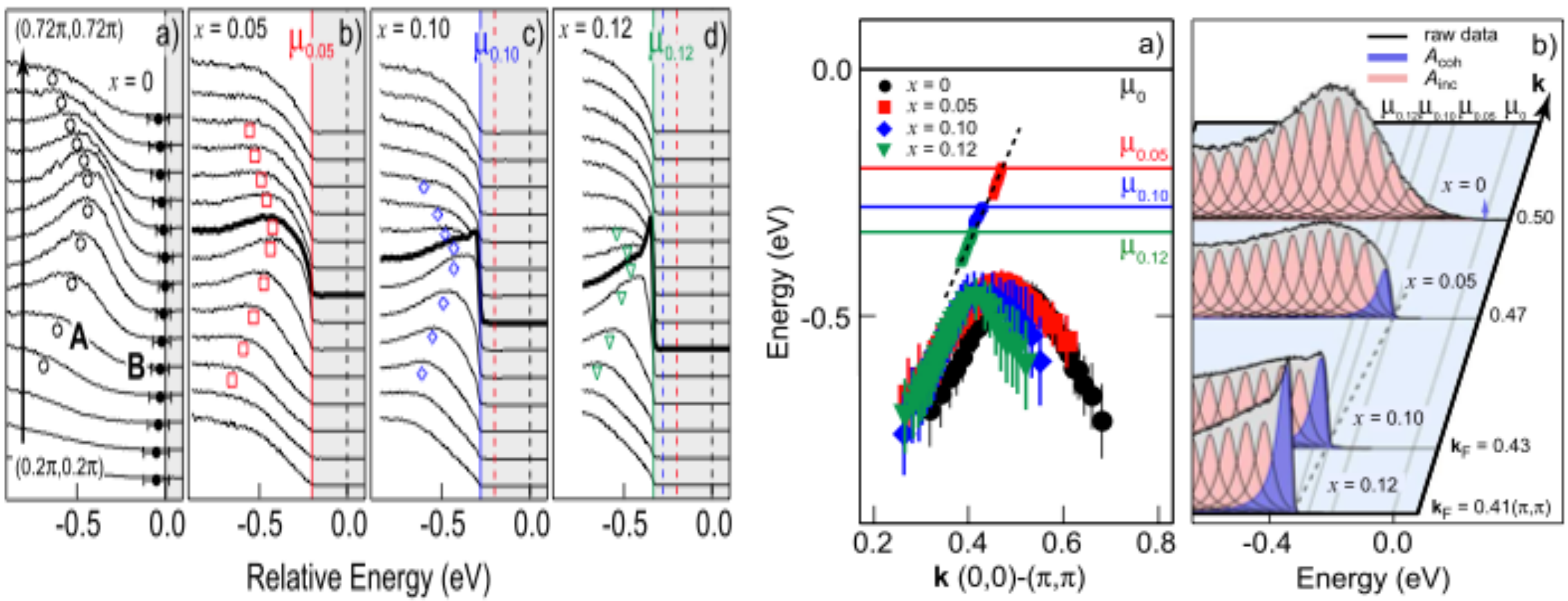
Nodal cut band dispersion vs hole doping level in $La_{2-x}Sr_xCuO_4$

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 $Ca_2CuO_2Cl_2$



K. Shen, Z-X Shen, PRL 2004

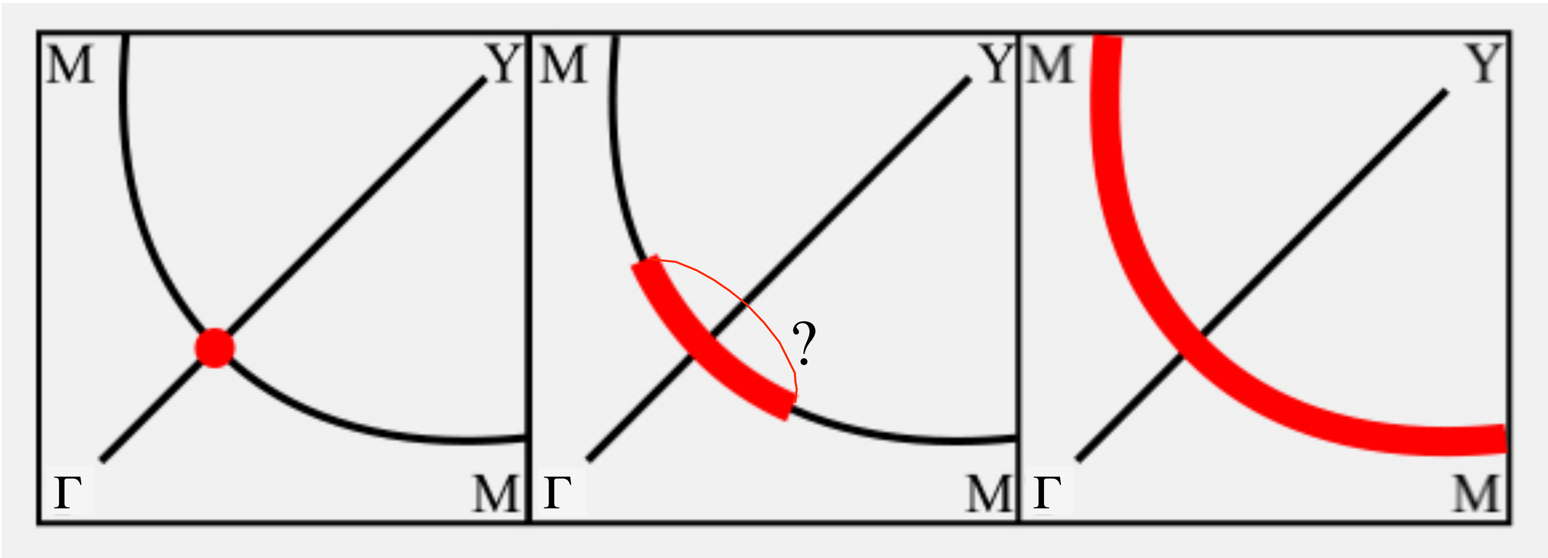
Claim: The majority of the dispersive peak is an incoherent superposition of many Franck-Condon-broadened loss peaks. The zero-loss peak with weight Z is the quasiparticle, with Z vanishingly small for low doping.

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 arc”, 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.

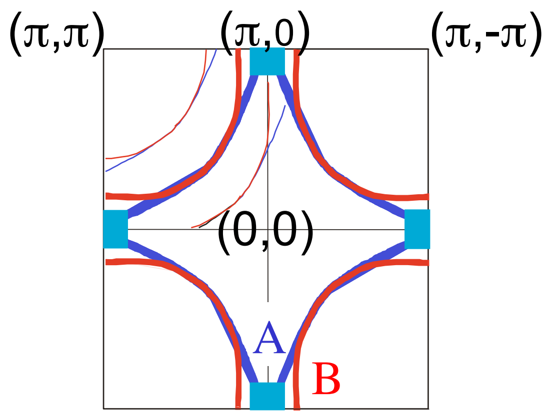


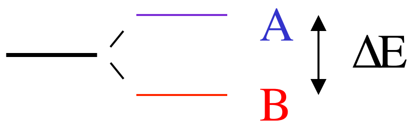
Truly truncated? Closed by a weak “shadow” piece on the back side? Made of quasiparticles?

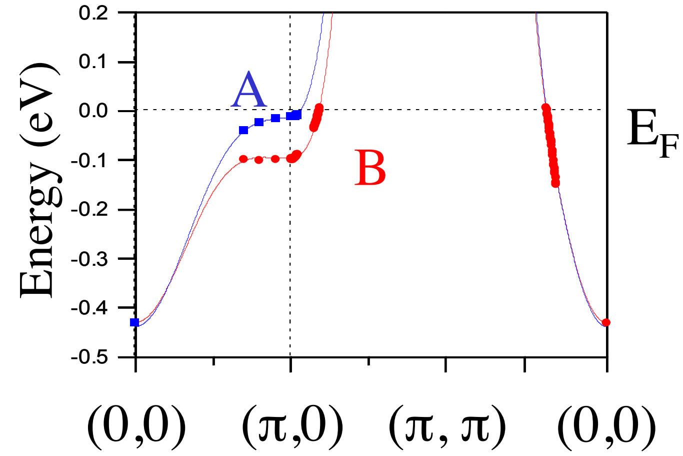
Will cover later in more detail.

Bilayer Splitting in double-layer cuprates

BILAYER SPLITTING = 2 PIECES OF FS   Bonding plus Antibonding band
Due to electronic coupling between the pair of CuO_2 planes per unit cell
Superstructure bands exist as well.

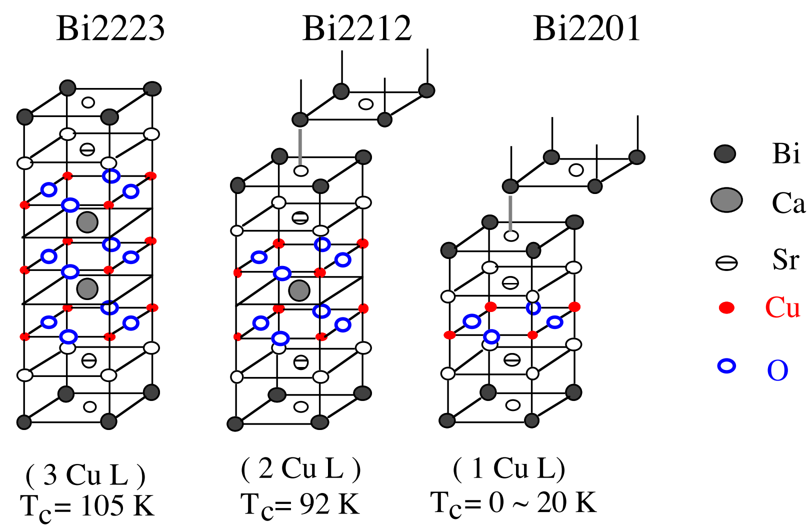






ΔE ~ 100 meV.

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



Angle Resolved Photoemission Spectroscopy (part 2)

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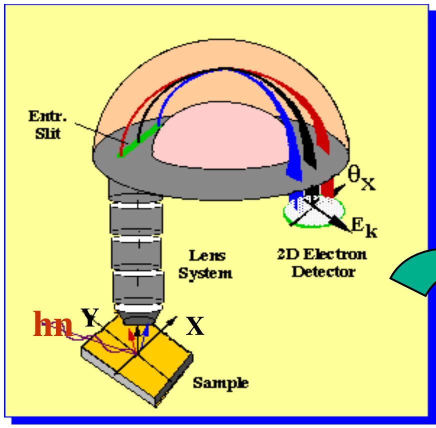
Plan

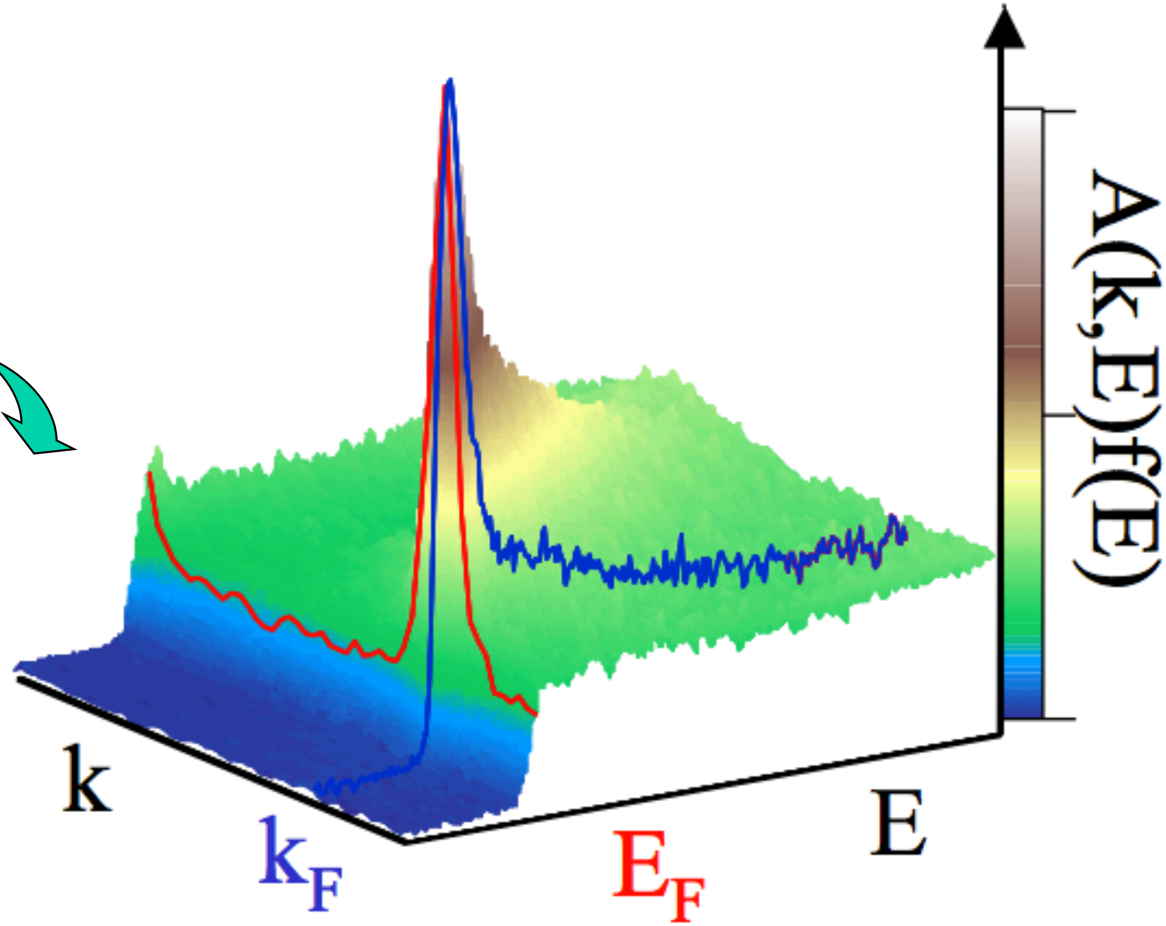
- Overview of 2D electronic detection, MDCs, EDCs, and self-energies.
- Studies of gaps (superconducting gaps and pseudogaps)
- Studies of mode coupling (dispersion kinks).

2D detection (in energy and momentum)

EDCs and MDCs

Two dimensional electron detection





Energy Distribution Curve (EDC)

Momentum Distribution Curve (MDC)

A.D. Gromko, University of Colorado Thesis

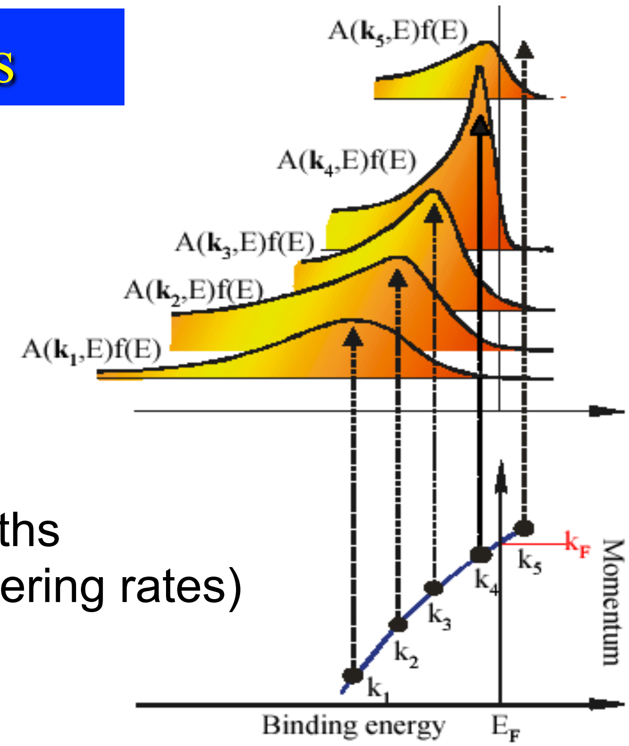
ARPES peak widths and lineshapes

Spectral Function A(k,ω) = -Im G(k,ω)

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

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?

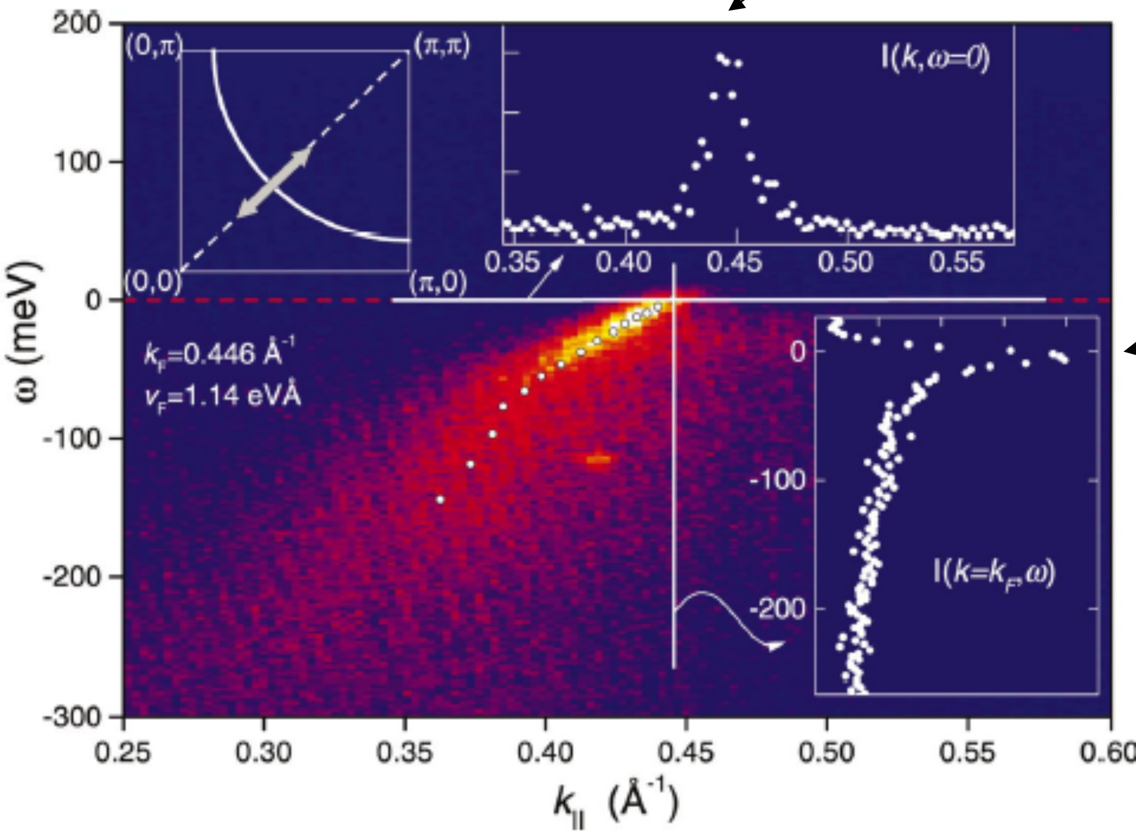
2D detection: high T_c superconductor $Bi_2Sr_2CaCu_2O_8$

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

24 SEPTEMBER 1999 VOL 285 SCIENCE

Momentum Distribution Curve (MDC)

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



Energy Distribution Curve (EDC)

Peak width $\Delta E = \hbar/\tau$

$1/\tau \sim$ scattering rate

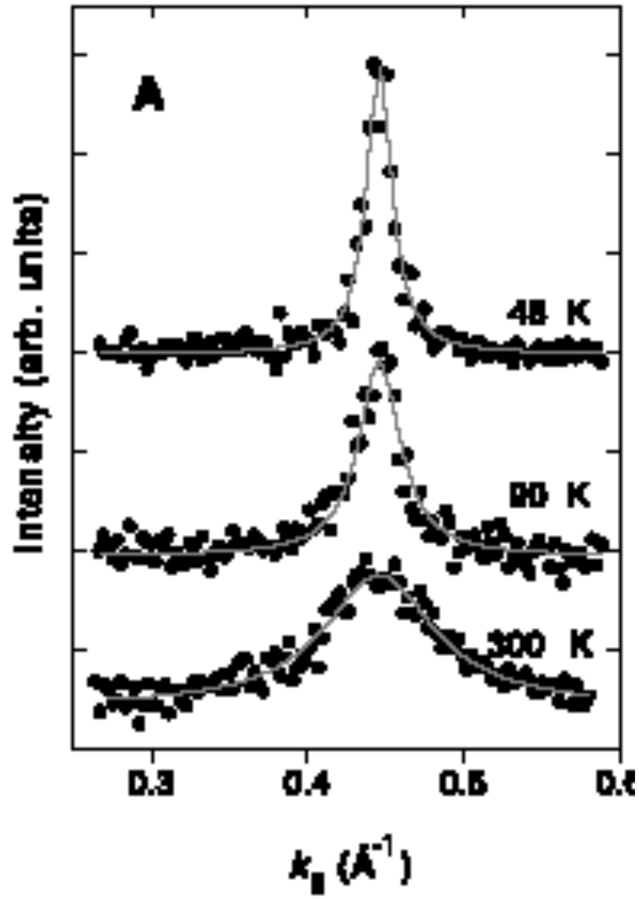
$\tau \sim$ quasiparticle lifetime

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

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

2D detection on the high Tc superconductor $Bi_2Sr_2CaCu_2O_8$

Valla et al., Science (1999)



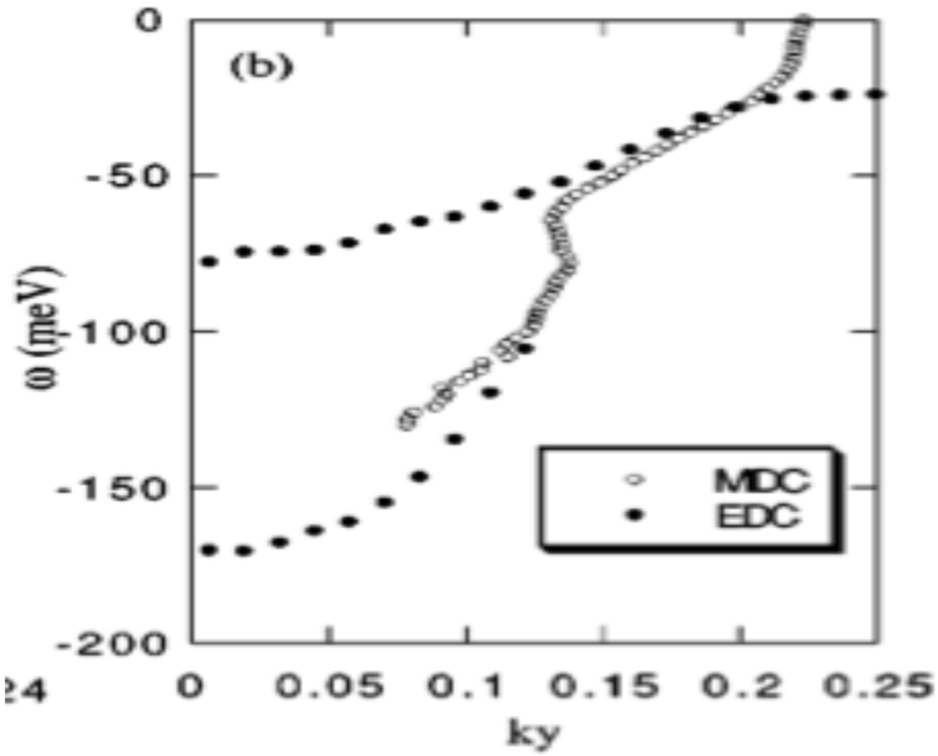
Lorentzian MDC fits as as a function of temperature.
Broader peaks at higher T → shorter photohole lifetimes.

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.

MDC vs EDC dispersion will disagree when there are broad peaks.

Superconducting state dispersion near the gap edge.
Calculated EDC and MDC dispersion.



M.R. Norman et al, PRB 2001

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

Superconcuting Gaps

Superconducting order parameter symmetry

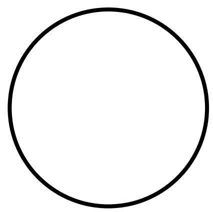
SC gap Δ = magnitude of order parameter. Varies as a function of k in a d-wave SC

$\Psi(r1,\sigma 1;r2,\sigma 2)=\psi(\text{orbital}) \bullet \chi(\text{spin})$

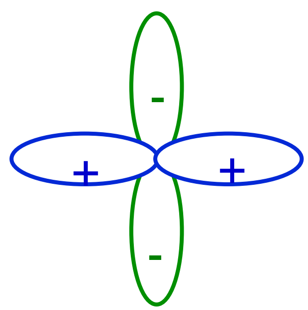
Antisymmetric under exchange

χ(spin) : known to be a singlet (S=0) ↓↑

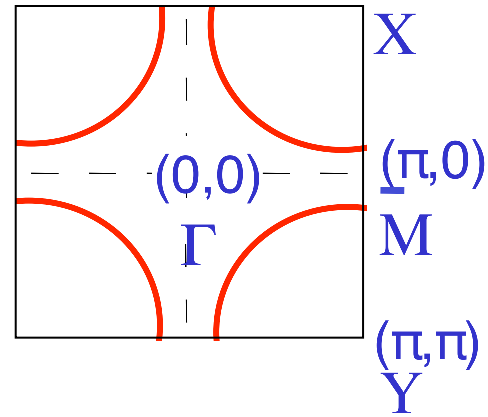
S = 0, l = 0
-- s-wave superconductor
(conventional SC)



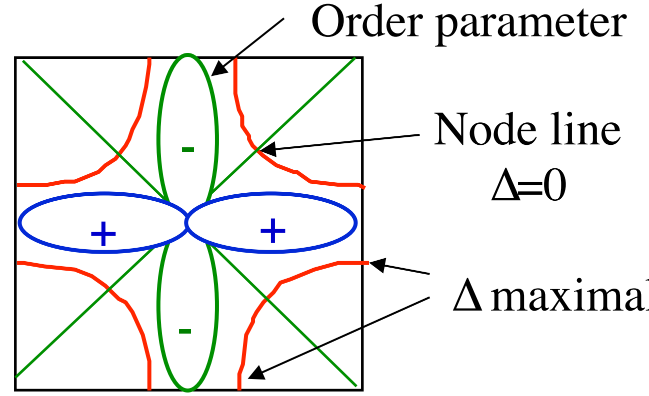
S = 0, l = 2
-- d-wave superconductor
(HTSCs - pretty sure)



Hole-like Fermi Surface

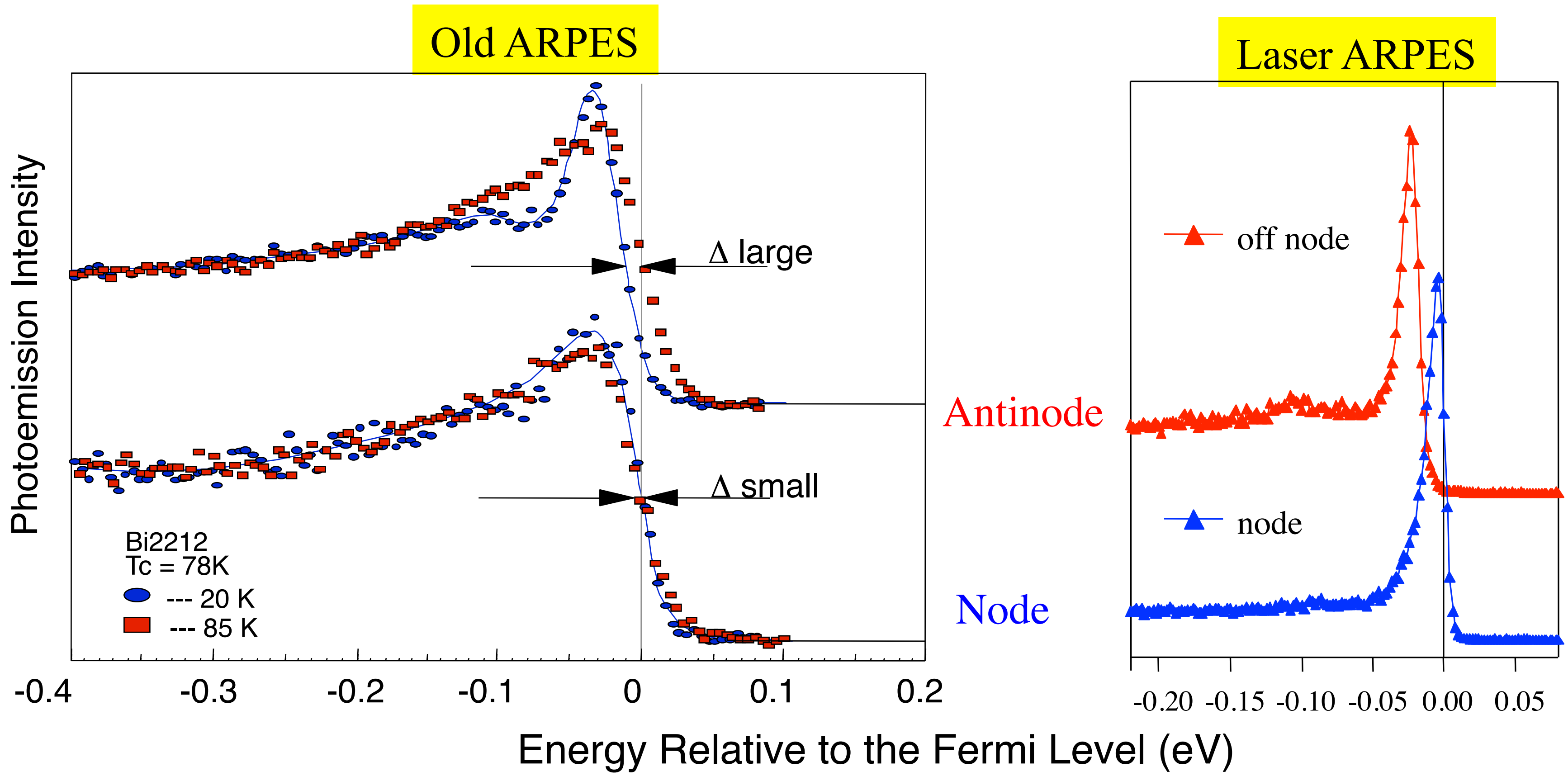


d-wave SC gap - maximal near (π,0)



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

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 Δ is small or T is large.

How to accurately determine the gaps when we don't understand the lineshape and when the peaks are broad?

a) Leading edge shift
b) Separation of peaks of symmetrized (about E_F) spectra
c) New TDoS method, using tunneling formulae.

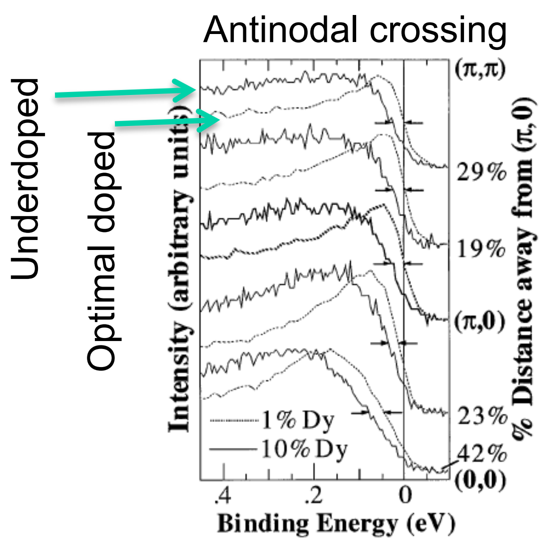
Pseudogaps and Fermi Arcs

Original ARPES pseudogap study in cuprates. Arcs and pockets.

VOLUME 76, NUMBER 25 PHYSICAL REVIEW LETTERS 17 JUNE 1996

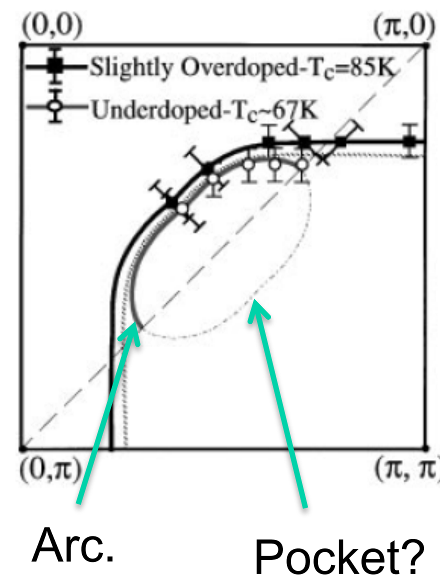
Unconventional Electronic Structure Evolution with Hole Doping in $Bi_2Sr_2CaCu_2O_{8+\delta}$: Angle-Resolved Photoemission Results

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



T=100K (above T_c)

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



- Pgap is max at (π,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?

Excitation Gap in the Normal State of Underdoped $Bi_2Sr_2CaCu_2O_{8+\delta}$

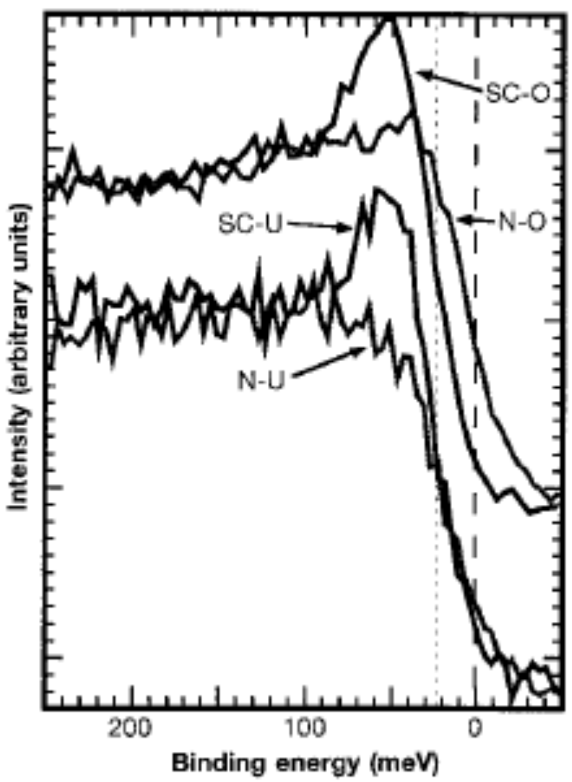
A. G. Loeser, Z.-X. Shen, D. S. Dessau,* D. S. Marshall, C. H. Park, P. Fournier,† A. Kapitulnik

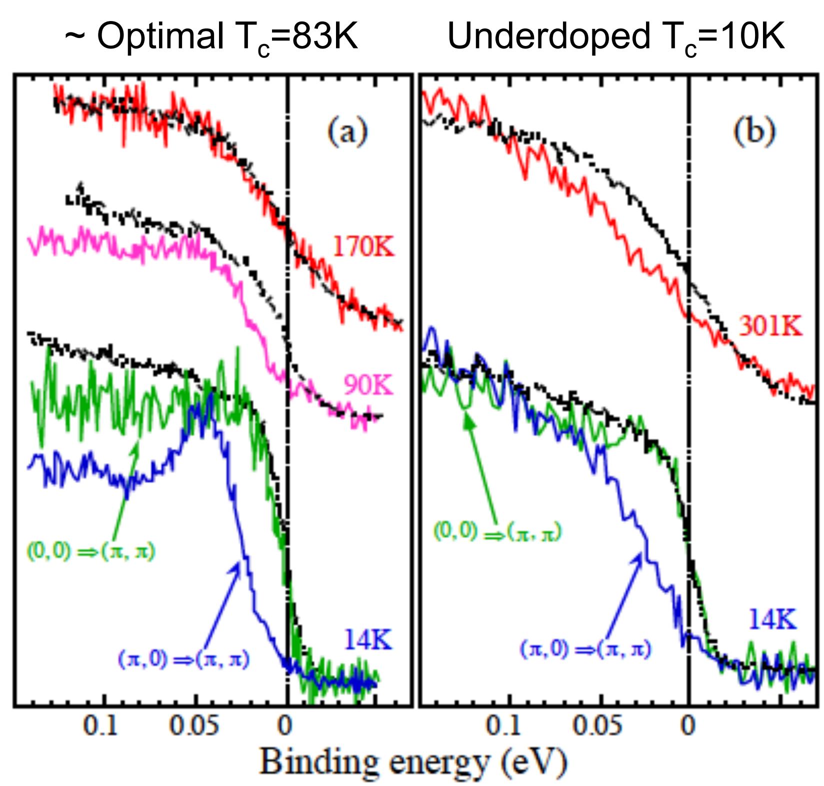
SCIENCE • VOL. 273 • 19 JULY 1996

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

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

Nature **382**, 51-54 (4 July 1996)





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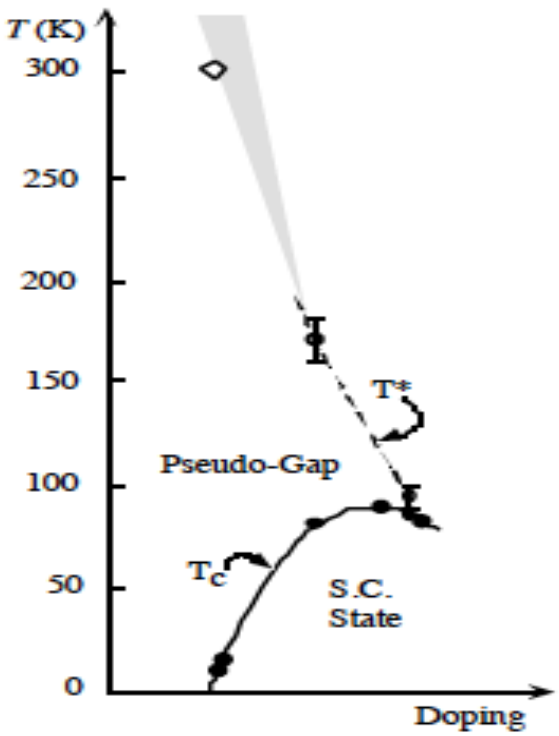
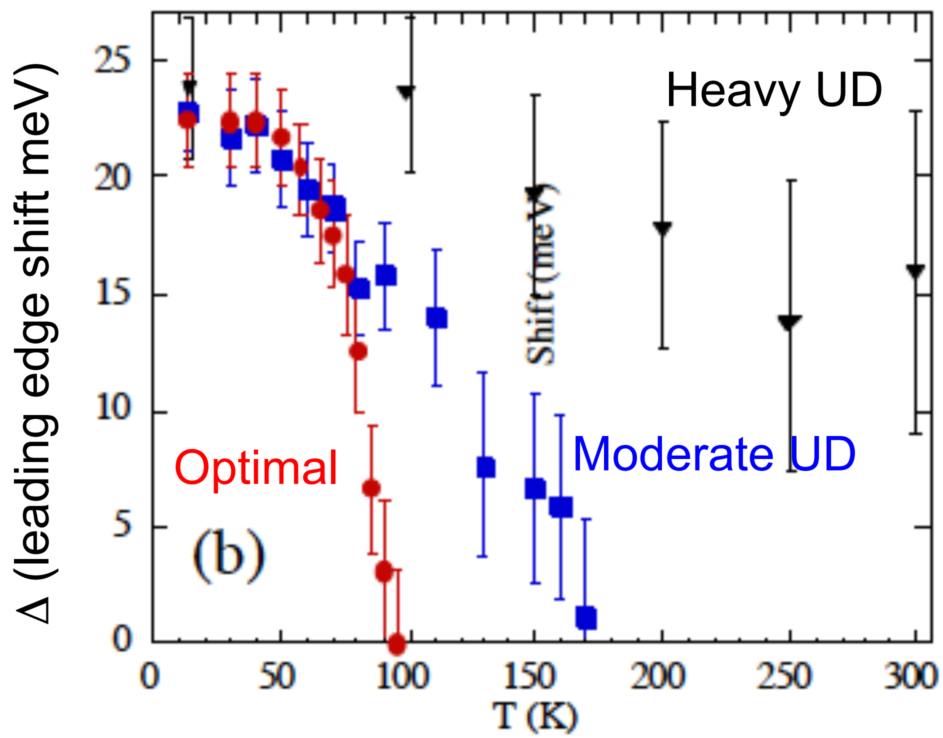




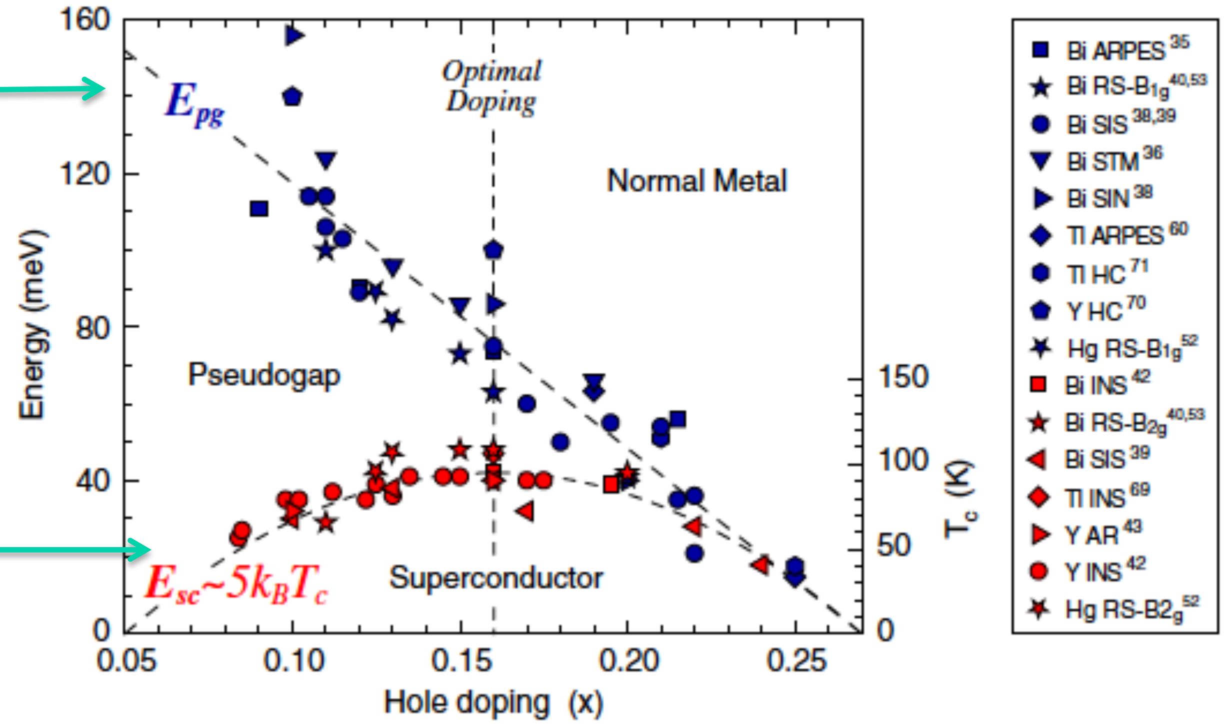
Nature **382**, 51-54 (4 July 1996)

IOP PUBLISHING REPORTS ON PROGRESS IN PHYSICS
Rep. Prog. Phys. 71 (2008) 062501 (9pp) doi:10.1088/0034-4885/71/6/062501

Two gaps make a high-temperature superconductor?

S Hüfner[1,2], M A Hossain[1,2], A Damascelli[1,2] and G A Sawatzky[1,2]

Almost exclusively antinodal measurements.



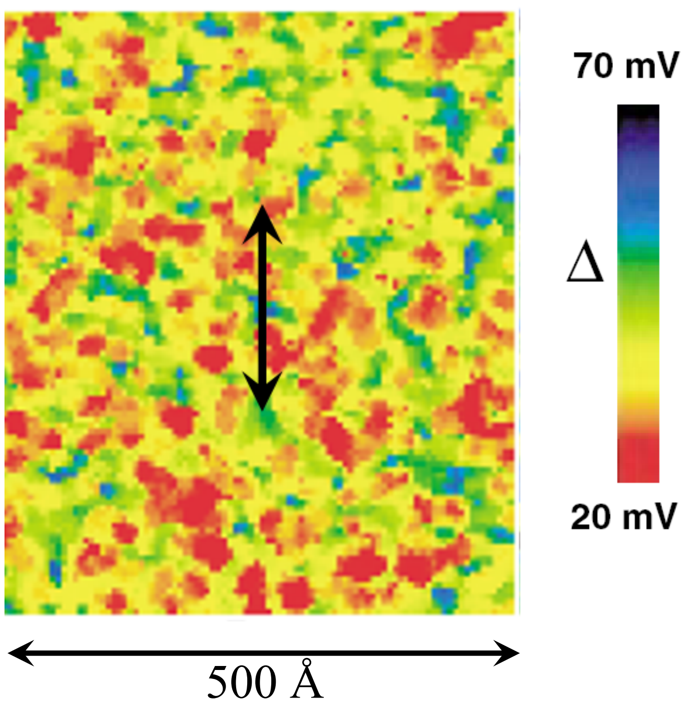
Nodal gap behavior?

- When measuring at the antinode are you measuring the max of the SC gap or something completely different (e.g. a gap from a competing order?)
- Is antinodal pseudogap a precursor to the SC gap, or is it a separate competing gap.
- Are there multiple types of pseudogaps (a competing order gap plus a prepairing gap)?

Homogeneous vs. heterogeneous broadening

Lots of heterogeneity observed in cuprates. It is likely due to dopant potentials, especially out of the planes giving strong forward scattering.

STM gap map



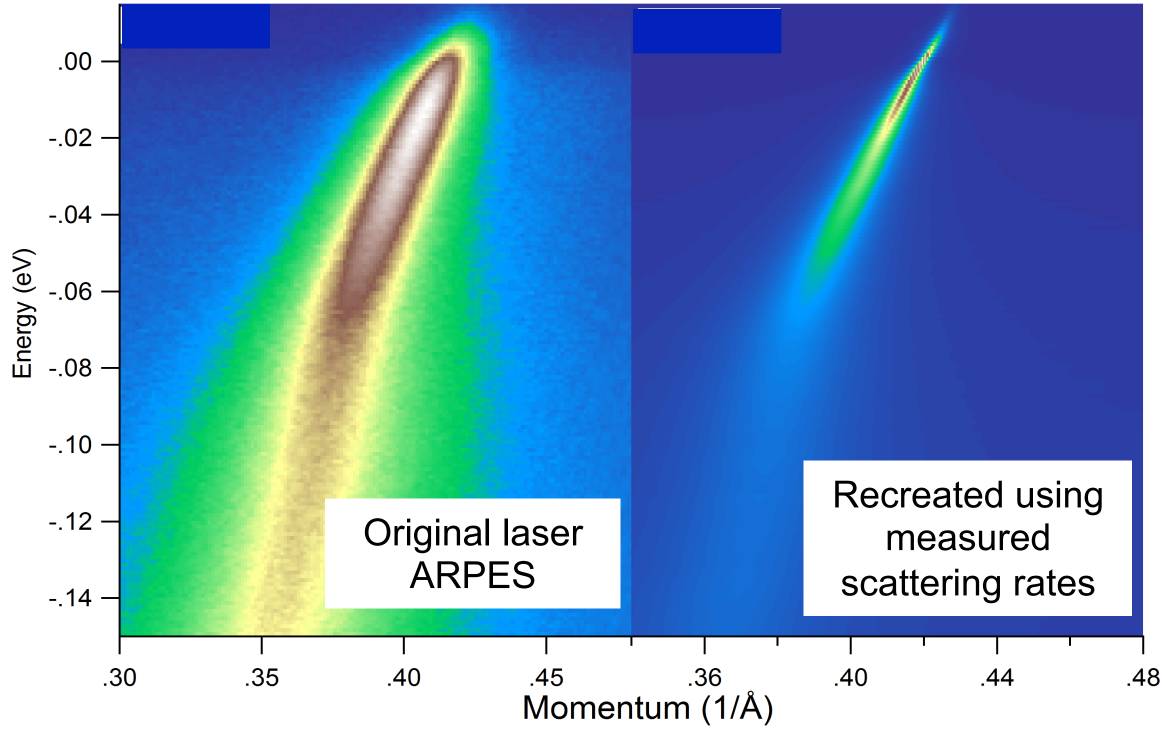
K. McElroy *et al.* PRL **94,** 197005 (2005)

Is it possible to separate out the heterogeneous (dirt) effects from the homogeneous effects?

When an ARPES peak is broad is it due to a self-energy effect (a true many-body interaction) or is it due to “dirt”, even if the dirt is an unavoidable part of creating the sample?

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

Optimal Bi2212
Nodal spectra

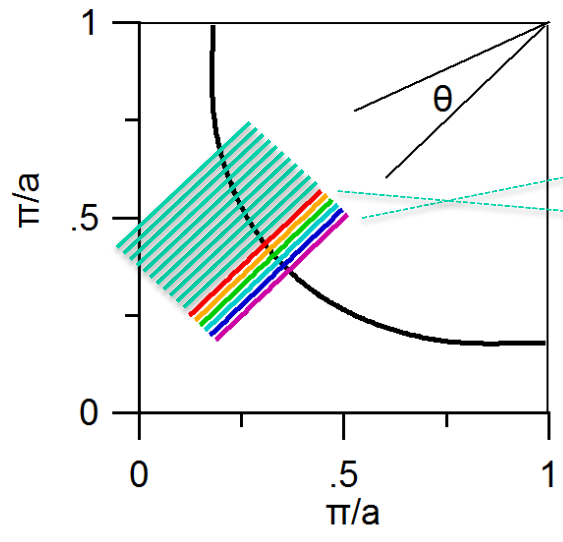


→Quantitative determination of gaps and scattering rates (self energies).
→Qualitatively different understanding of many aspects of the physics.

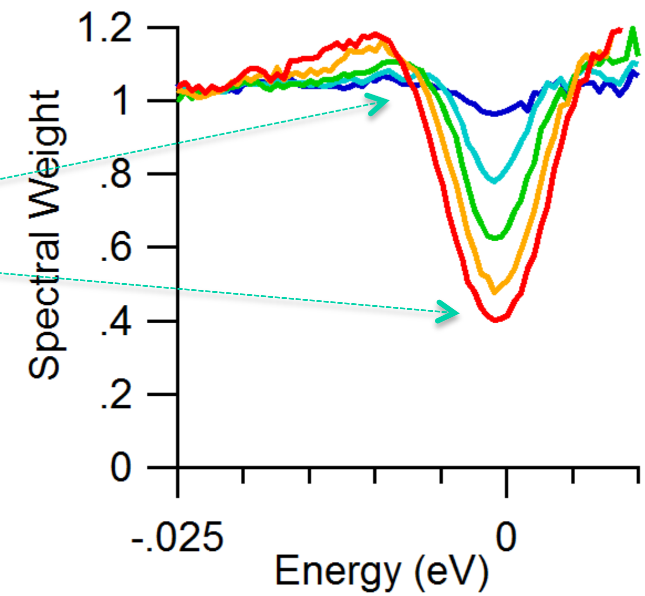
T. J. Reber, D.S.D. et al. Nature Physics **8**, 606–610 (2012)

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.

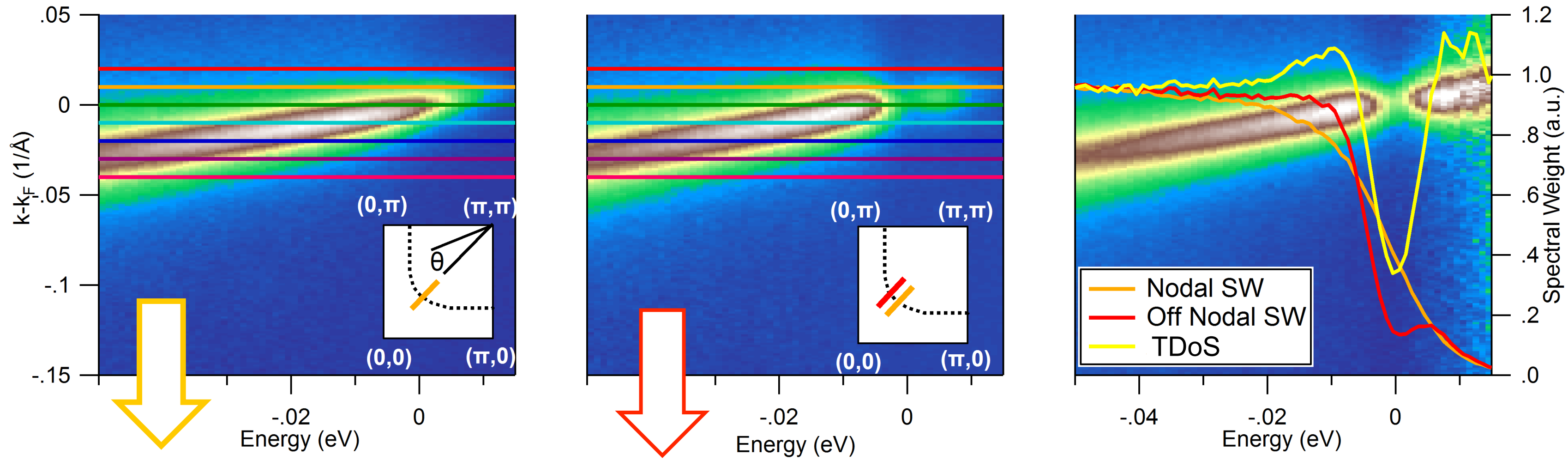


Quantitative determination of gaps and scattering rates (via Dynes tunneling formula).

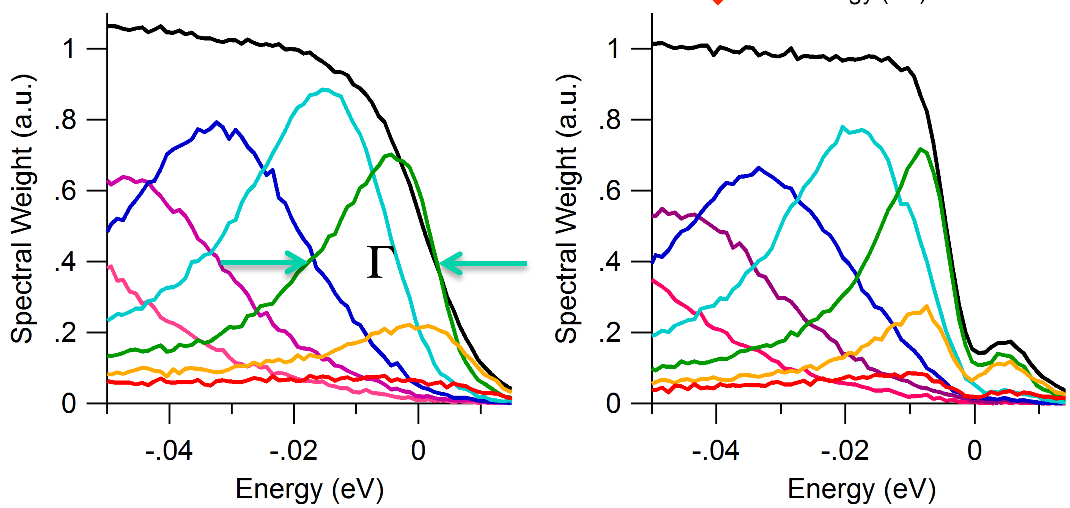
Qualitatively different understanding of many aspects of the physics.

T. J. Reber et al. Nature Physics **8**, 606–610 (2012)

Creating the Tomographic Density of States (TDoS)



Sample:
Bi2212
T: 50 K
T_C: 91 K
hv:7 eV



Colored: EDCs along one cut.
Black: Sum of ~ 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) ~ 15 meV or greater. Full scattering, including heterogeneous contribution.
TDoS scattering rate ~ 2-3 meV – homogeneous contribution?

Fitting to Dynes's Tunneling Formula (1978)

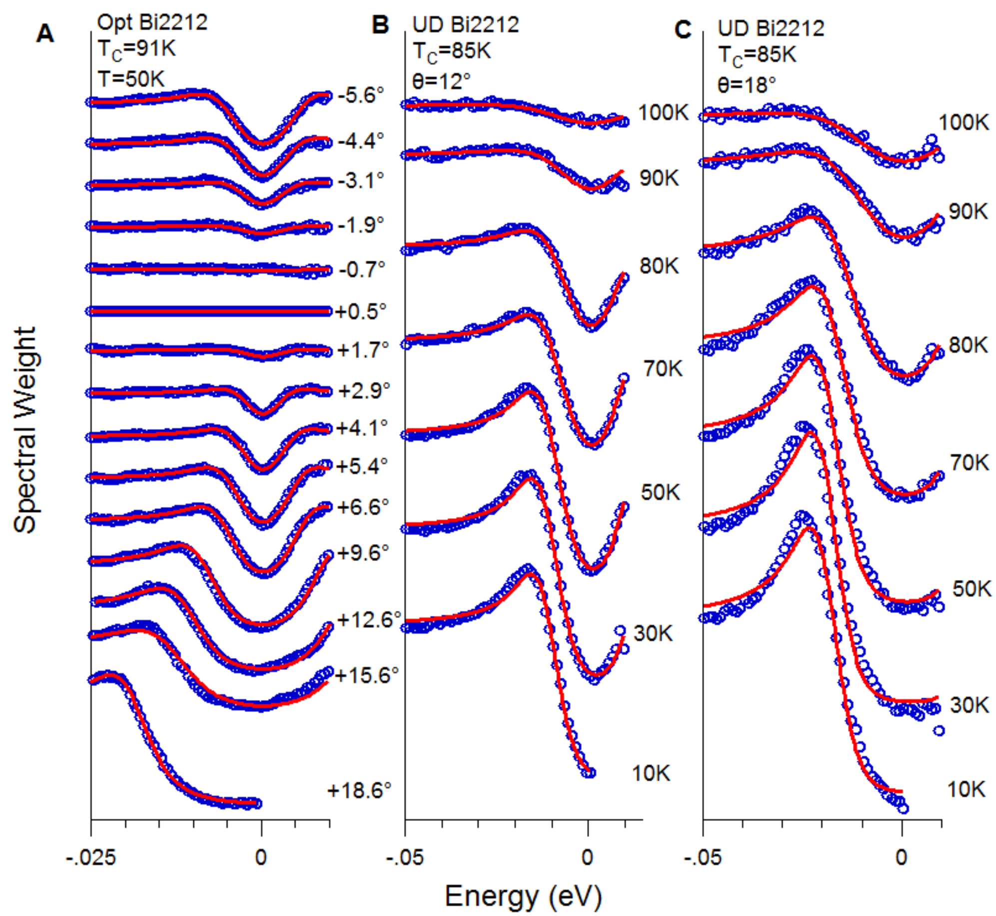
$$I_{TDoS}(\omega) = \rho_{Dynes}(\omega) = \mathrm{Re}\frac{\omega + i\Gamma}{\sqrt{(\omega + i\Gamma)^2 - \Delta^2}}$$

Represents a broadened BCS DOS.

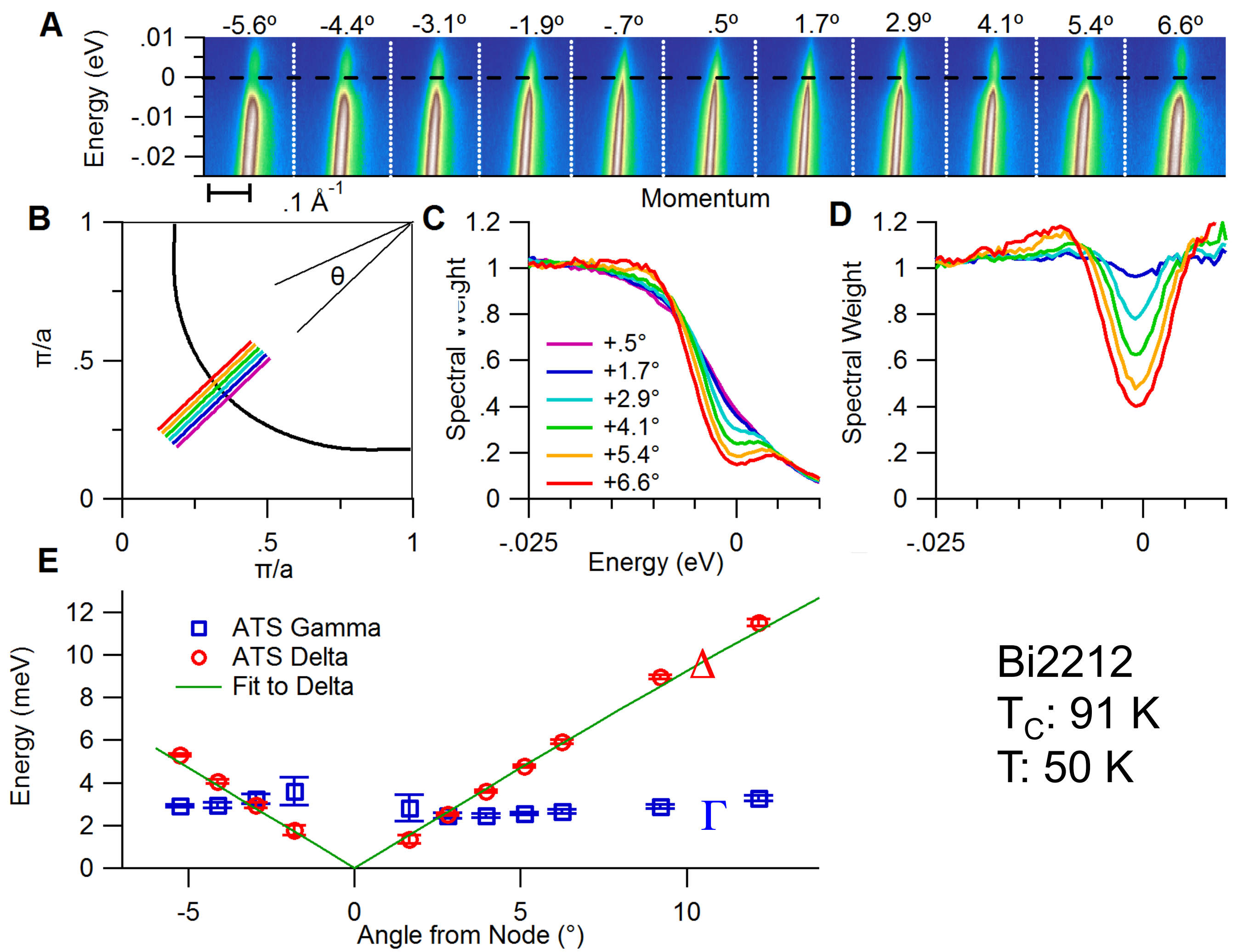
The TDoS are well fit by the Dynes formula over the full range of accessible angles and temperatures.

Each fit gives: pairing strength Δ, and pair-breaking rate Γ.

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



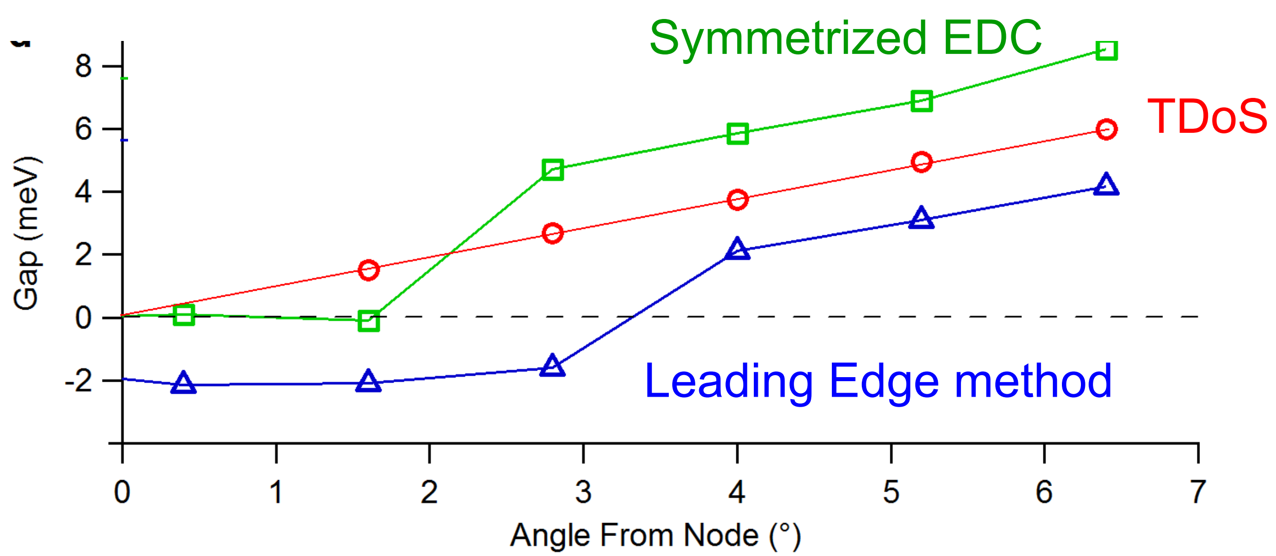
Near-Nodal Angular Evolution of TDoS



Bi2212
T_C: 91 K
T: 50 K

The TDoS extracts a d-wave Δ with a nearly isotropic Γ in the near nodal region. Improved accuracy and precision over all other techniques for determining Δ or Γ.

Gap magnitudes:
Comparison to Leading Edge and Symmetrized EDCs



Sample:
Bi2212
T: 50 K
T_C: 91 K
hv:7 eV

Both conventional techniques (Leading Edge and Symmetrized EDCs) fail near the node, giving a finite arc where the extracted gap is zero or negative.

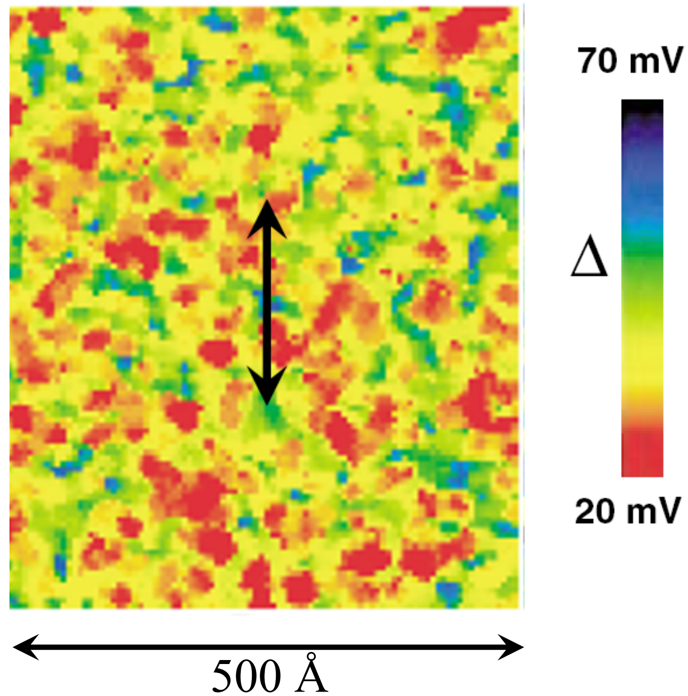
An artificial arc forms when $\Gamma \sim> \Delta$.

Reber et al. Nature Physics 2012

Homogeneous vs. heterogeneous broadening

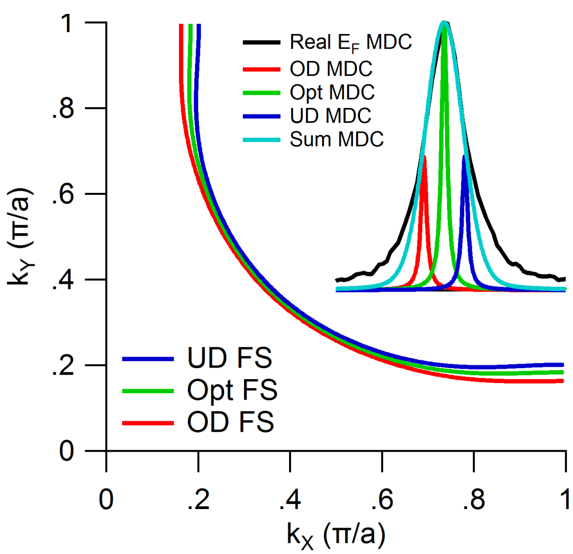
Lots of heterogeneity observed in cuprates. It is likely due to dopant potentials, especially out of the planes giving strong forward scattering.

STM gap map



K. McElroy *et al.* PRL **94,** 197005 (2005)

Dopant inhomogeneity effectively gives multiple FS's (Wise, Hudson et al., Nat. Phys 2009)

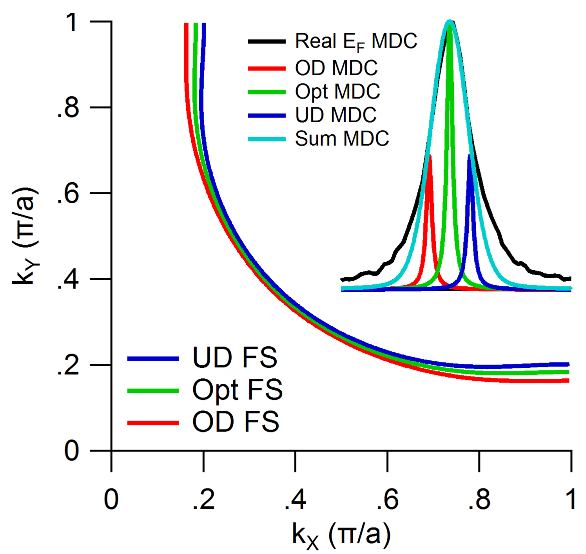


Broadens EDCs and MDCs but not TDoS.

Homogeneous vs. heterogeneous broadening

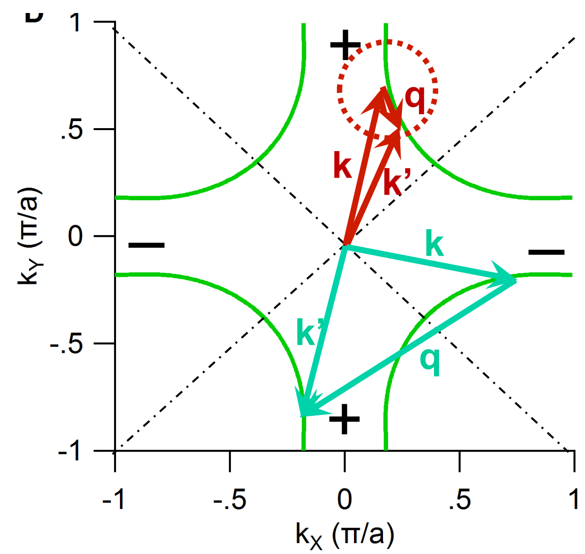
TDoS scattering rates of 2-3 meV are much smaller than the full ARPES scattering rates (15-20 meV). TDoS scattering rates are consistent with optics and STM.

Dopant inhomogeneity effectively gives multiple FS's (Wise, Hudson et al., Nat. Phys 2009)



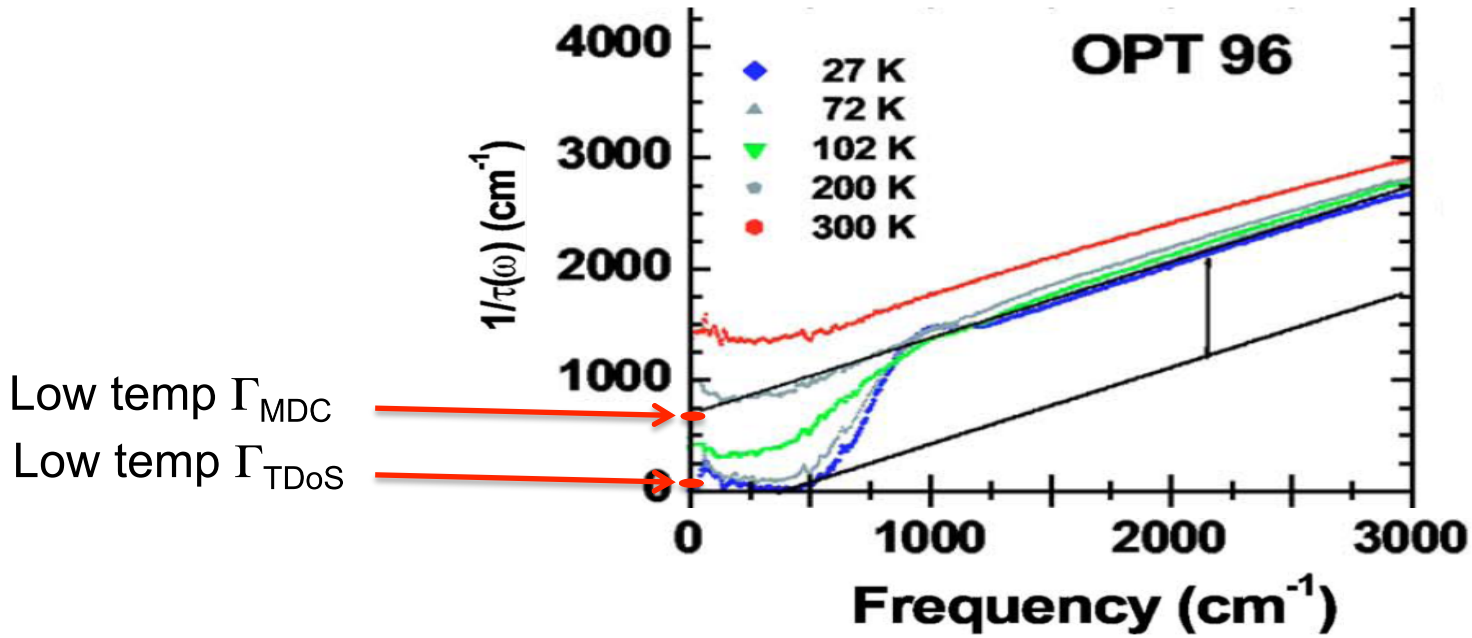
Broadens EDCs and MDCs but not TDoS.

Forward scattering from out-of-plane disorder. Non pair breaking. Affects EDC and MDC but not TDoS.



Back scattering from in-plane disorder. Pair breaking. Affects EDC, MDC and TDoS.

Comparison to Optics

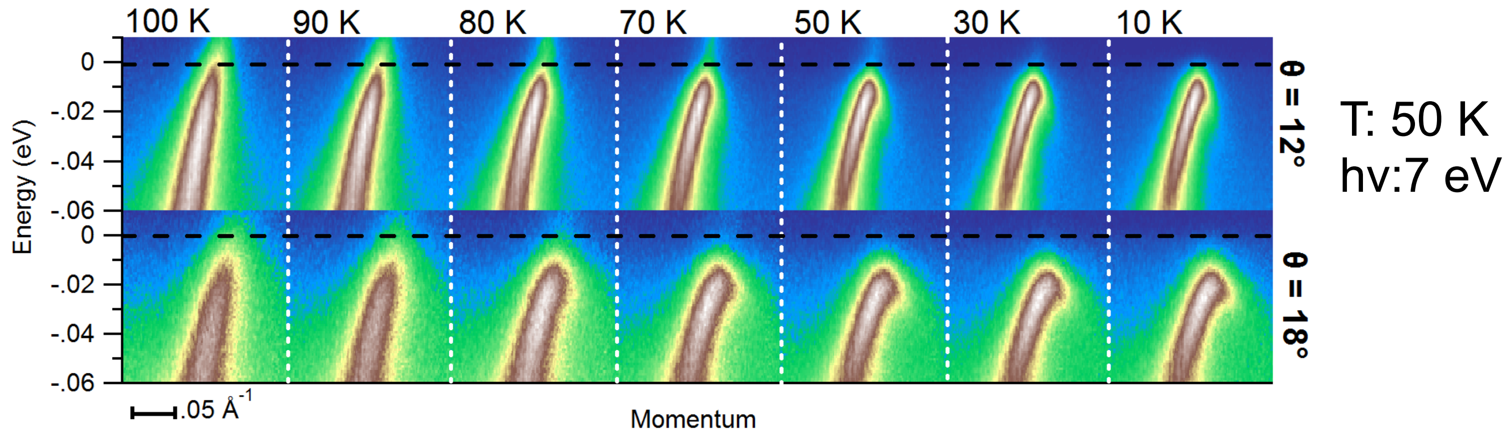


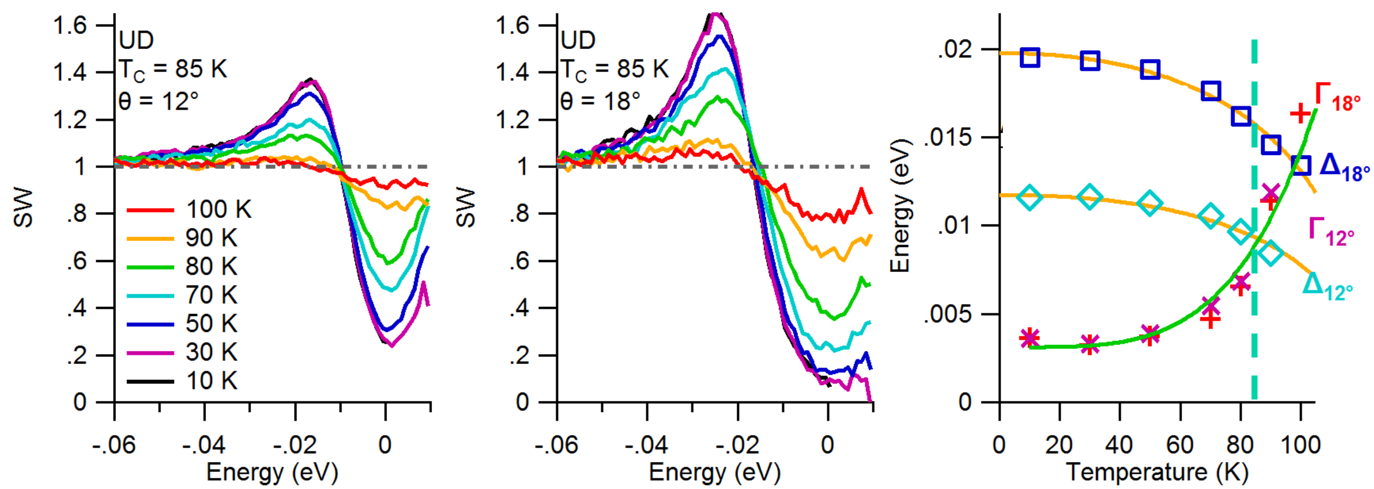
Hwang, Timusk & Gu, *Nature* 2004

TDoS scattering rates more consistent with optics and STM.

Temperature-dependence at two near-nodal angles

(Lightly underdoped T_c=85K Bi2212)

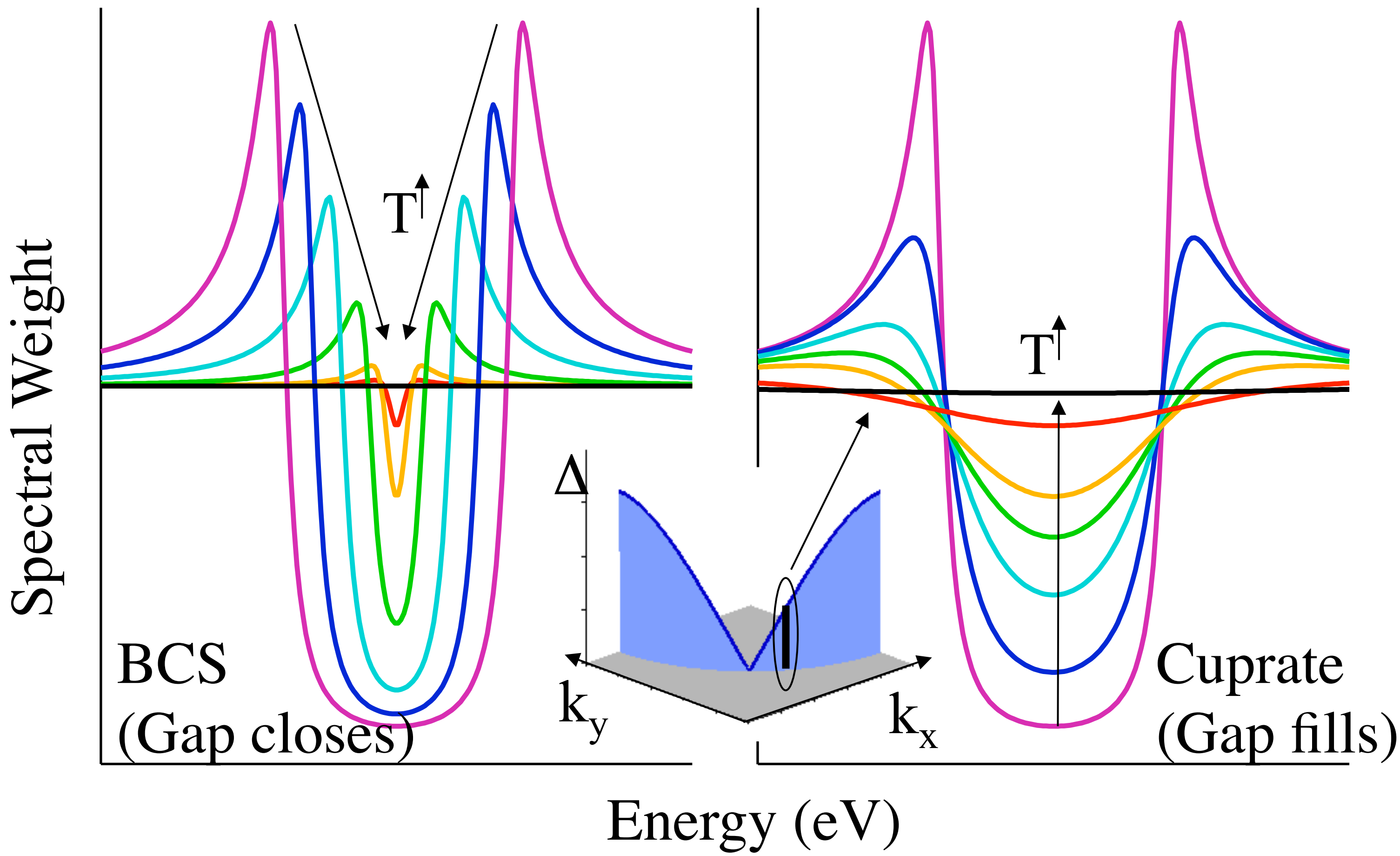




Near-nodal gap smoothly evolves through T_C, indicating that pre-formed pairs exist in the pseudogap state.

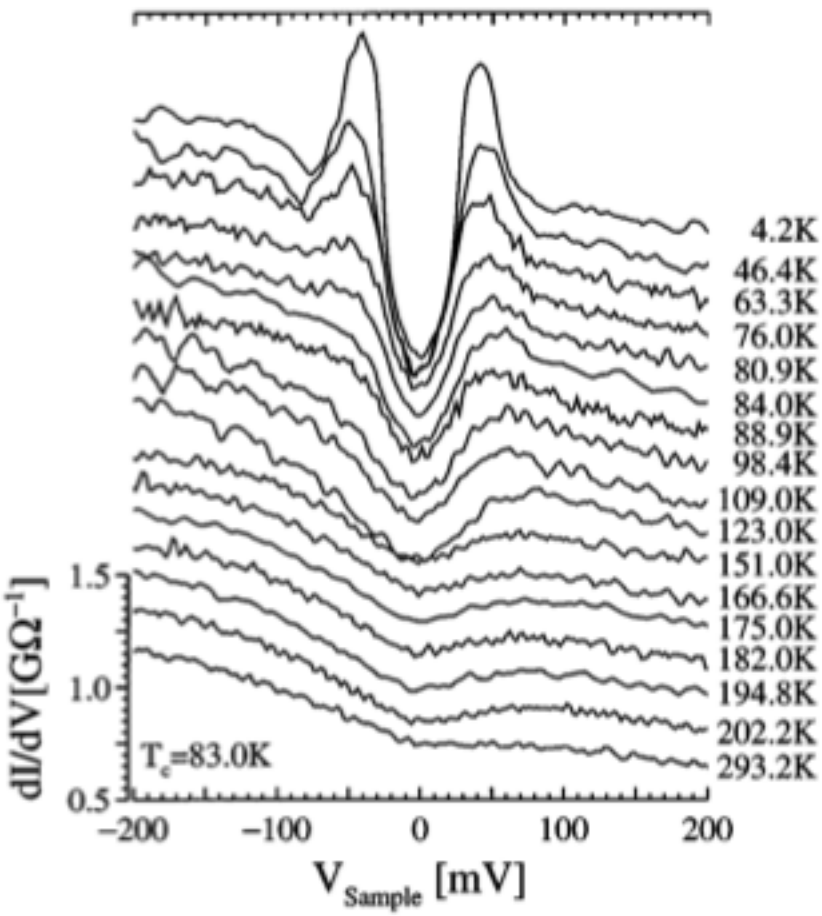
While Δ has shrunk by 30% by T_C, Γ has grown by nearly 300%. The rapid increase of pair-breaking scattering shifts weight from the peaks into the gap, filling it.

Closing/Filling of the gaps with temperature

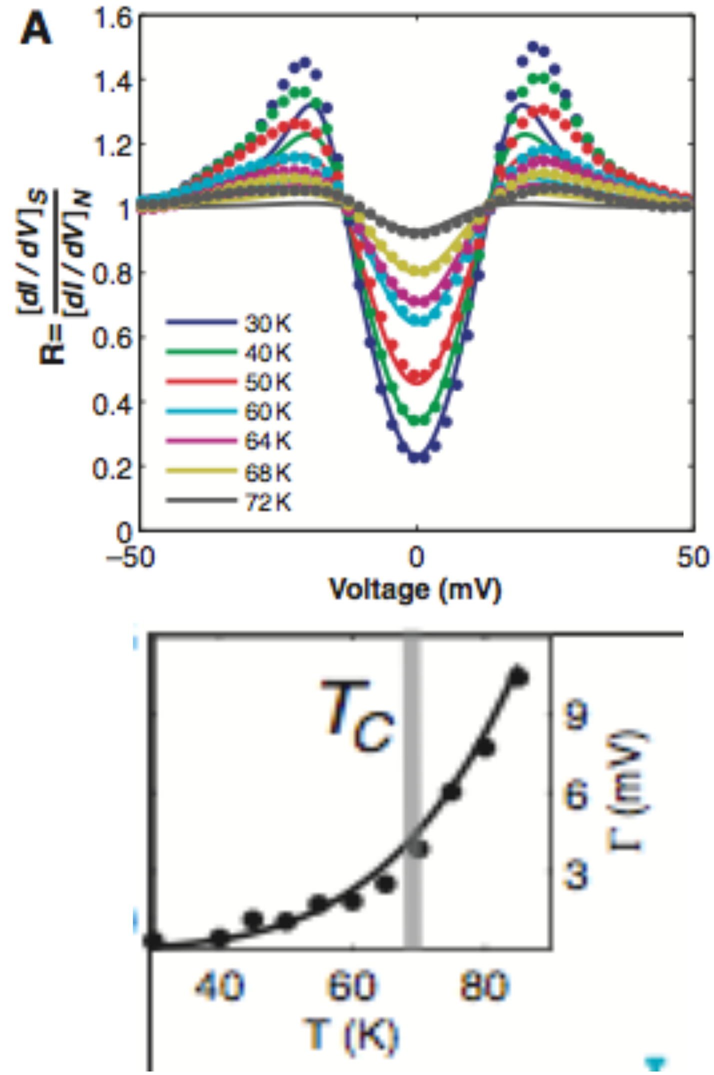


The filling of the gap in cuprates is due to the rapidly rising Γ (scattering rate) with temperature. This is a phenomenology observed in essentially all spectroscopies on cuprates, but has been difficult to quantify.

Filling of the gap from STM experiments



Renner, Fisher et al, PRL (1998)

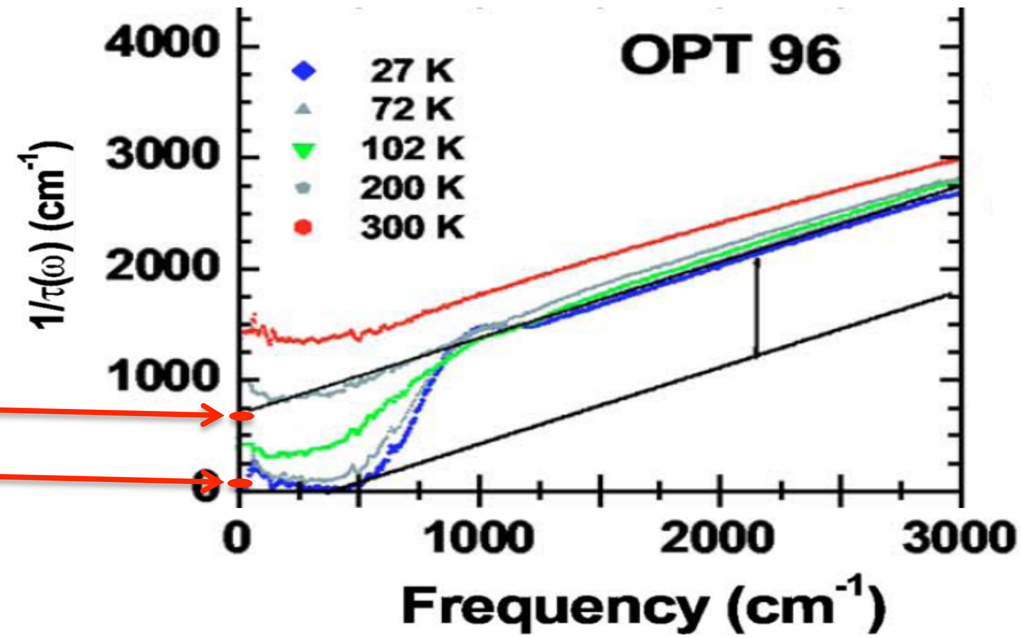


Pasupathy, Yazdani, et al. Science (2008)

Scattering rates from optics

Low temp Γ_{MDC}

Low temp Γ_{TDoS}

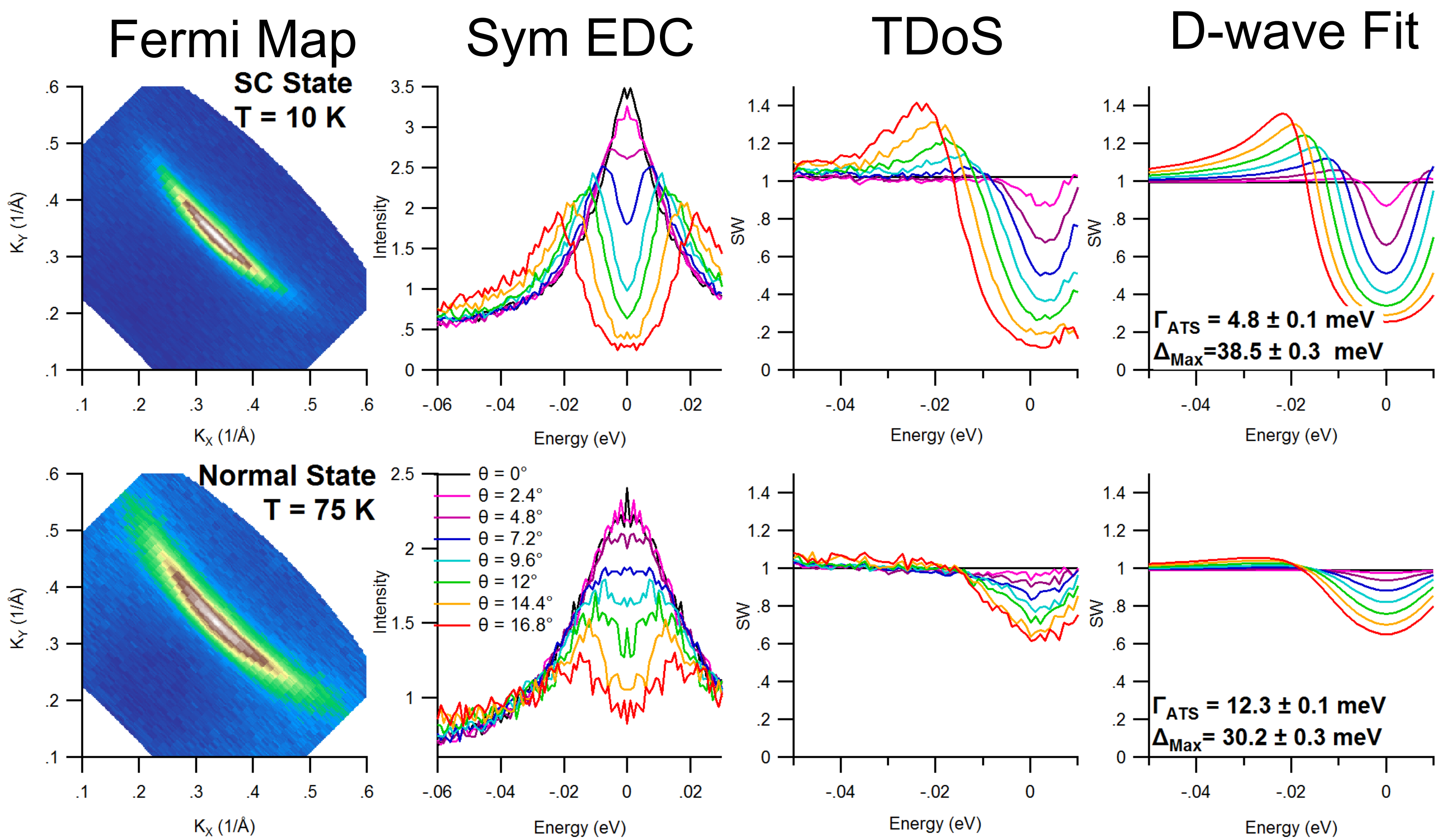


Hwang, Timusk & Gu, *Nature* 2004

TDoS scattering rates more consistent with optics and STM.

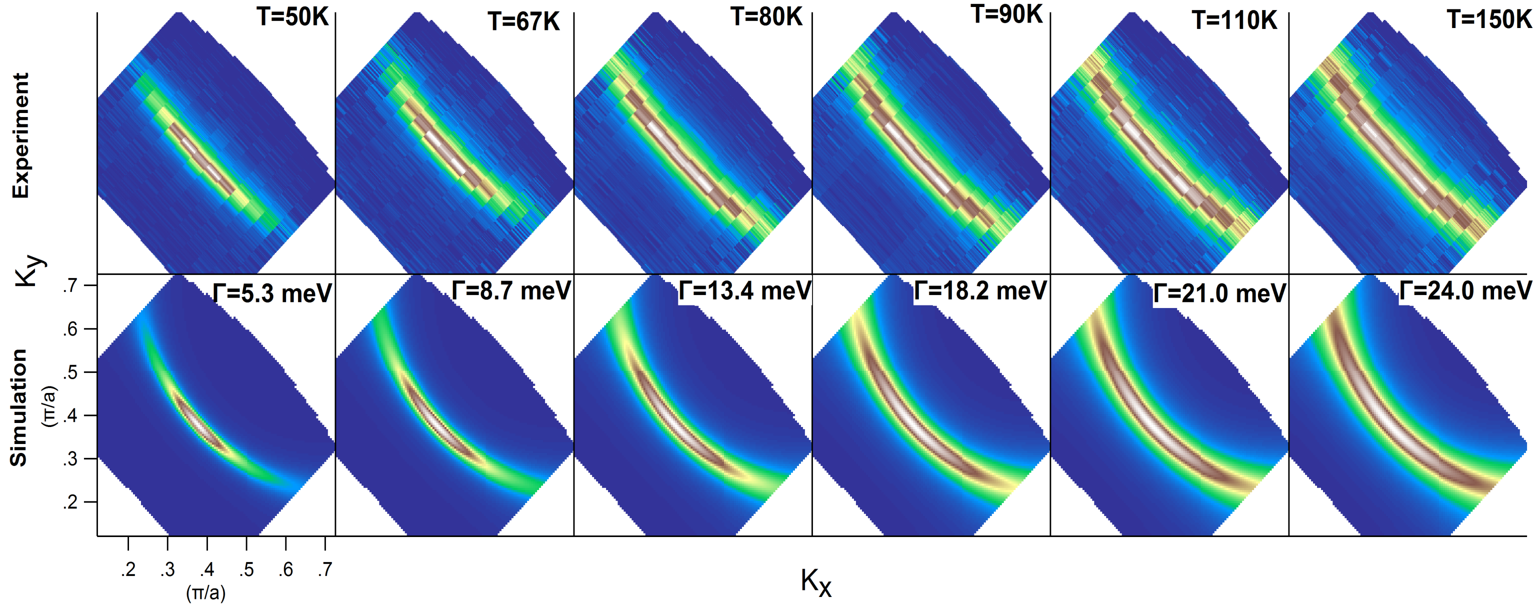
Formation of the Fermi Arc

UD Bi2212
T_C: 65 K
hv:7 eV

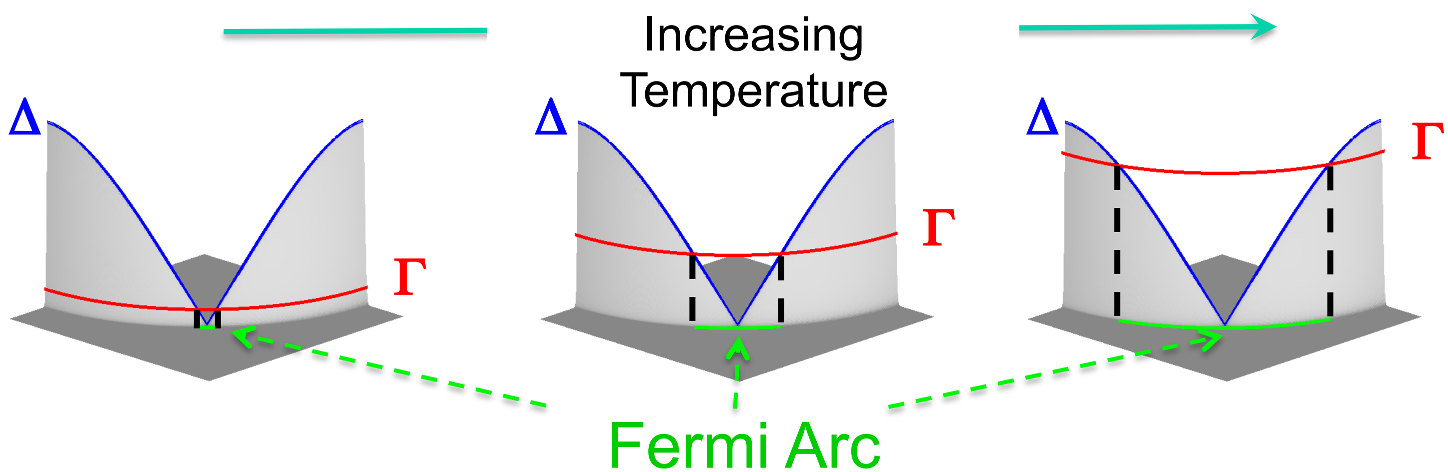


The Fermi arc can be fully accounted for by the rapidly increasing Γ shifting incoherent weight into the gap.

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

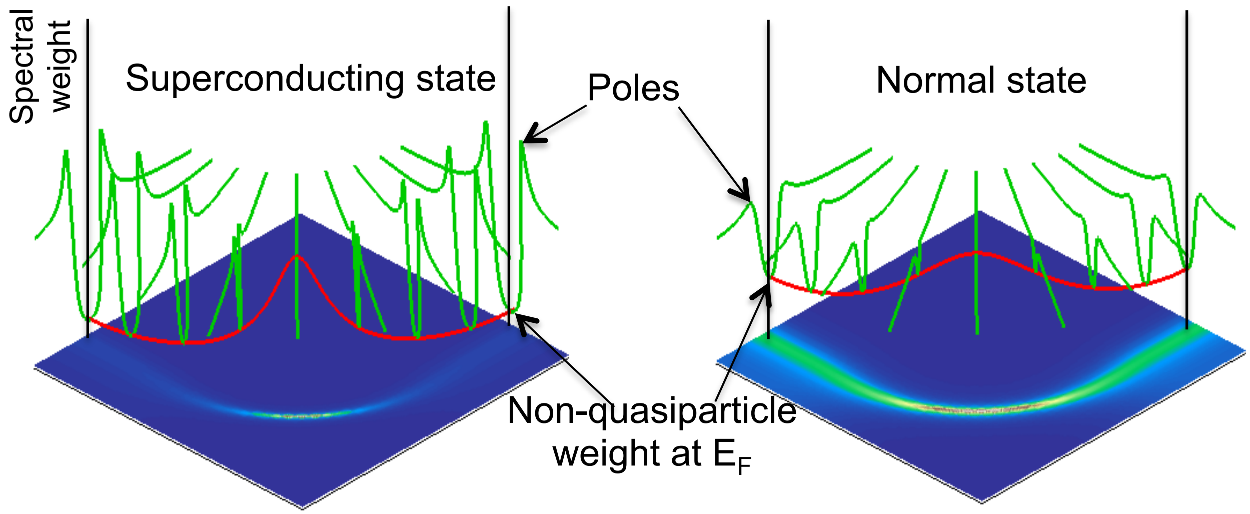


Sample:
UD
Bi2212
T_C: 67 K
hv:7 eV



T. J. Reber et al. Nature Physics **8**, 606–610 (2012)

Non-quasiparticle weight at E_F



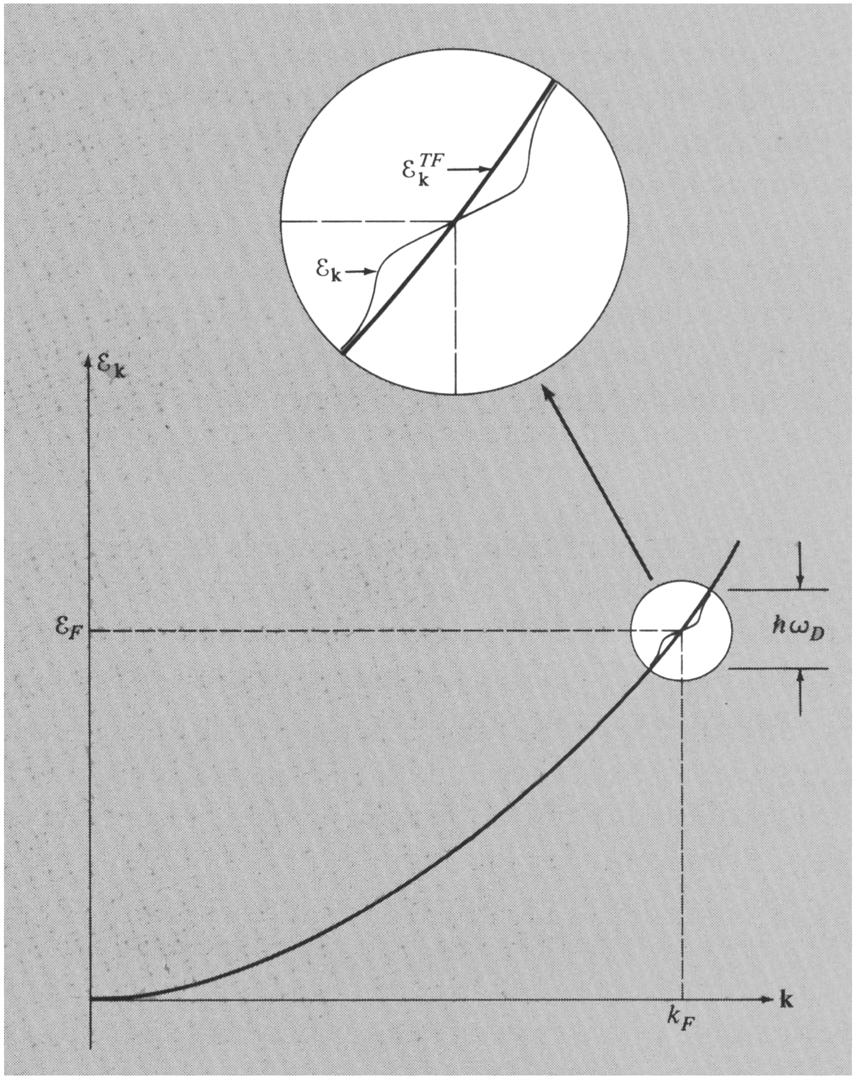
The weight at the FS that makes the arcs is not due to a qp pole, but rather is weight scattered up to E_F by the strong pair-breaking scattering rate Γ.

This non-qp spectral weight (plus a nodal qp) is what is available for transport, thermodynamics, etc.

Kinks and dispersion anomalies

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

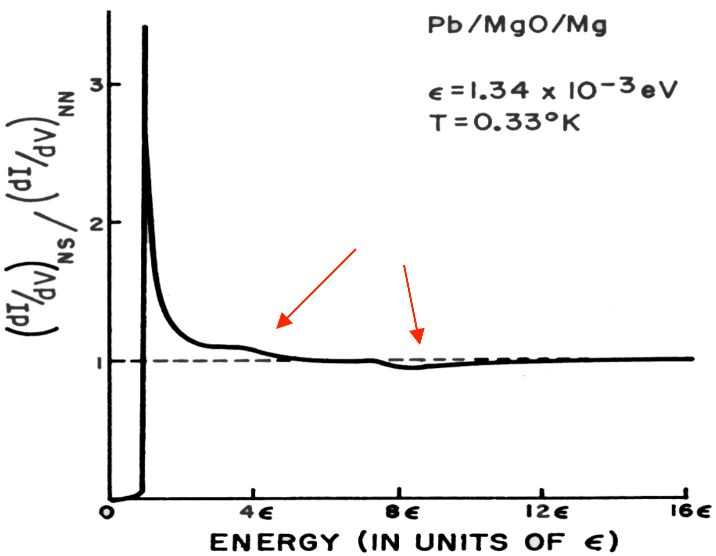


Self energies in conventional superconductors Via Structure in the tunneling density of states

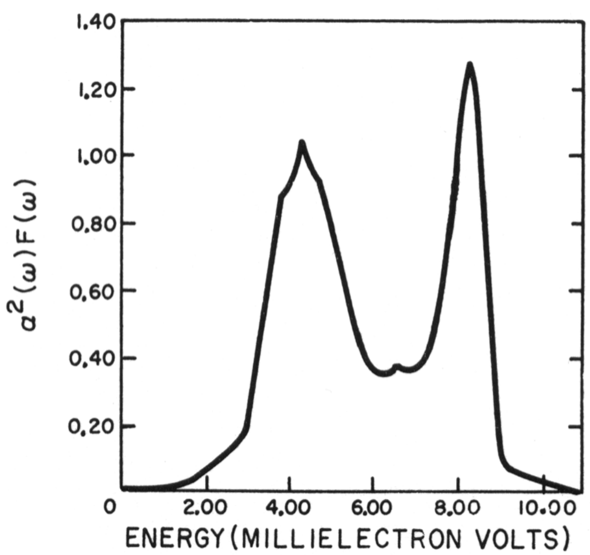
==> Confirmation that phonons mediate the pairing

From Nobel Lecture, John Bardeen, 1972

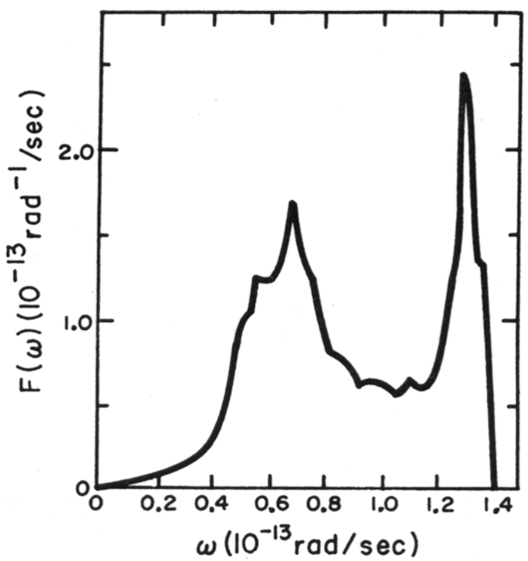
Tunneling Spectrum (Density of States)



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.

VOLUME 83, NUMBER 10 PHYSICAL REVIEW LETTERS 6 SEPTEMBER 1999

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

T. Valla,[1] A. V. Fedorov,[1] P. D. Johnson,[1] and S. L. Hulbert[2]

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

"spectral function" = ARPES weight (k,ω)

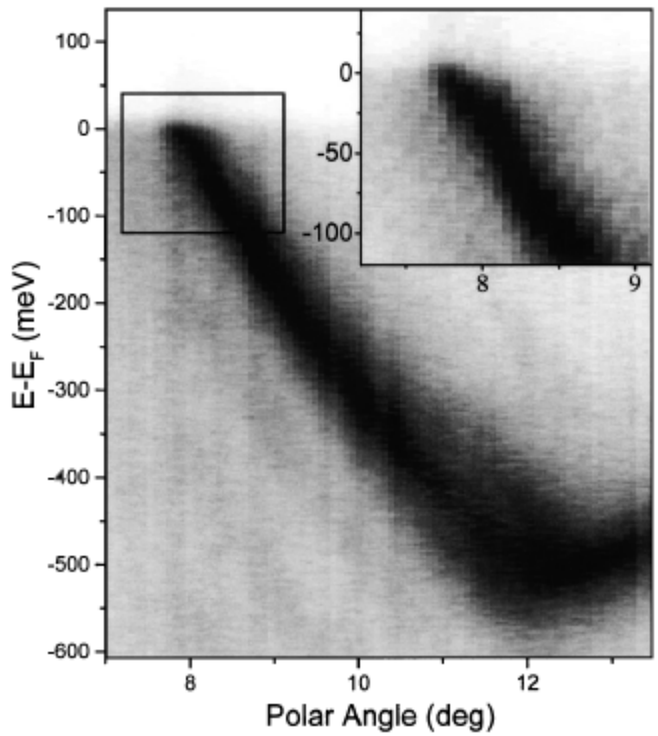
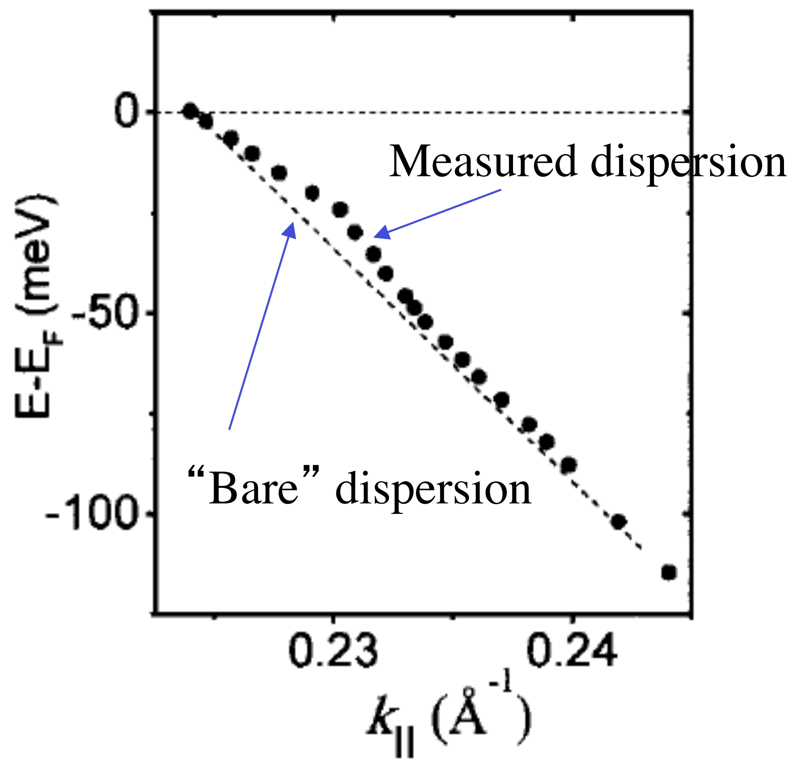


FIG. 1. ARPES intensity plot of the Mo(110) surface recorded along the $\overline{\Gamma}$-$\overline{N}$ line of the surface Brillouin zone at 70 K. Shown in the inset is the spectrum of the region around k_F taken with special attention to the surface cleanliness.



"Kink effect"

VOLUME 83, NUMBER 10 PHYSICAL REVIEW LETTERS 6 SEPTEMBER 1999

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

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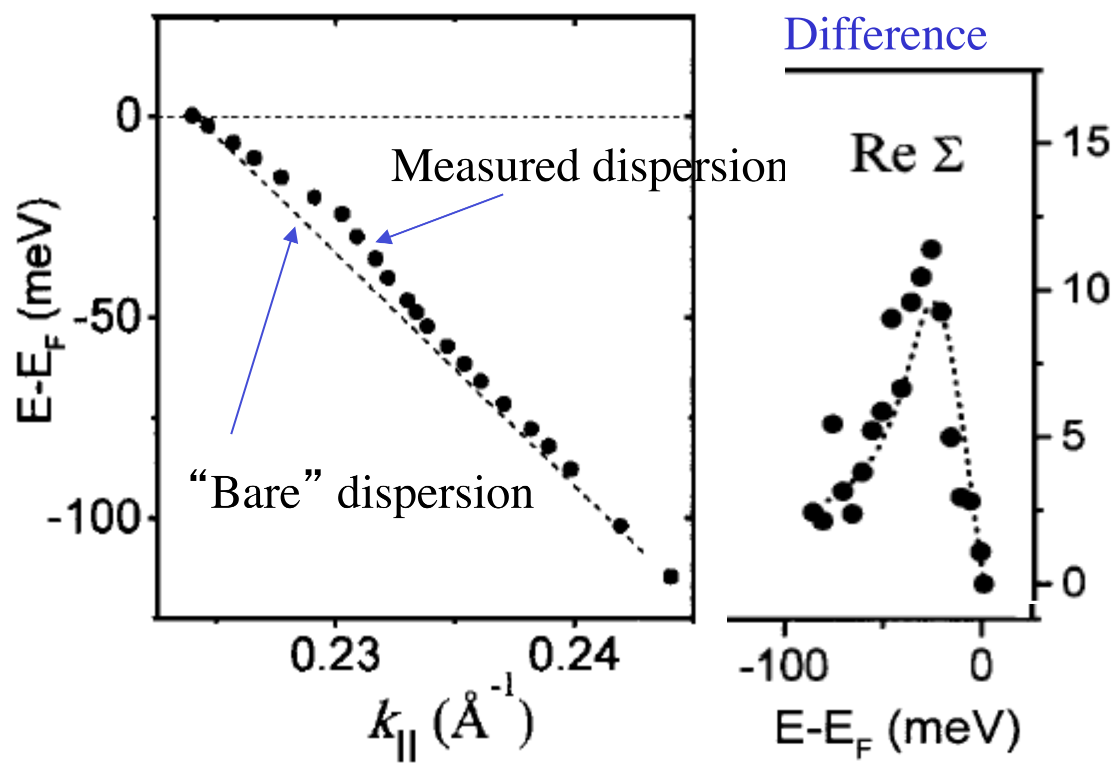
$$A(\mathbf{k},\omega) \propto \frac{\mathrm{Im}\Sigma(\mathbf{k},\omega)}{[\omega - \varepsilon_{\mathbf{k}} - \mathrm{Re}\Sigma(\mathbf{k},\omega)]^2 + [\mathrm{Im}\Sigma(\mathbf{k},\omega)]^2}$$

"spectral function" = ARPES weight (k,ω)



A(k,ω) peaks when $[\omega-\varepsilon_k-\mathrm{Re}\Sigma]=0$ or when
$\omega=\varepsilon_k+\mathrm{Re}\Sigma$
Bare band ε_k: when ReΣ=0
Measured: ReΣ=finite.

Σ = electron "self energy". Here the "kink" is due to electron-phonon scattering. (Phonon lives at kink scale or ~ 30 meV).

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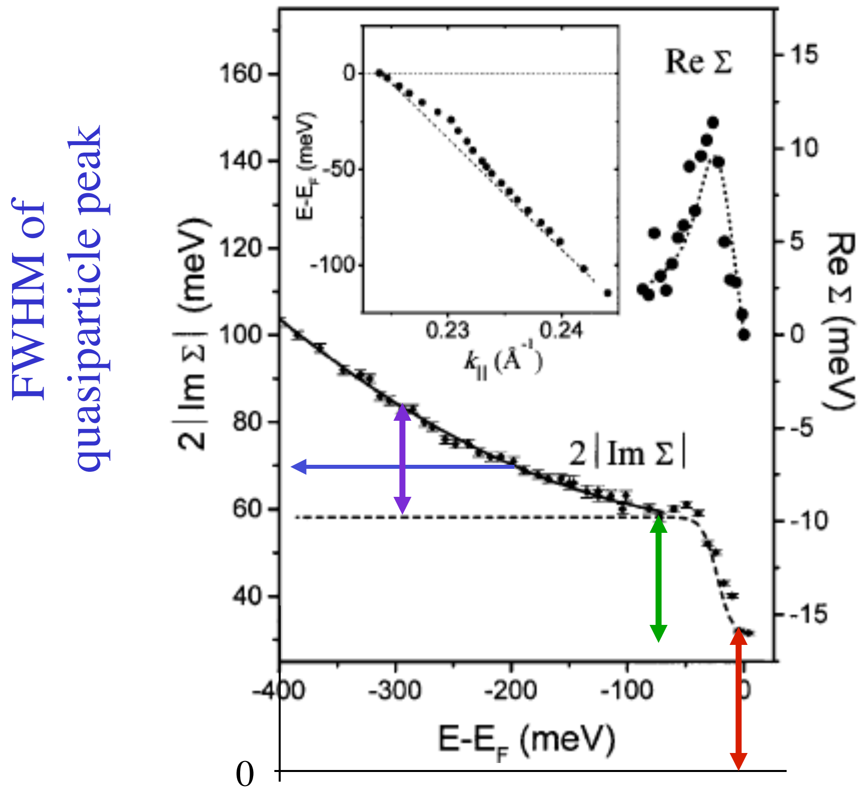


ImΣ = width of spectral peak
Measurable in the same spectra.

ImΣ and ReΣ related through Kramers-Kronig relations (weighted integral over all energies).

Electron-electron scattering

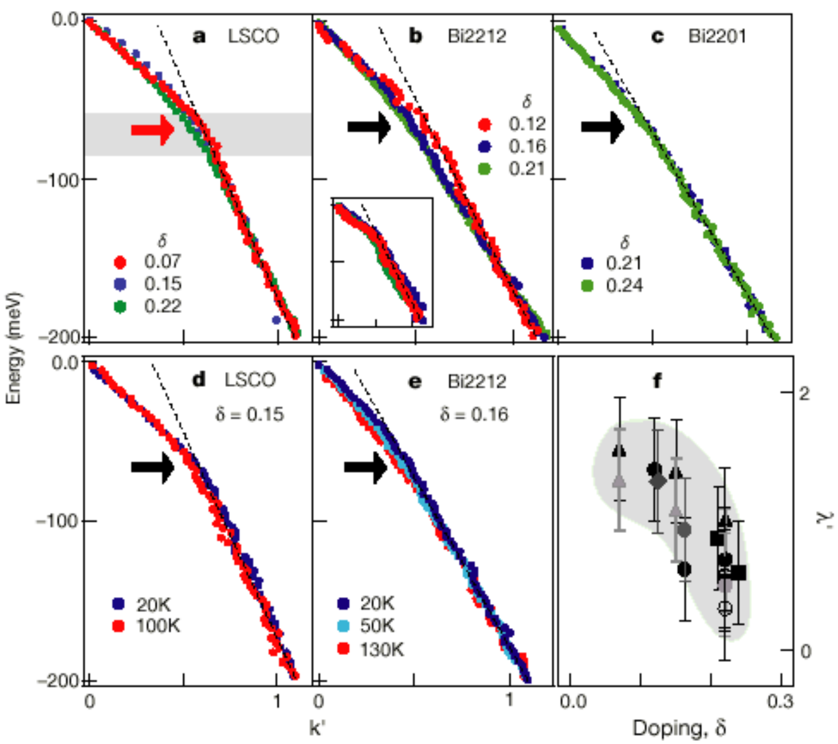
Coupling to phonons

Impurities, finite resolution, final state effects, etc.

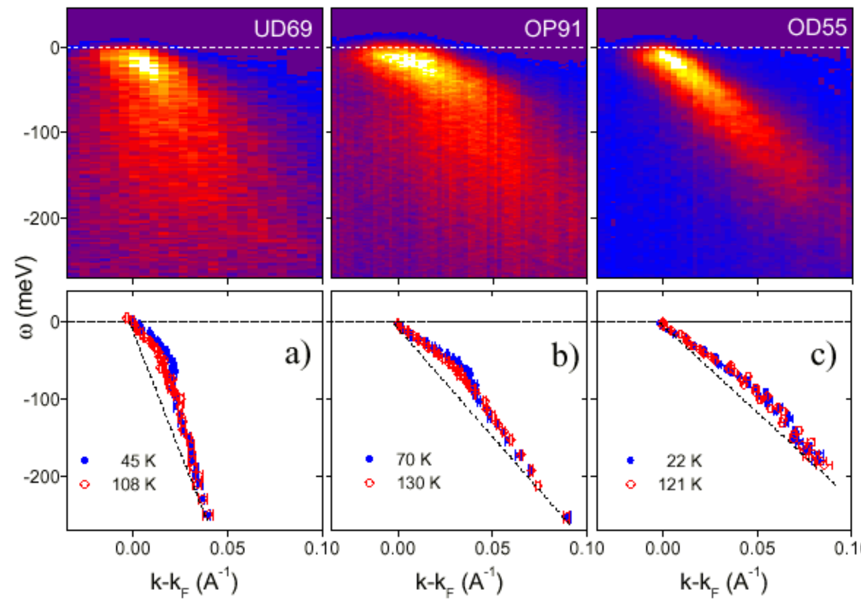
In principle the ARPES spectral function contains all the info about the single-particle many-body fermionic interactions. This plus bosonic measurements from neutrons or inelastic x-rays should give a nearly complete picture of the many-body physics.

kinks in cuprates
(π,π) direction (nodal direction of d-wave gap)

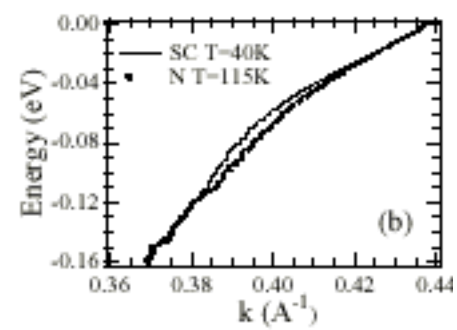
Stanford Group
Lanzara et al.
Nature (2001)



Brookhaven Group
Johnson et al.
PRL (2001).



Argonne Group
Kaminski et al.
PRL (2001)



Kink energy scale ~ 70 meV

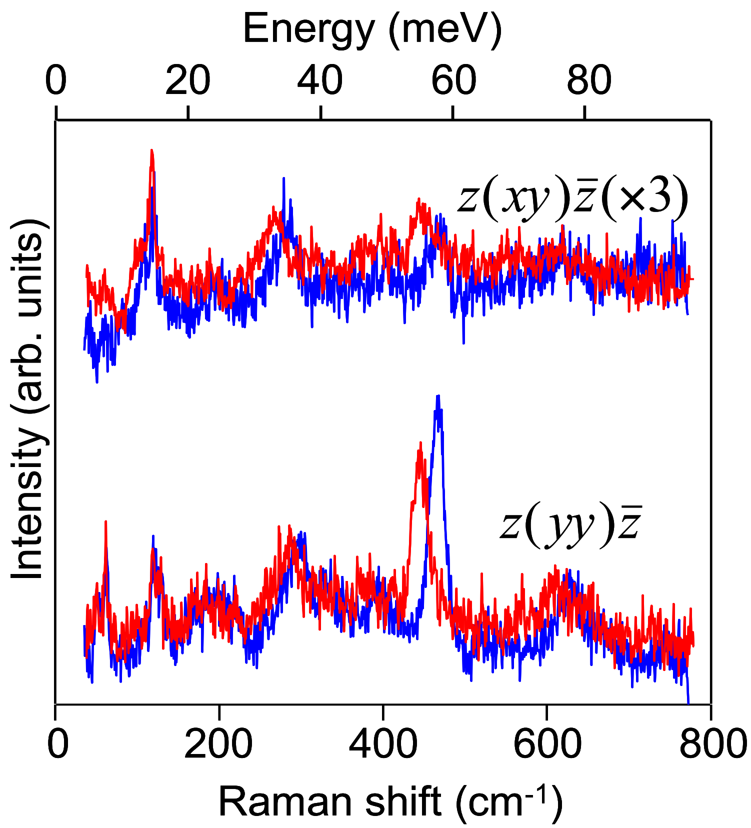
kinks

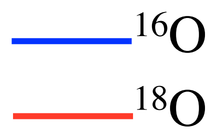
- A kink in the dispersion muct be associated with a step increase in the width/scattering rate.
- Most common explanation is coupling to a boson.
- Strong kinks → strong electron-boson coupling → candidate for the glue (among other things)

Main suggestions for origin of the nodal kink:

- Coupling to a phonon. In particular the in-plane oxygen-stretch LO phonon.
- Coupling to the "41 meV" magnetic resonance mode

Isotope substitutions in Bi2212
Way to fingerprint a mode coupling as phonon originated or not



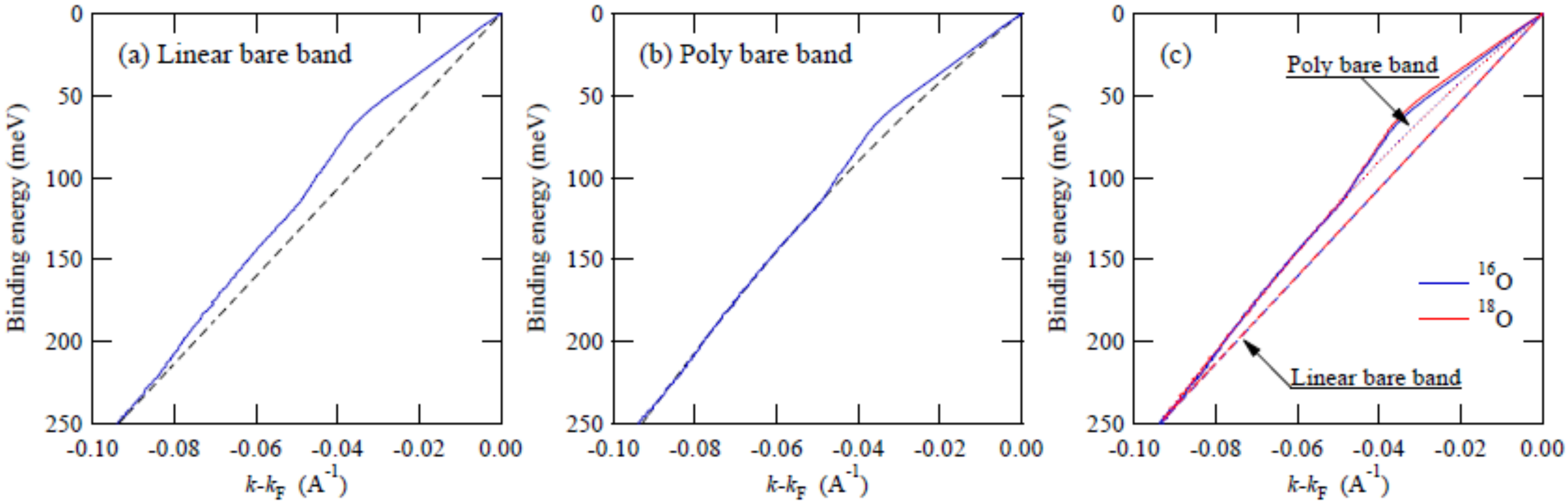


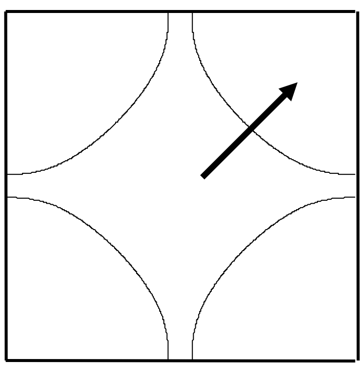
Throughout this presentation

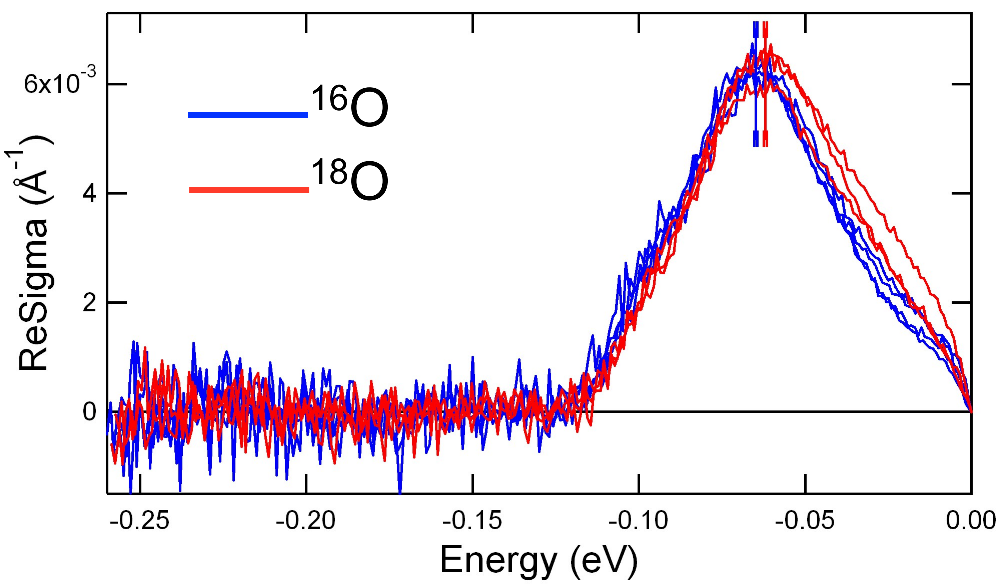
Raman on our samples:
- near full substitution of ^{18}O for ^{16}O
- ~ 3 meV softening with substitution

-Same samples as used by J.Lee and J.C. Davis for isotope studies using STM

Search for a low energy scale (few meV) shift of the nodal kink



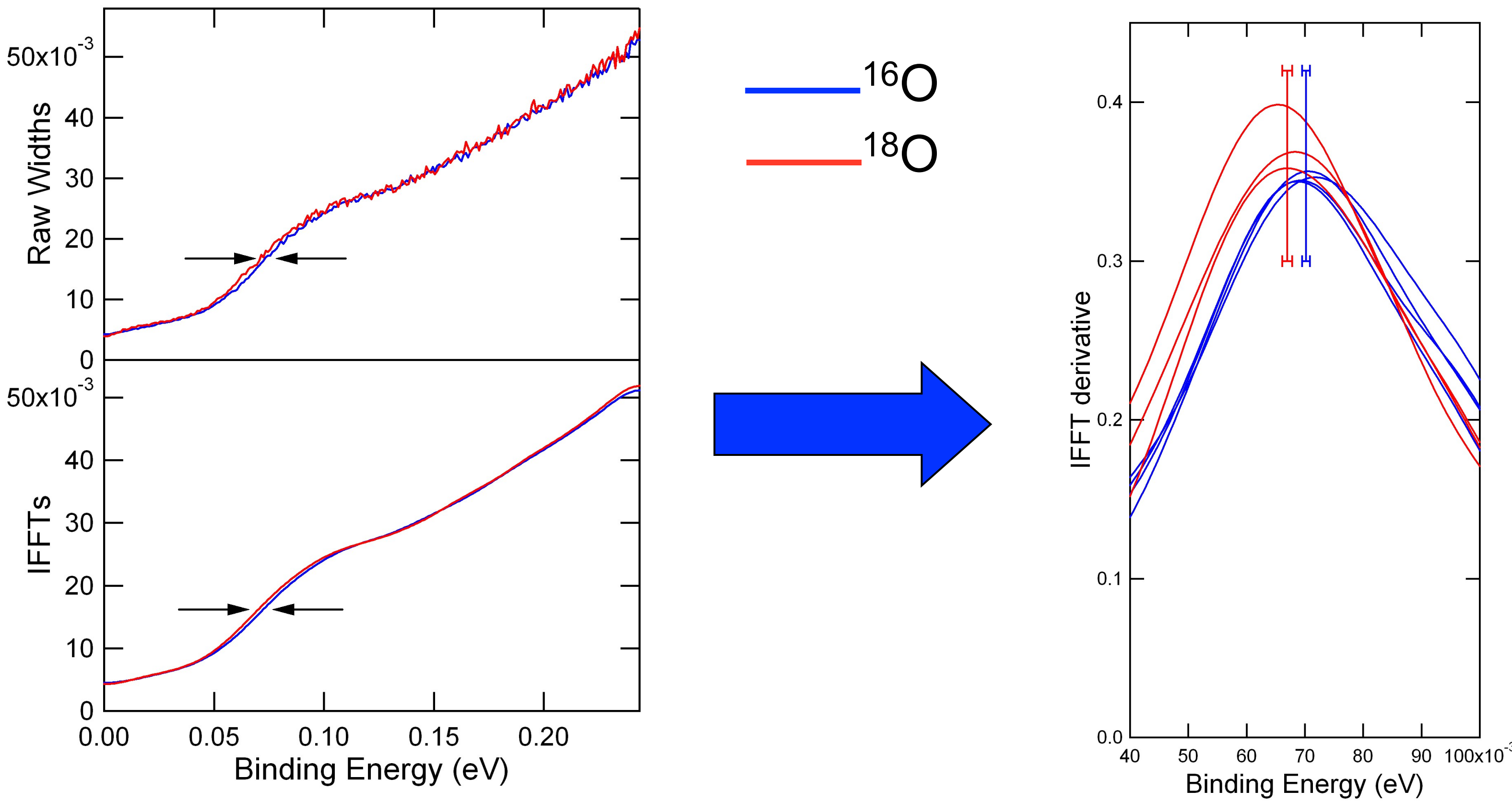




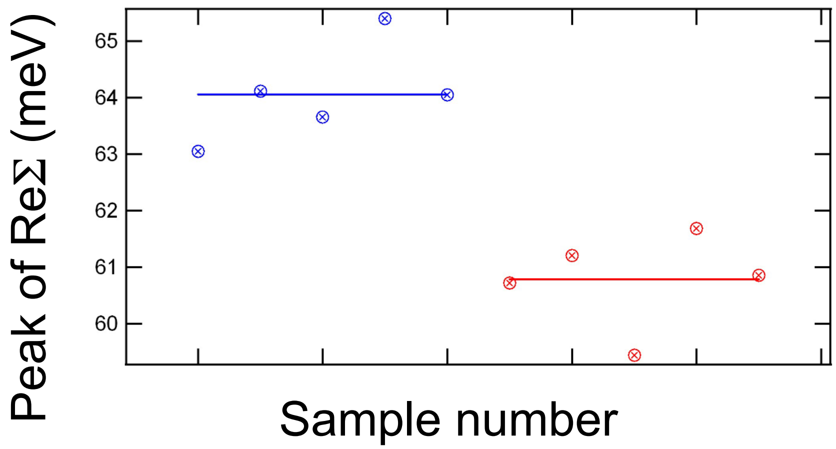
Search for a low energy scale (few meV) shift of the kink, version 2

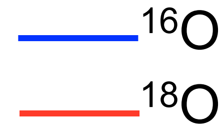
Kink energy analysis method for ARPES widths (ImΣ)

a) Using ARPES widths (ImΣ), no assumed background is needed
b) Take derivative to try to find a well-defined peak

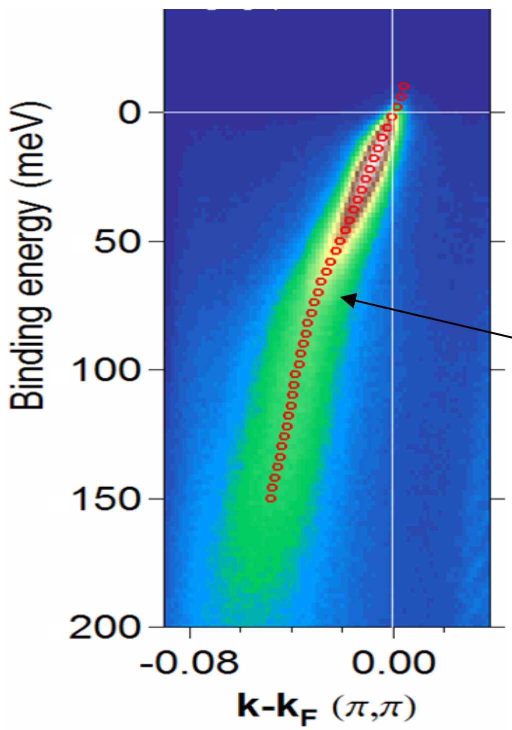


Isotope Effect: Two methods, consistent results





Kink softening of 3.4 ± 0.5 meV



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

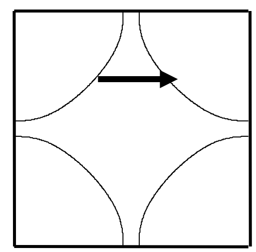
H. Iwasawa, D.S.D. et al., PRL 101, 157005 (2008)

Boson coupling

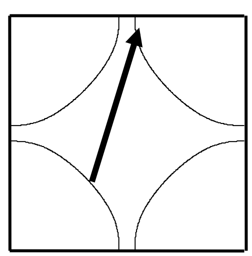
•STM (Davis group) (52 meV, gap referenced) mainly picks up antinodal states mode ~ 52 meV {*Nature*, **442**, 546 (2006)}

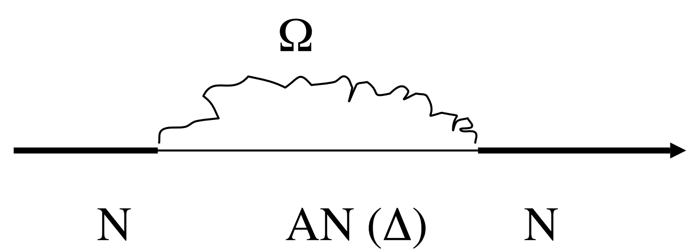
•ARPES (65 meV relative to E_F, node)

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

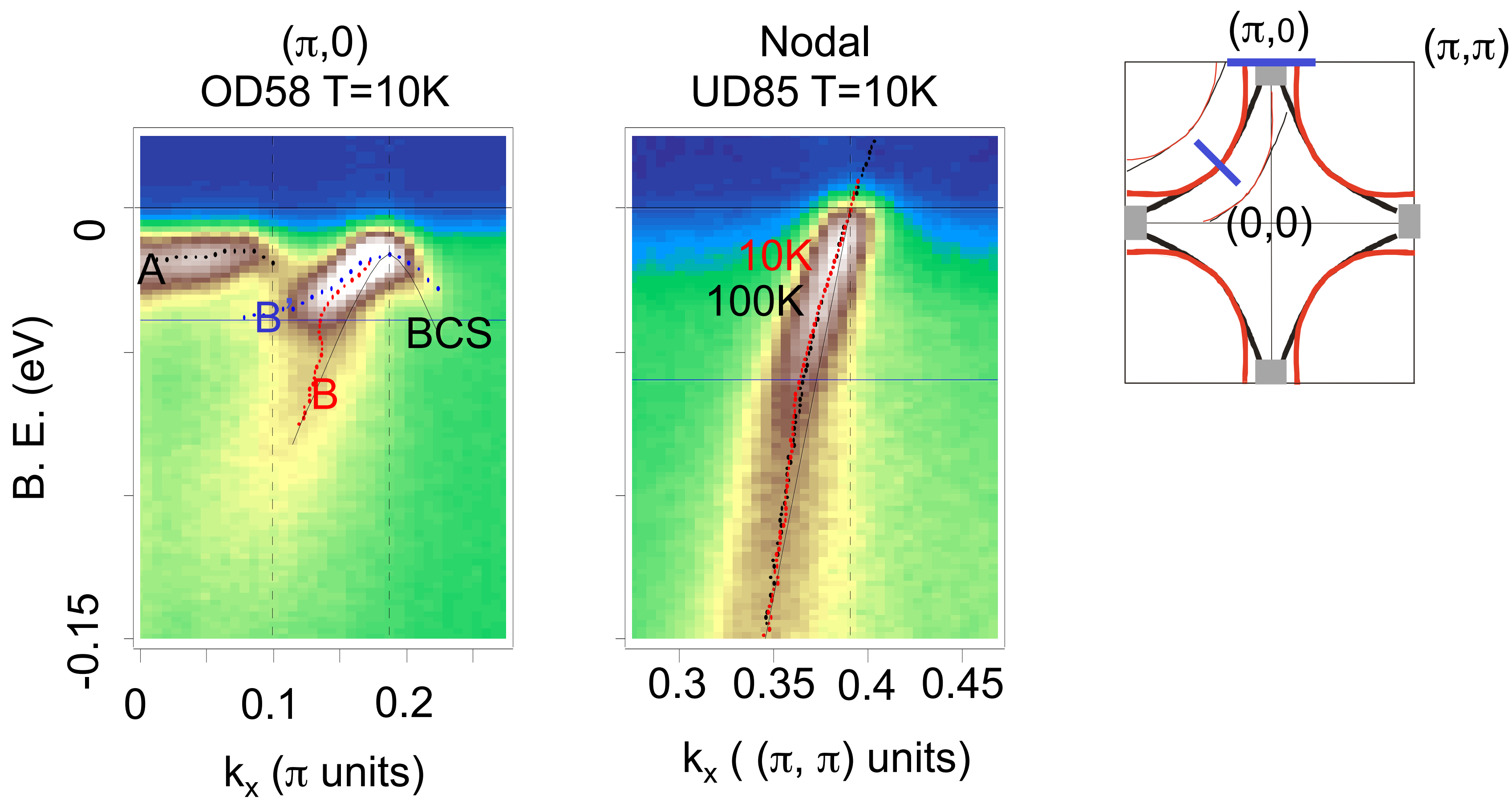


- if nodal-antinodal (e.g. B_{1g}) then gap referencing (to an average around the FS) needed. Mode ~ 30-40 meV.





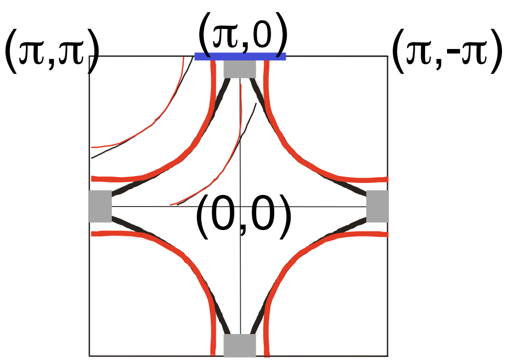
(π,0) kink vs. nodal kink

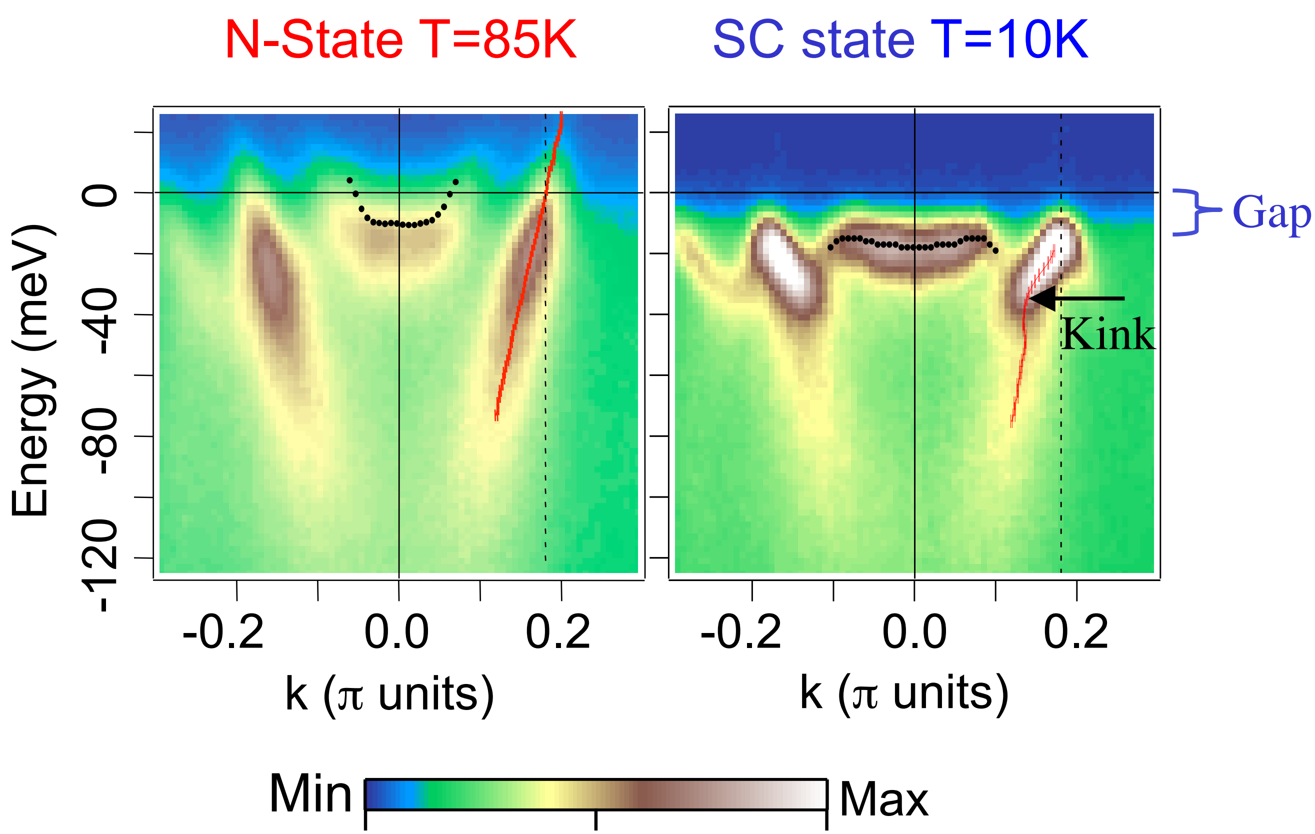


(π,0) kink is much stronger than nodal kink,
shows much stronger T dependence, and is at a different (lower) energy.

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

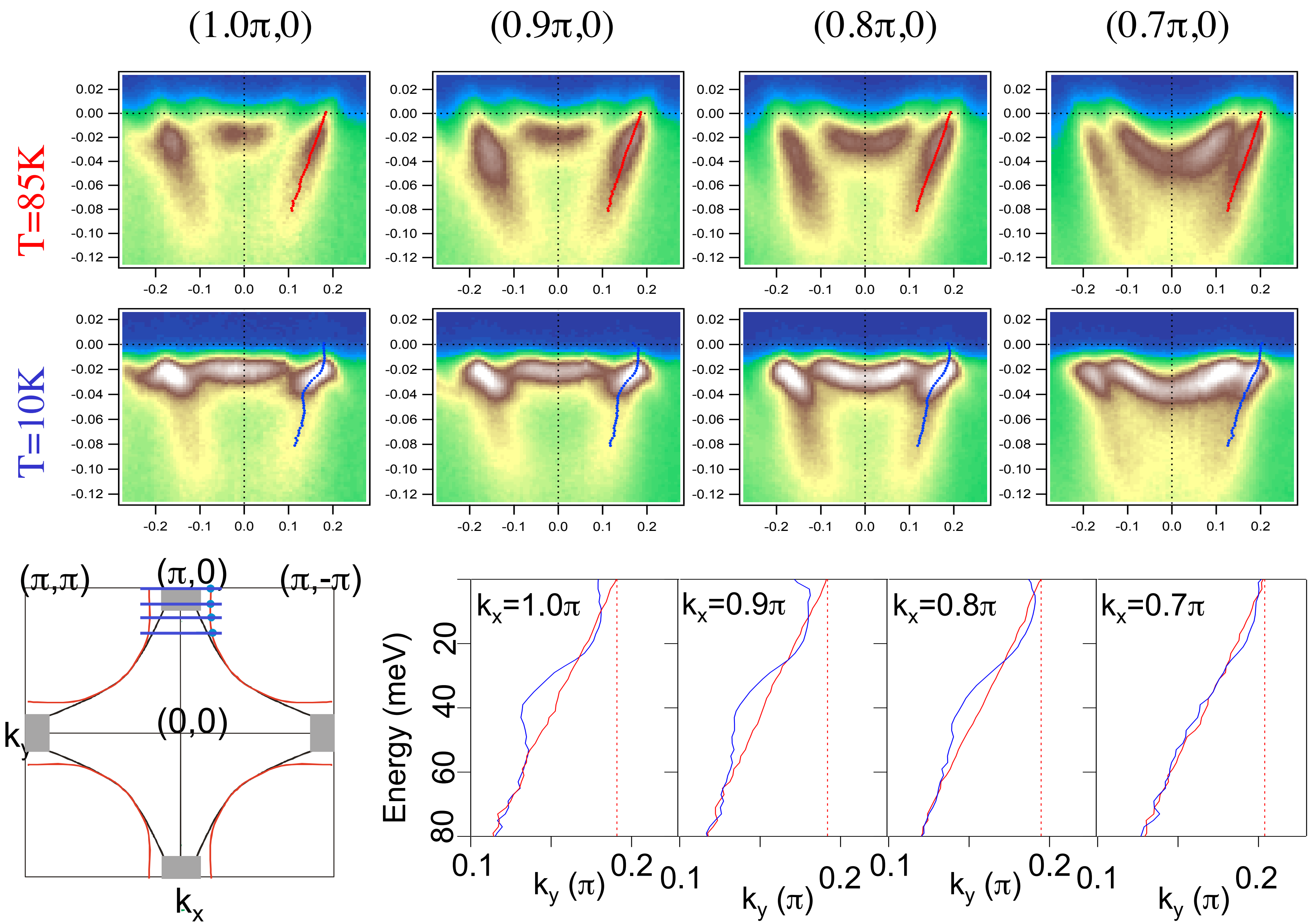
Antinodal Data: Tc=58K Overdoped Bi2212



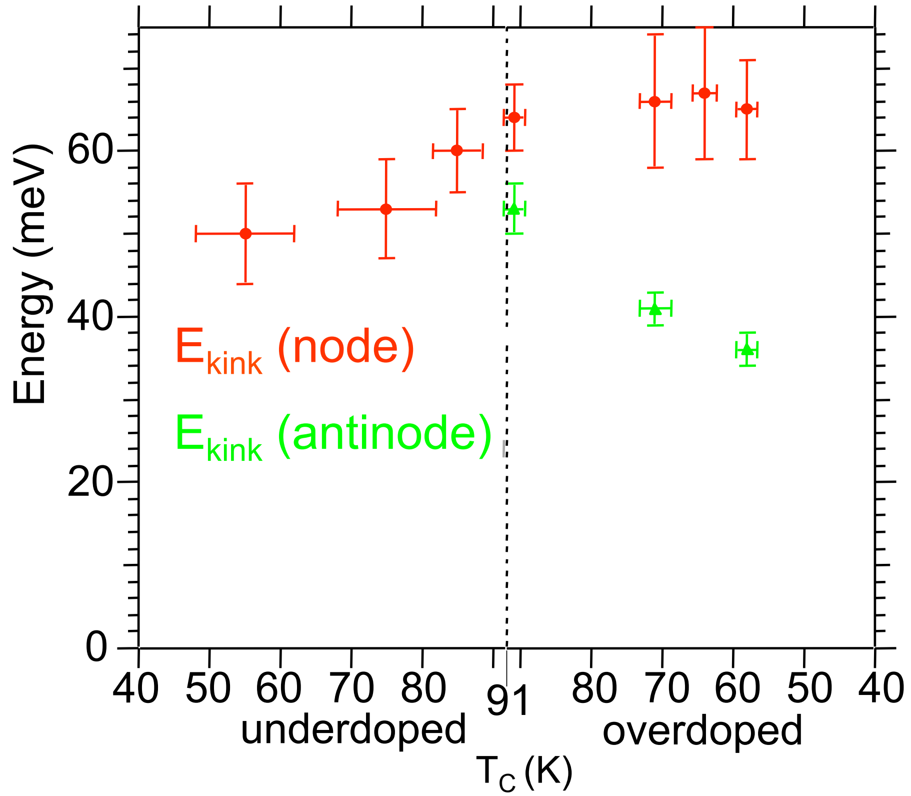


A.D. Gromko, D.S.D. et al. Phys. Rev. B **68**, 174520 (2003).

k-dependence of the kink near (π,0) T_c=71K OD Bi2212



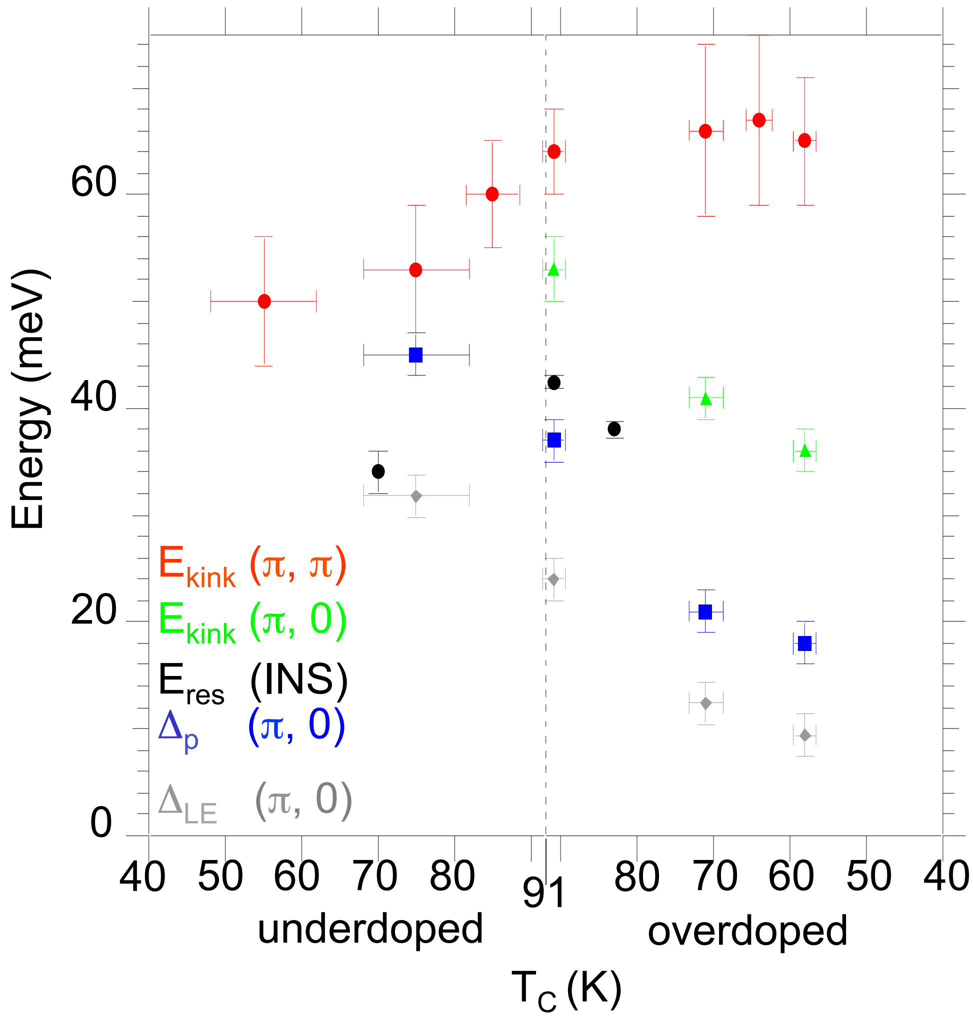
Doping dependence of kink energies (Bi2212)



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

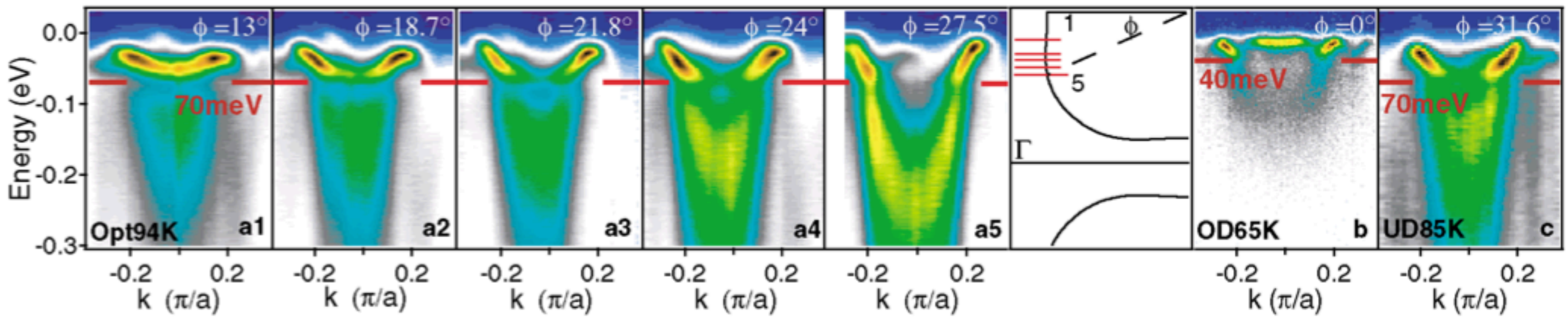
- Nodal and Antinodal kinks have different energy scales, different k-dependence, different T dependences ==> different phenomena.

Energy Scale summary - kinks, gaps, and magnetic resonance
Doping study



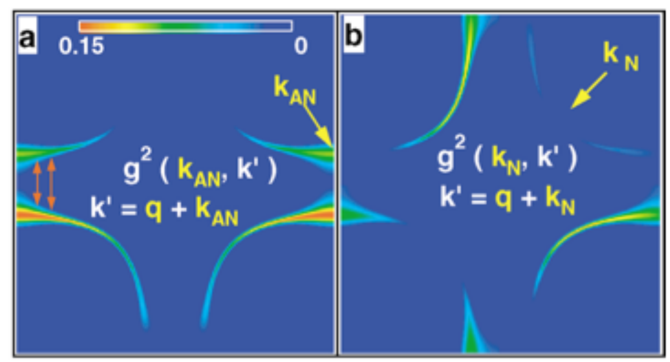
- (π,π) and (π,0) kinks have different energy scales, different k-dependence, different T dependences ==> different phenomena
- Naive picture - $E_{kink}=E_{res}+\Delta_p$ ==> E_{kink} lower than expected. $E_{res}+\Delta_{LE}$ closer.

Other studies on the (π,0) kink



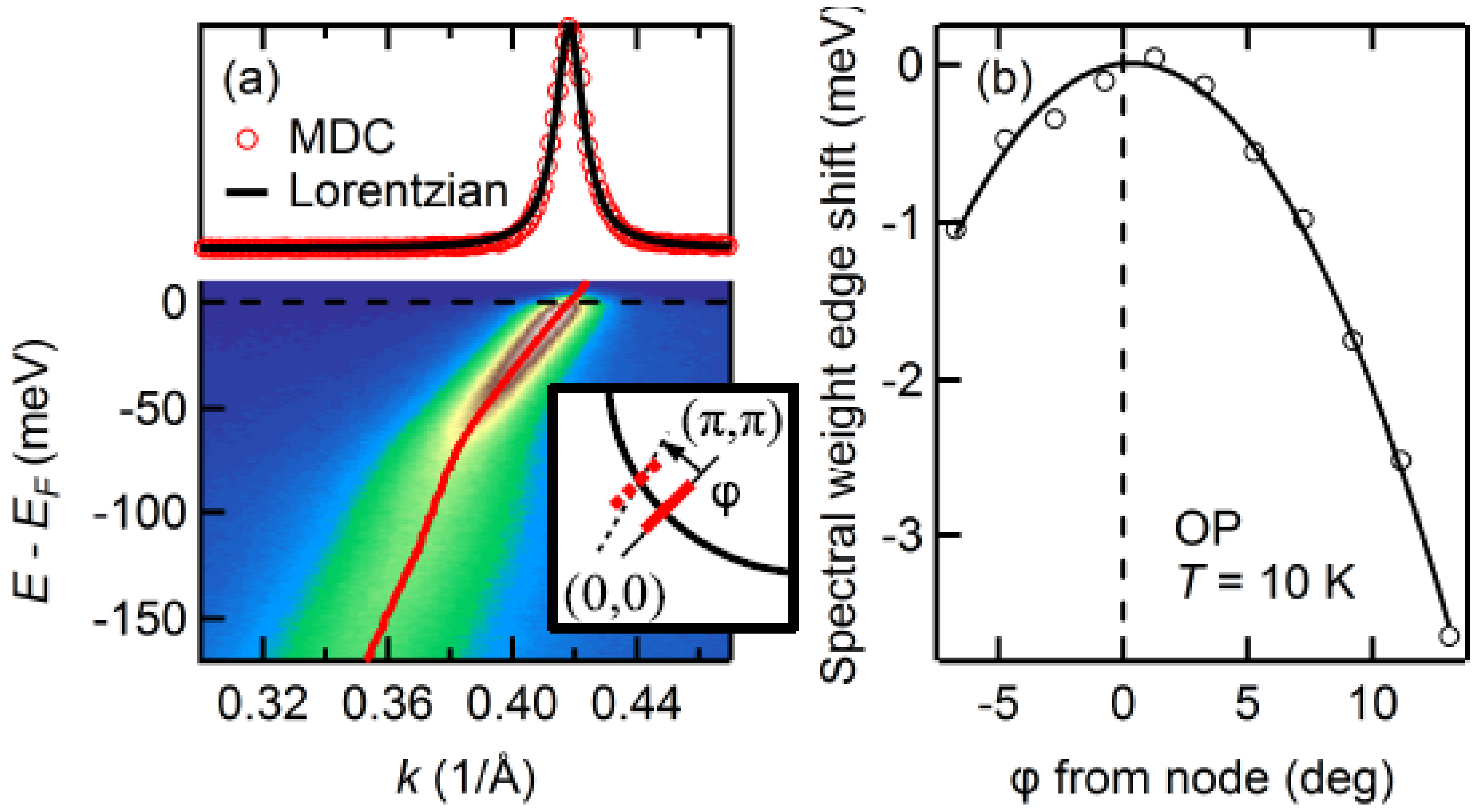
Calculation of $g^2(k,k')$
(electron-phonon vertex)

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



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

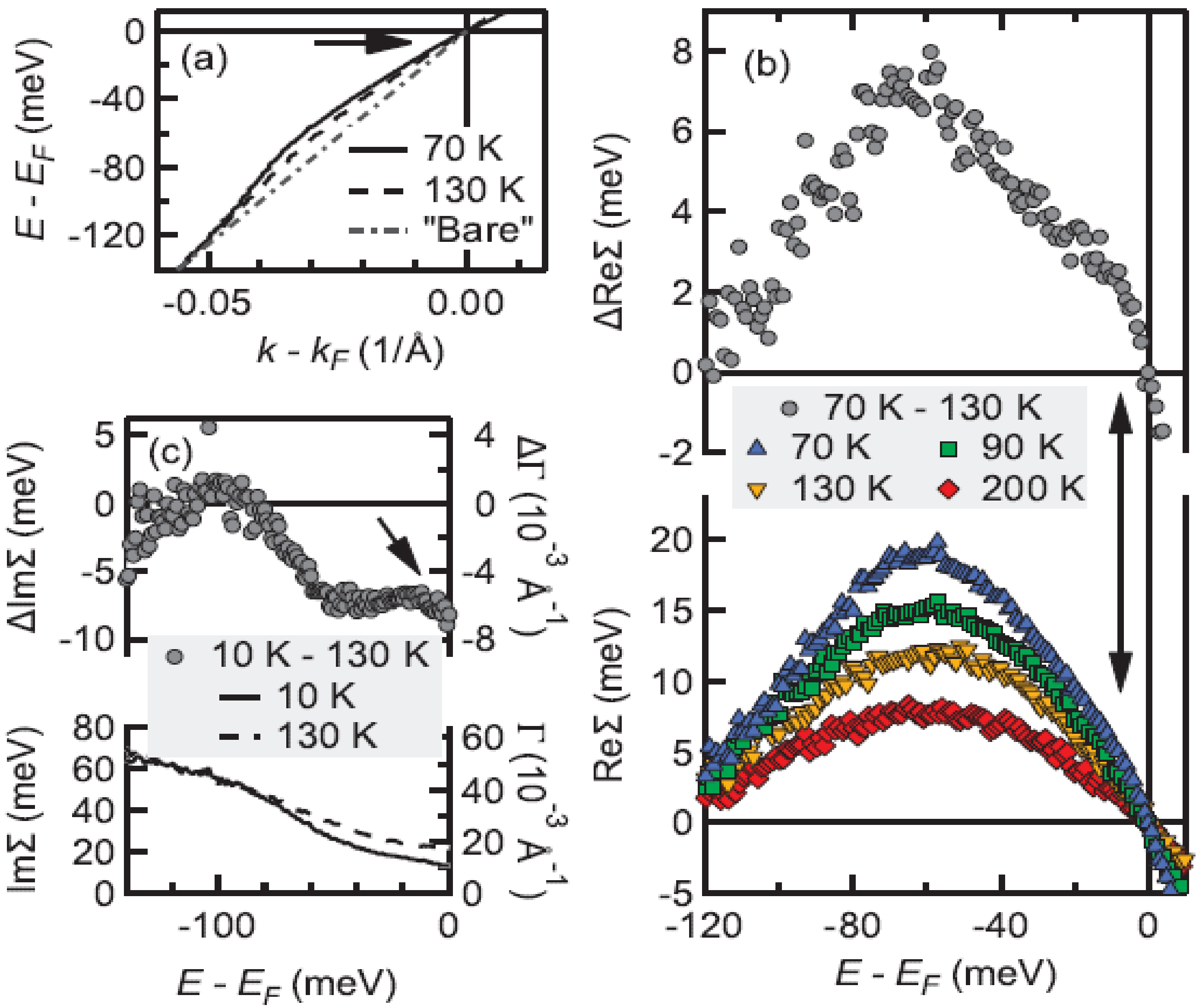
A very low energy (~ 10 meV scale) kink along the nodal direction.



Kink is not visible in this energy window of the data.

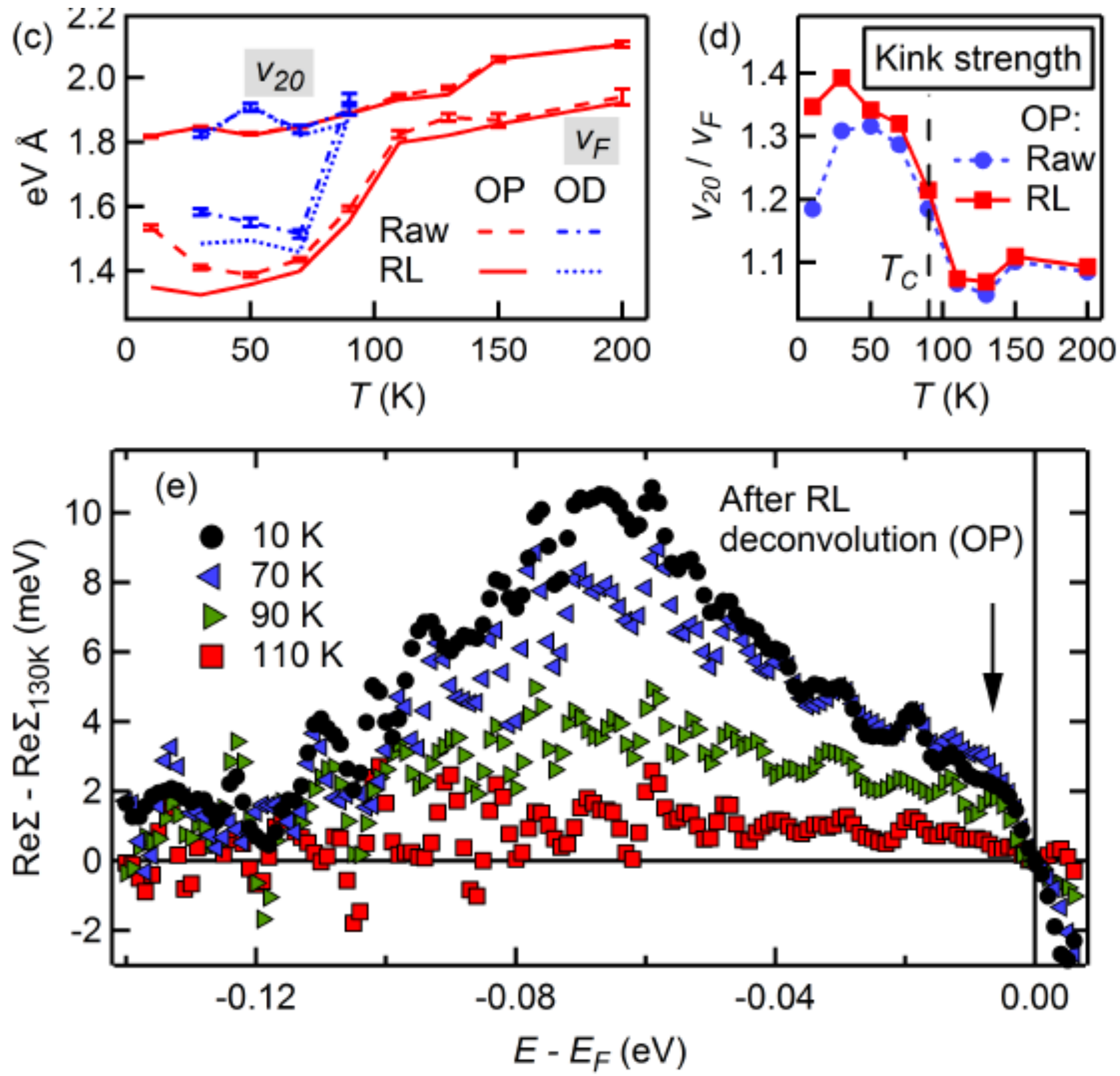
N.C. Plumb, D.S.D. PRL (2010)

T-dependent effect in ReΣ and ImΣ

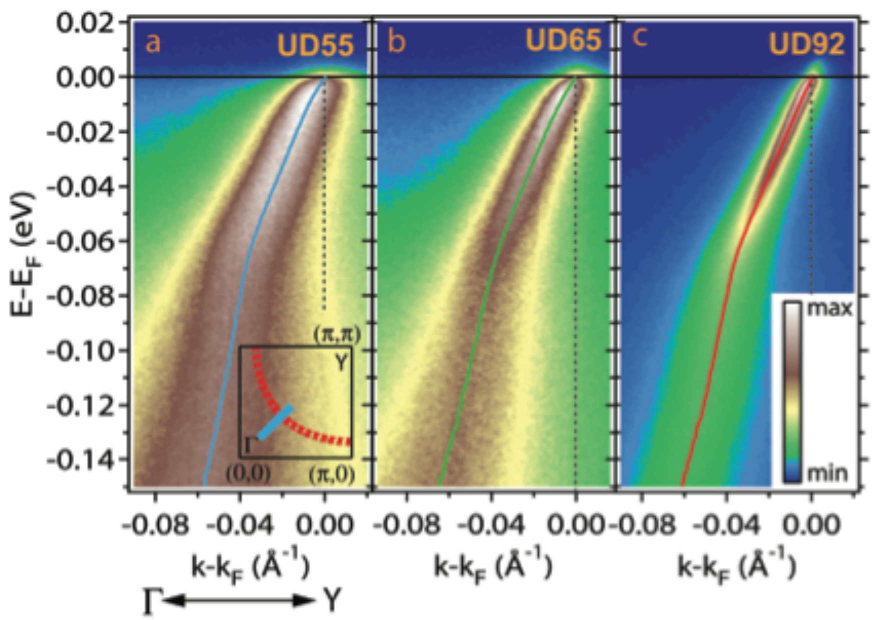


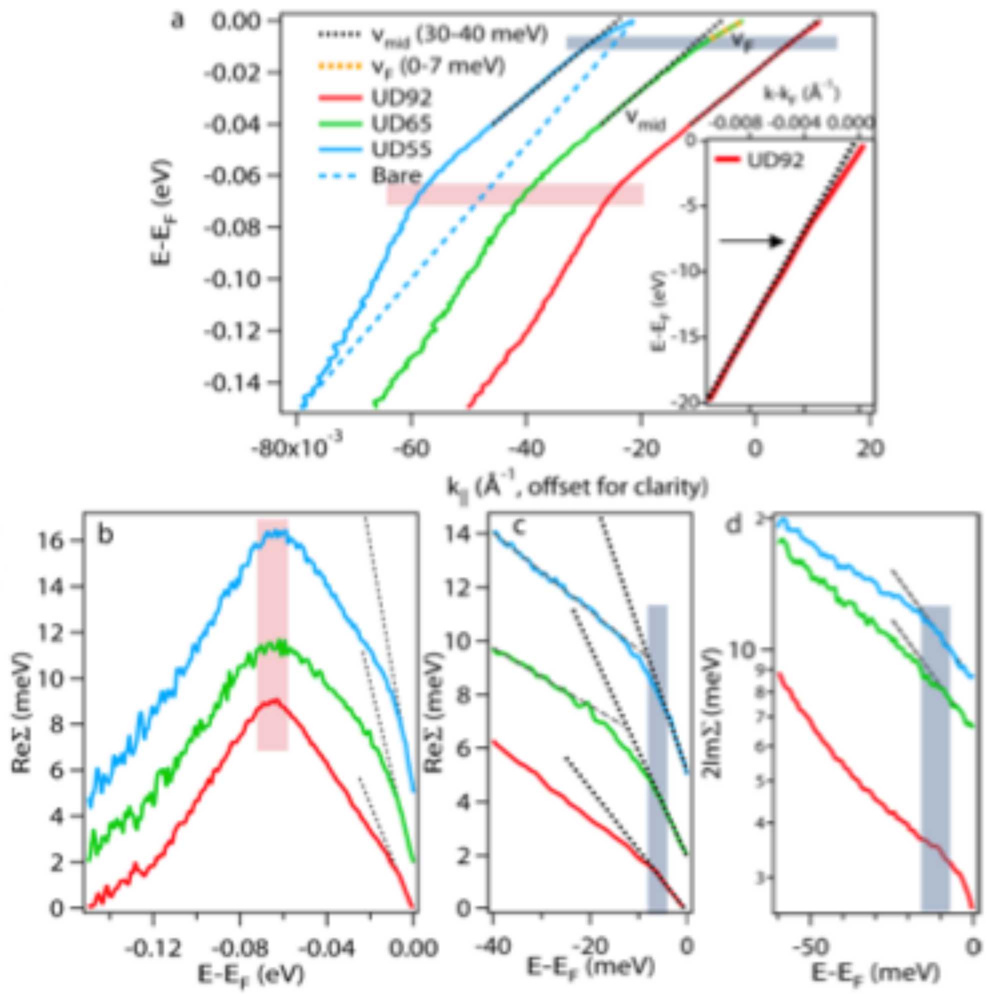
N.C. Plumb, D.S.D. PRL (2010)

Kink turns on at T_c (effect on v_F). v_{20} has no anomaly at T_c



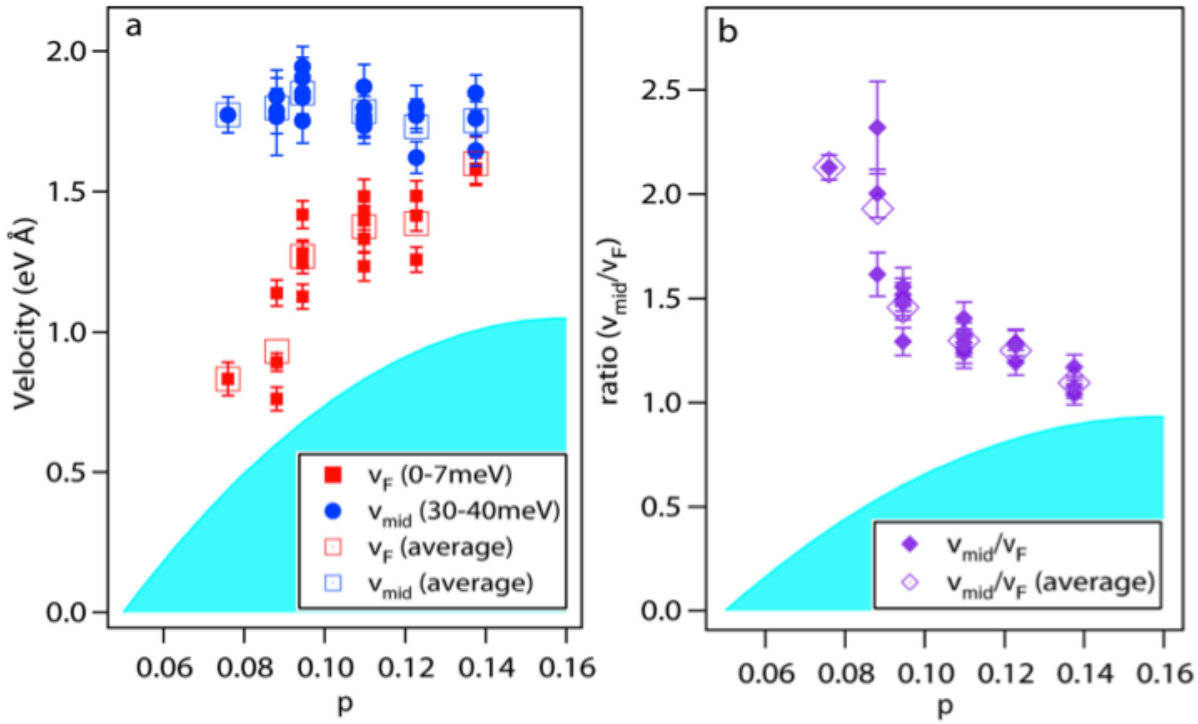
Doping dependence of the low energy (< 10 meV) kink





Vishik, Shen 2010

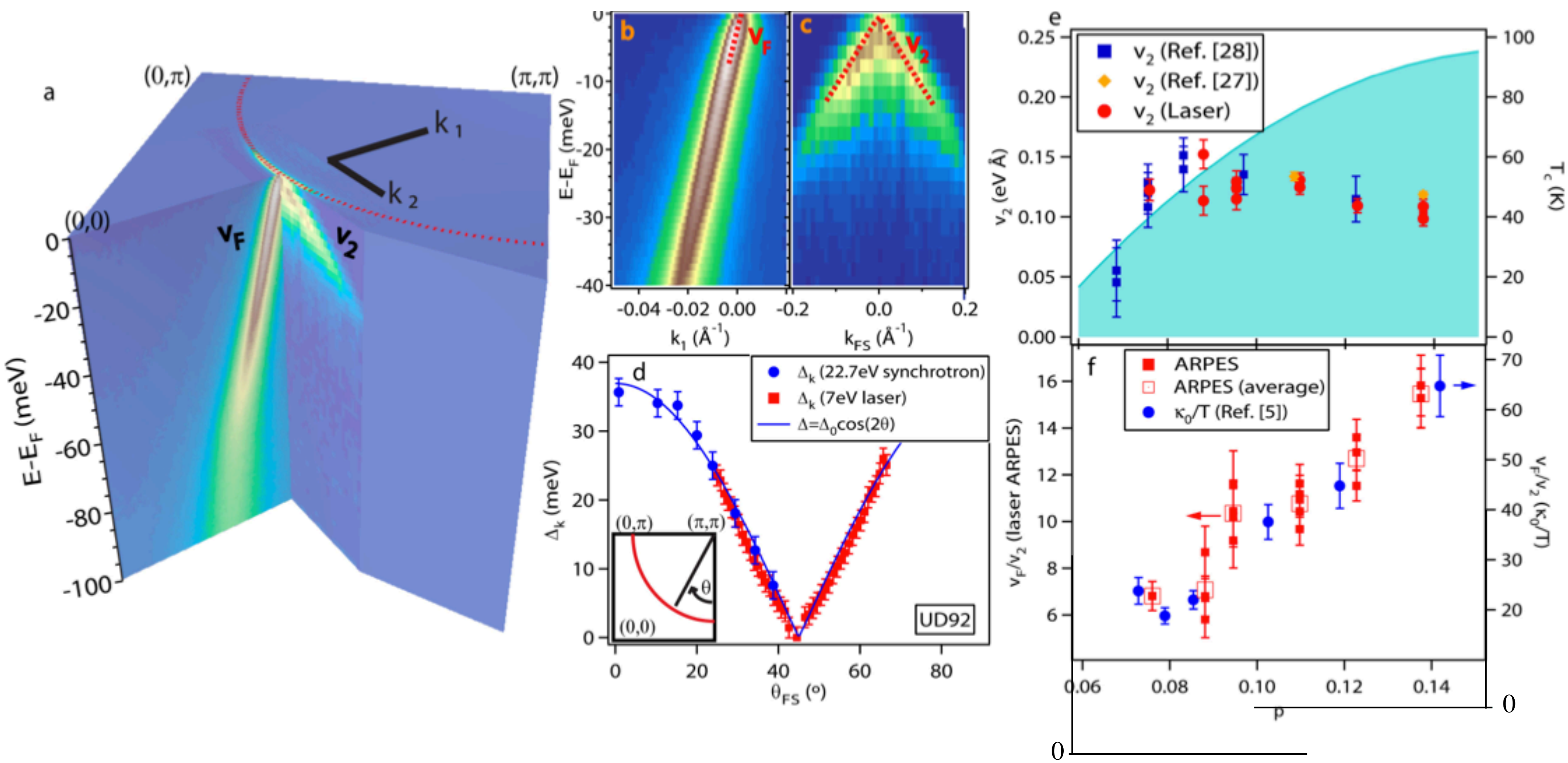
Doping dependence of the low energy (< 10 meV) kink



Low E kink stronger for UD samples.

Vishik, Shen 2010

Knowledge of low energy v_F allows connection to thermal conductivity

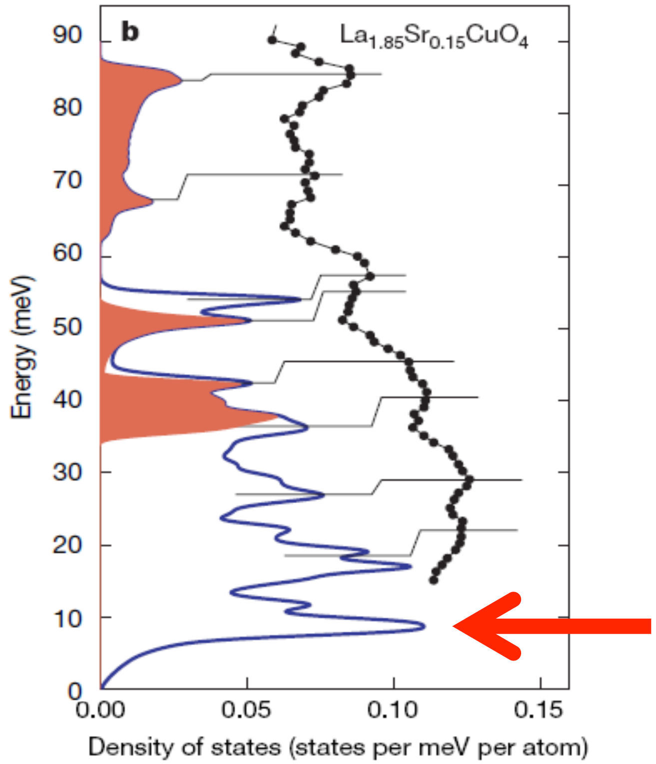


Thermal conductivity

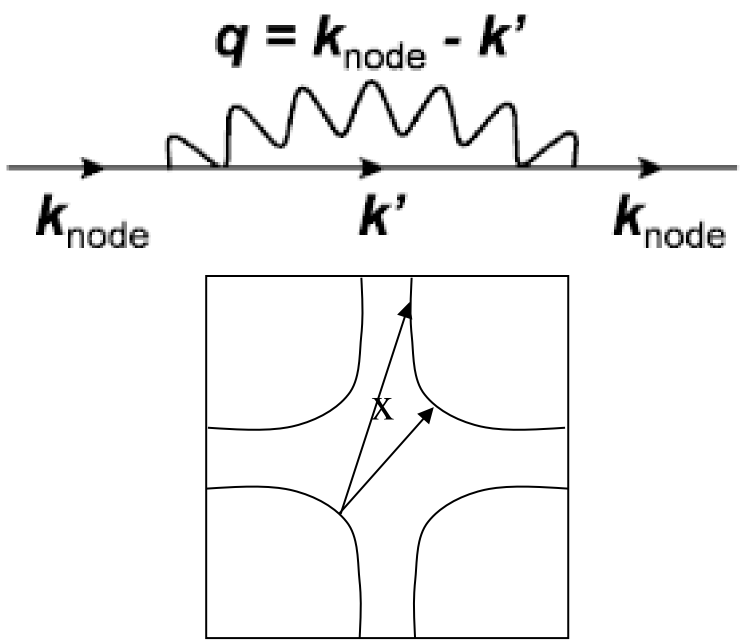
$$\kappa_0/T = \frac{k_B^2}{3\hbar}\frac{n}{d}\left[\frac{v_F}{v_2} + \frac{v_2}{v_F}\right],$$

Vishik, Shen 2010

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)

Chubukov, Eremin (spin-Fermion)

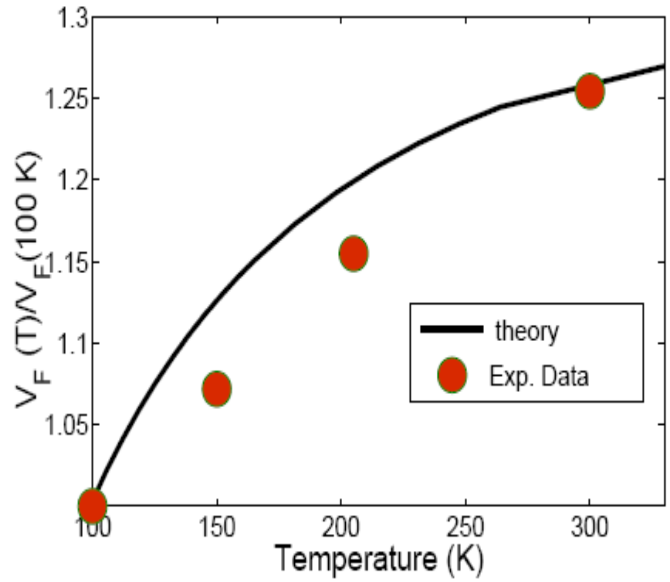
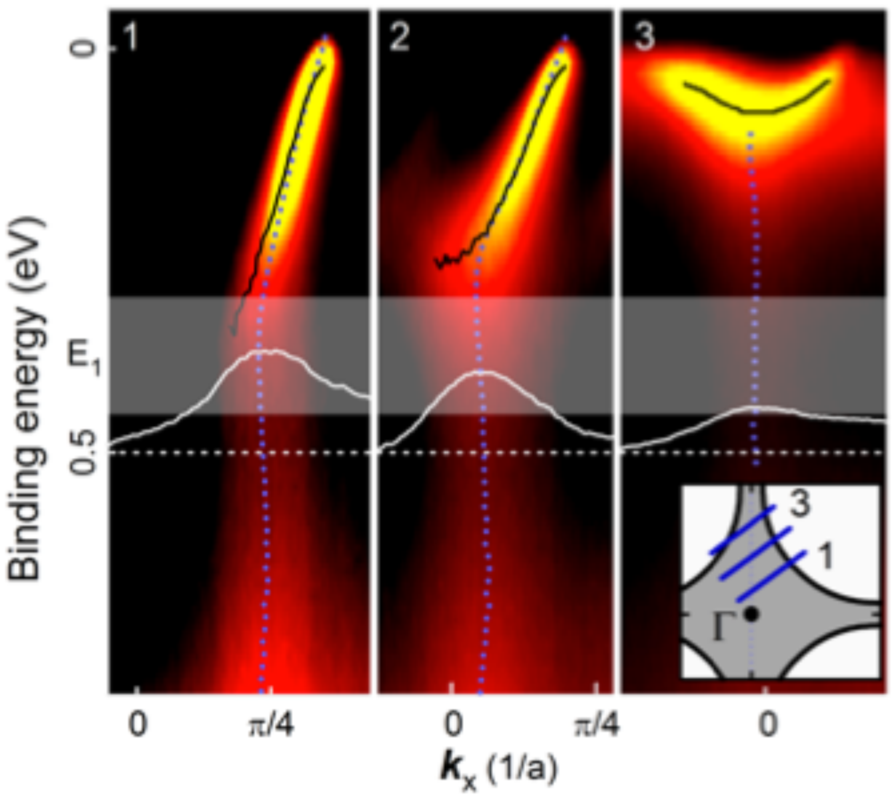


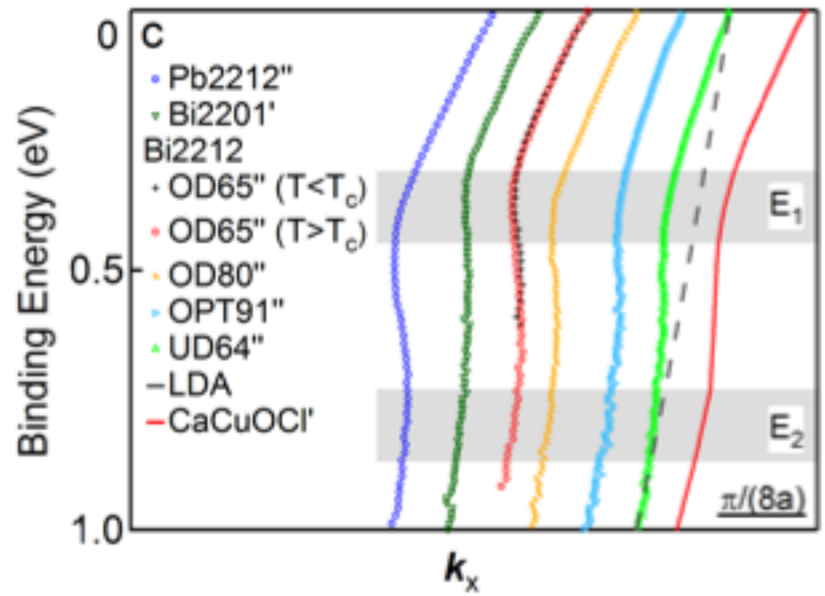
FIG. 1: (color online) Calculated temperature dependence of the nodal Fermi velocity between 100K and 250K. The circles are experimental data from Dessau et al.,

From Σ_2 (usually neglected)

High energy anomaly or kink



MDC-derived dispersion



Graf, Lanzara 2006

A new energy scale (~ 0.3 eV)? Interplay of different energy scales?
An issue of background/scattered weight?

Can discuss this more later.