ARPES studies of cuprates

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Physics 250 (Special topics: spectroscopies of quantum materials)

UC Davis, Fall 2016

Goals of lecture

- Understand why gaps are important and various ways that gap is extracted in ARPES experiments
- Superconducting gap
  - How does one know it is a superconducting gap?
  - Momentum dependence of d-wave superconducting gap
- Pseudogap: enhance understanding of what it is exactly
- Electron-doped cuprates

What kind of gaps are there in condensed matter?

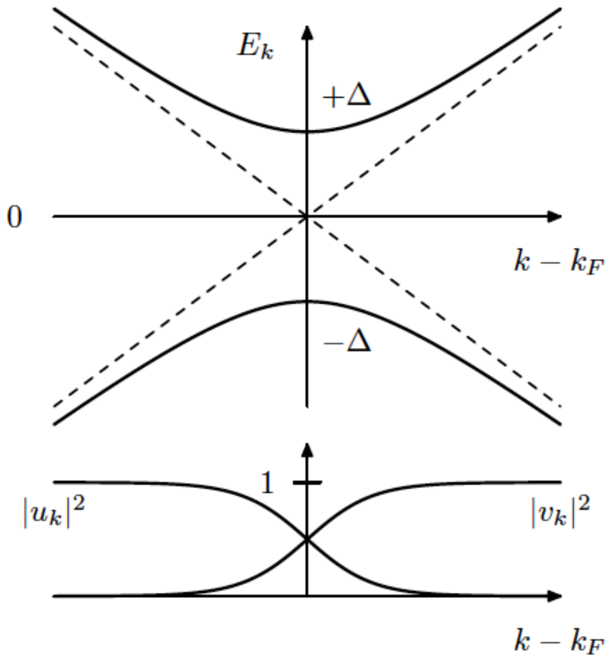
- Band gaps
- CDW gaps
- SDW gaps
- Superconducting gaps
- Hybridization gaps
- Pseudogaps

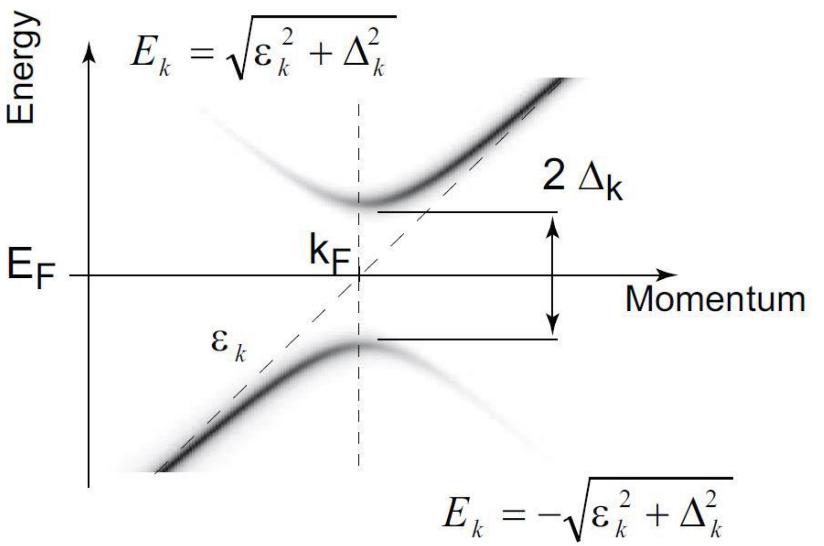
Why is it important to measure gaps?

Bogoliubov quasiparticles

$$\begin{pmatrix} \epsilon_{\mathbf{k}} - \epsilon_F & \Delta \\ \Delta^* & -(\epsilon_{\mathbf{k}} - \epsilon_F) \end{pmatrix} \begin{pmatrix} u_{\mathbf{k}} \\ v_{\mathbf{k}} \end{pmatrix} = E_{\mathbf{k}} \begin{pmatrix} u_{\mathbf{k}} \\ v_{\mathbf{k}} \end{pmatrix}$$

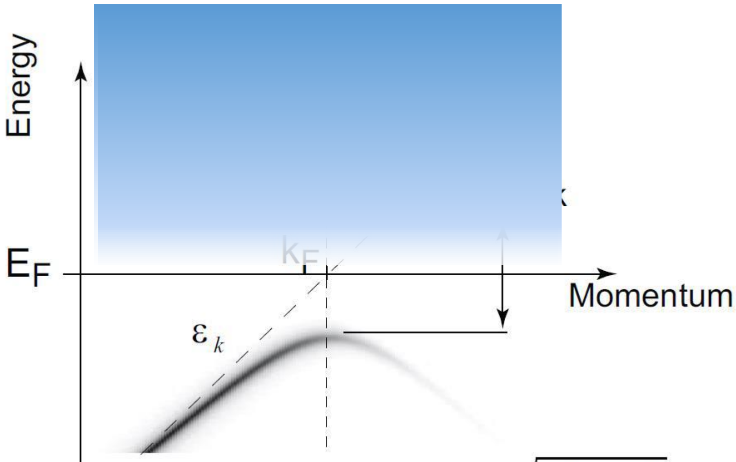
Solutions to the matrix equation are simple.



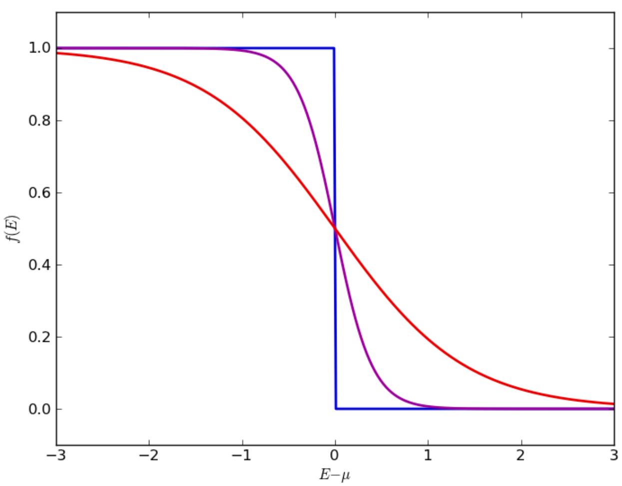


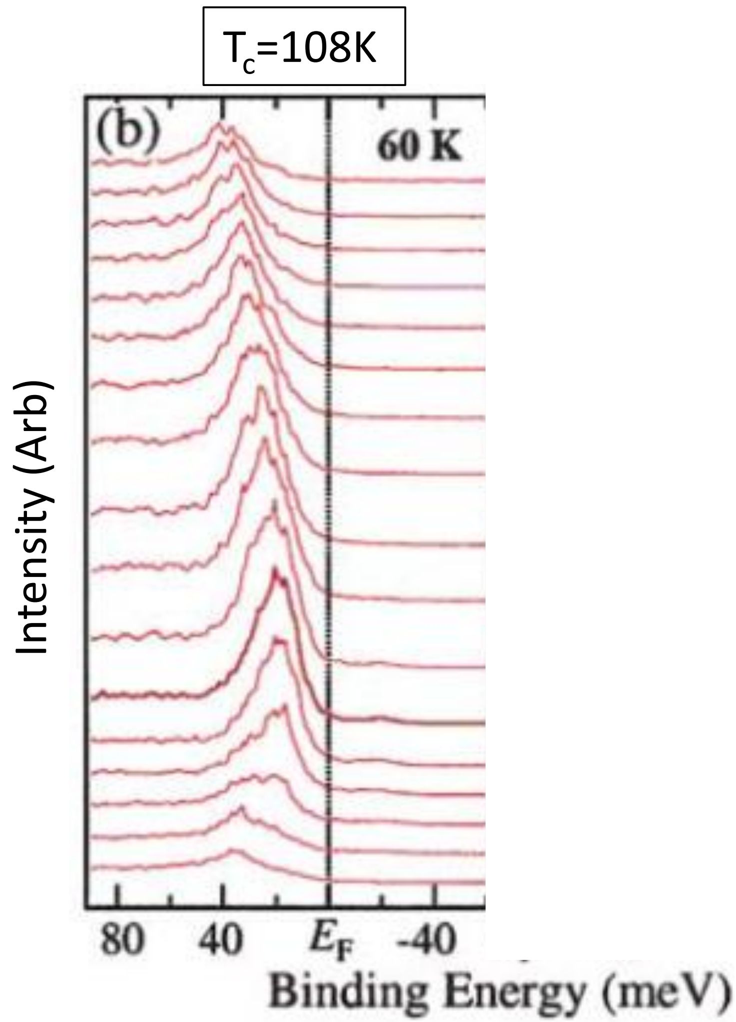
At k_F: $|u_k|^2 = |v_k|^2$.
Superposition of hole and electron states, with probabilities $|u_k|^2$ and $|v_k|^2$.

Observing Bogoliubov quasiparticles in ARPES



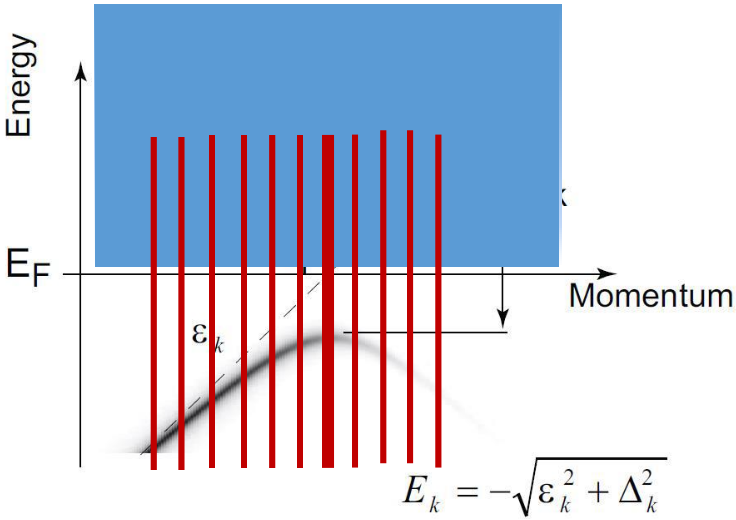
$$E_k = -\sqrt{\varepsilon_k^2 + \Delta_k^2}$$





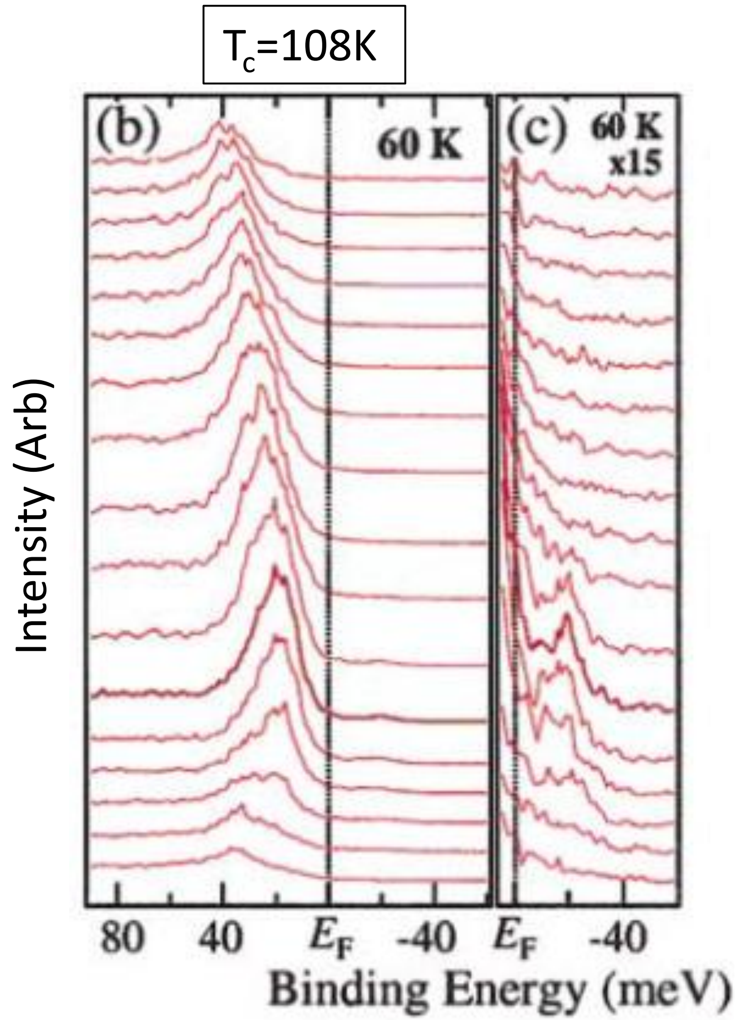
Matsui *et al.* PRL **90** (2003)

Observing Bogoliubov quasiparticles in ARPES



Energy distribution curves (EDCs)

- **Intensity** as a function of **binding energy** at **fixed momentum**
- Usual way of studying gaps

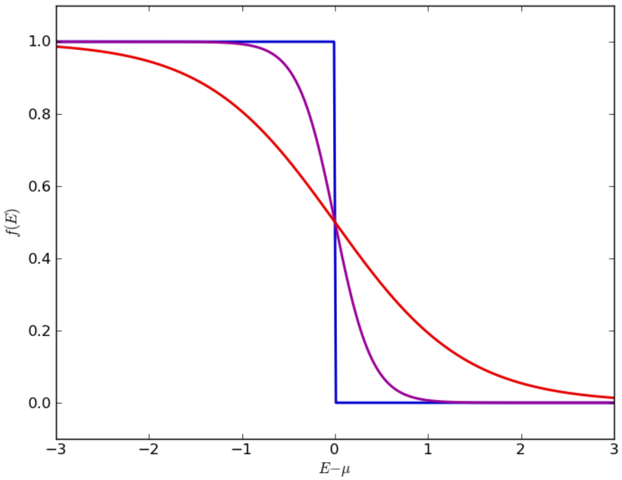


Matsui *et al.* PRL **90** (2003)

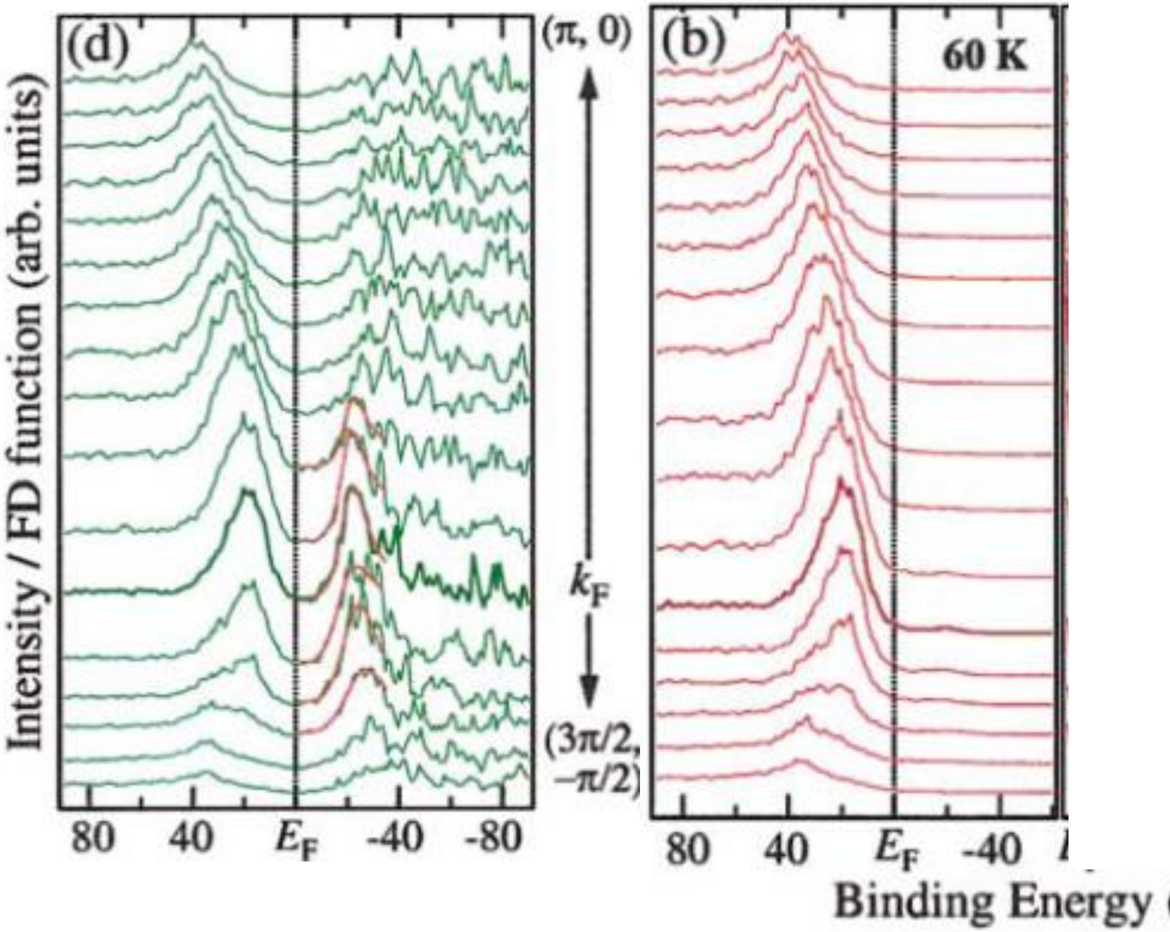
Assessing a gap, step 1: remove Fermi-Dirac cutoff

How?

- One way: divide spectrum by Fermi-Dirac function, convolved with instrument energy resolution
- Necessary if gap edge is sufficiently close to E_F

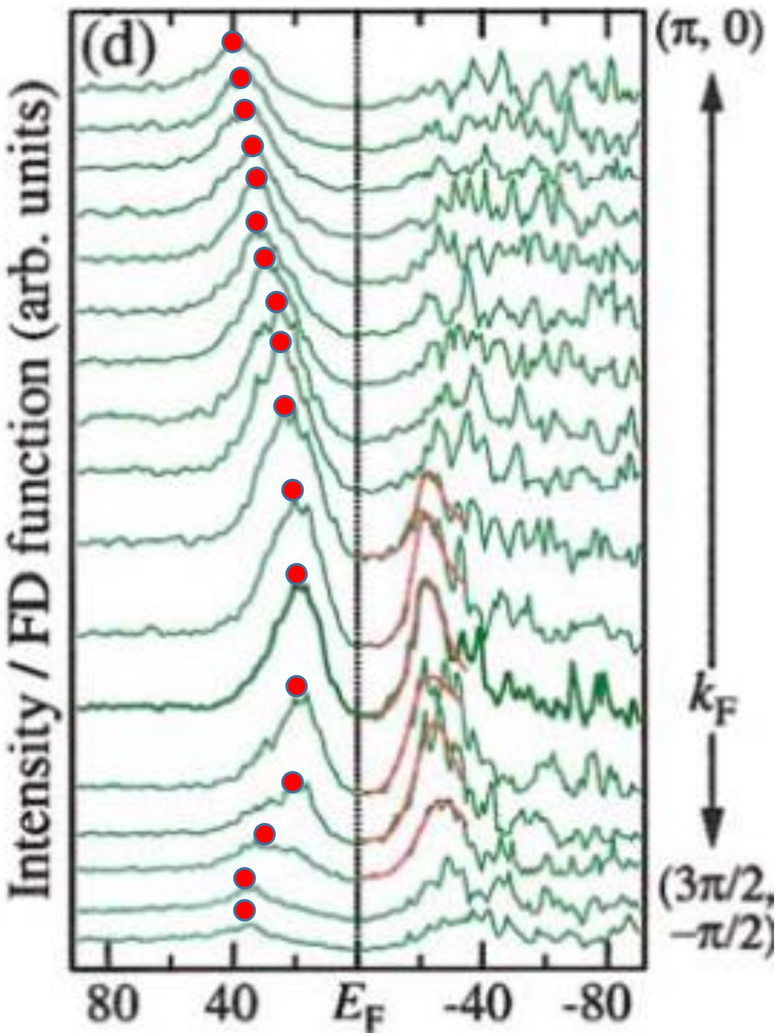


T_c=108K



Matsui *et al.* PRL **90** (2003)

Assessing a gap, step 2: quantify gap

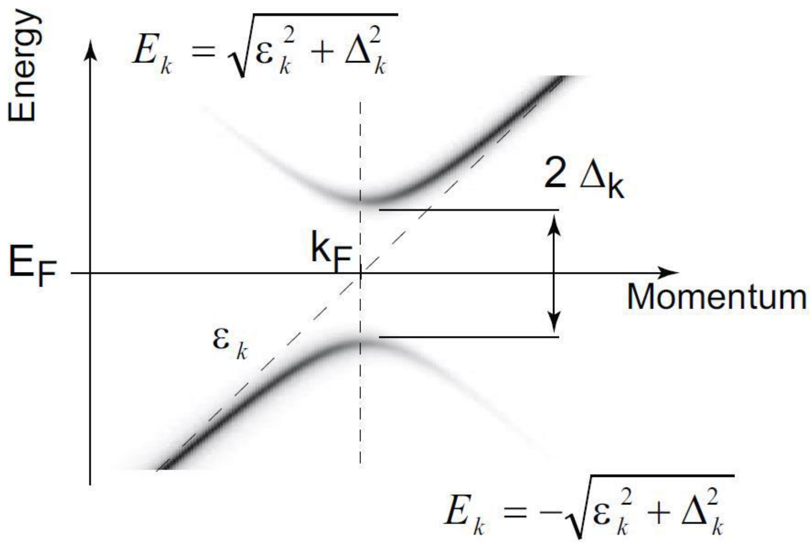


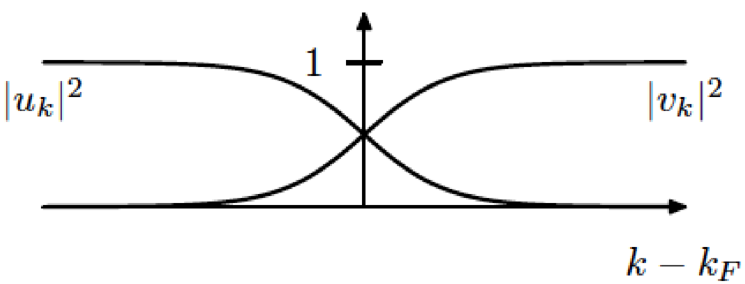
Matsui *et al.* PRL **90** (2003)

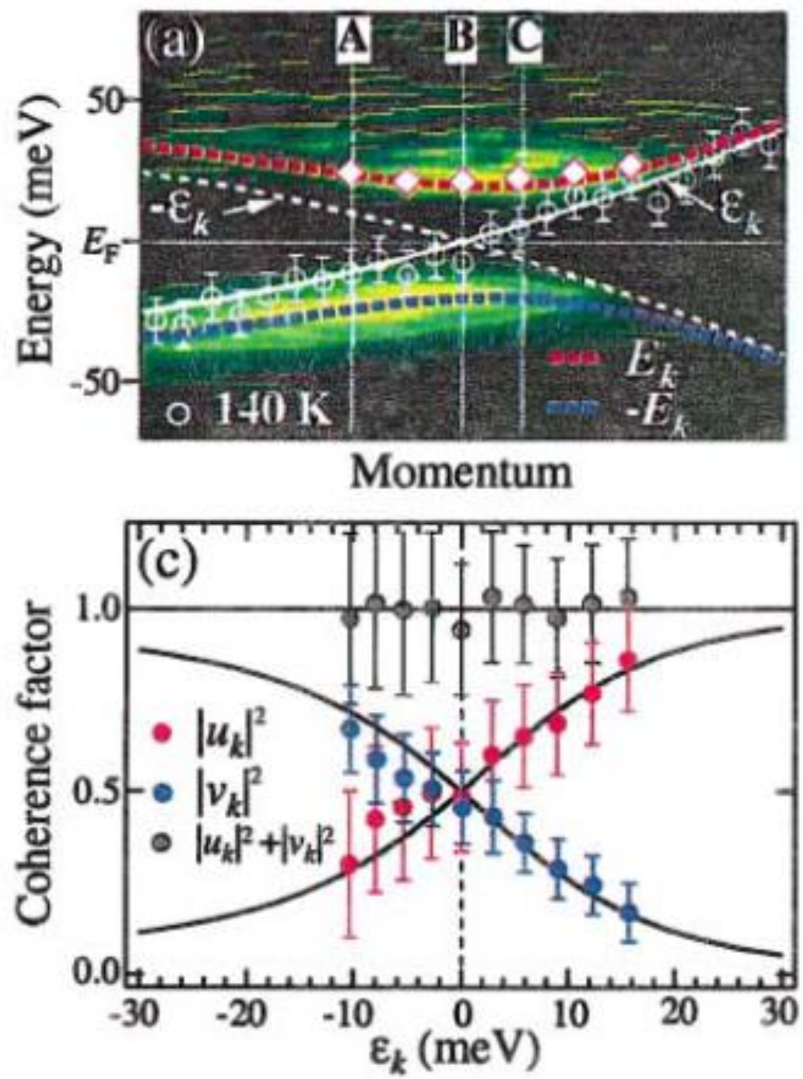
In this paper, $\Delta(k)$ along the cut was quantified by fitting to two lorentzians

- Peak position→Δ
- Peak intensity→$|u_k|^2, |v_k|^2$

Comparison to BCS theory





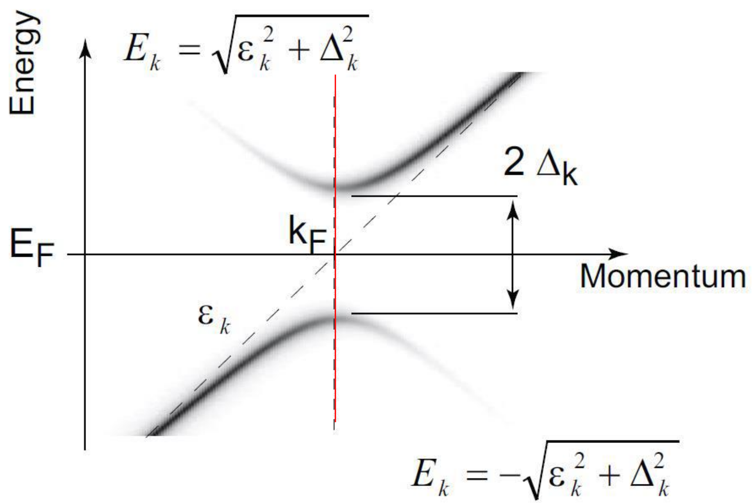


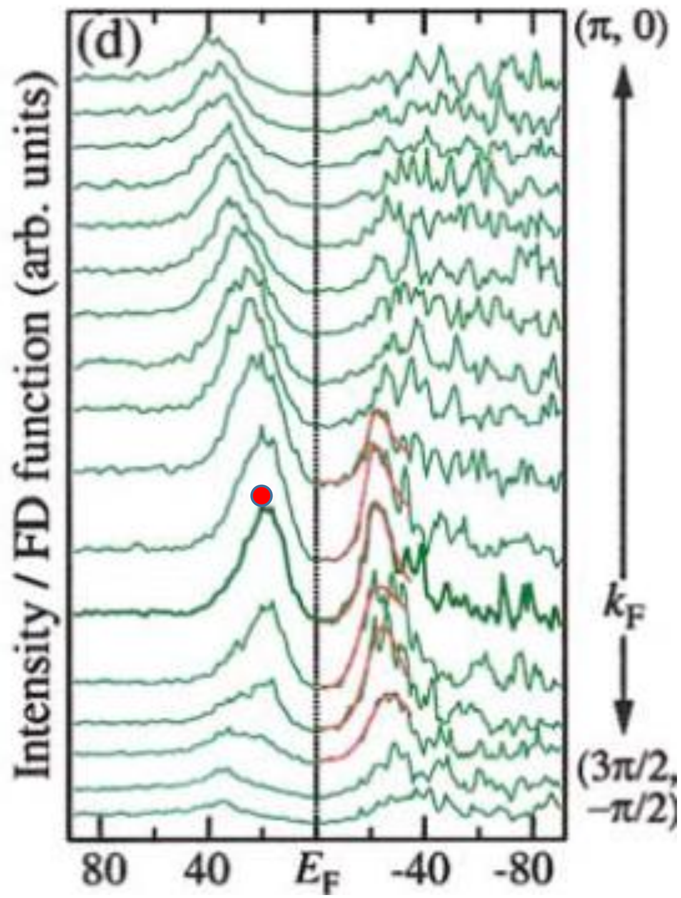
What correspondences between theory and experiment are there?

Matsui *et al.* PRL **90** (2003)

Mini-conclusions

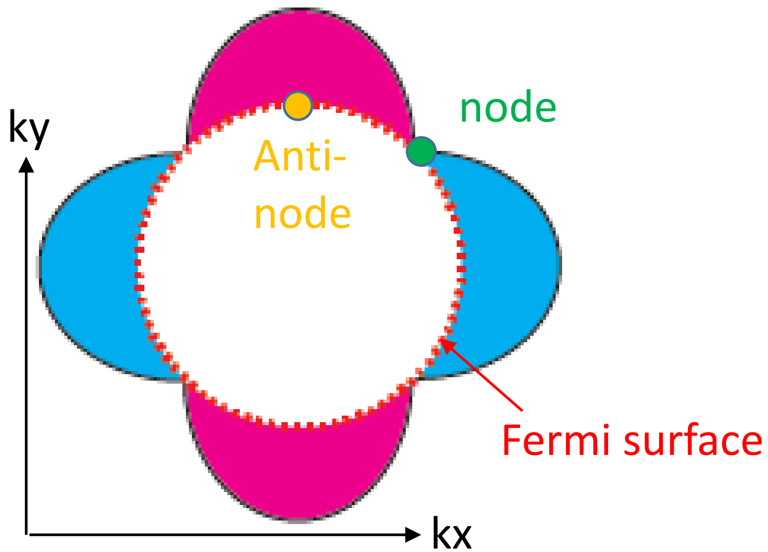
- In superconducting state of cuprates **quasiparticles** appear to follow the same phenomenology as in BCS superconductors
- Superconducting gap can be quantified by
  - Dividing out Fermi-Dirac function
  - Finding k_F
  - Measuring energy position of quasiparticle peak





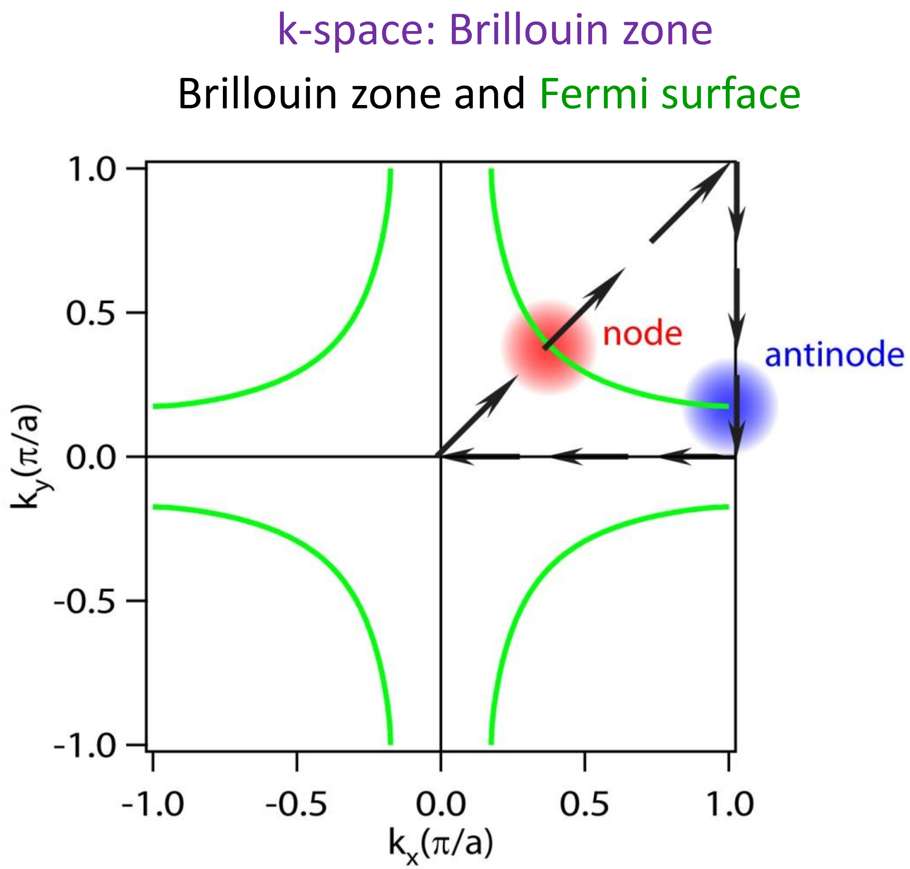
Superconducting gap is defined at k_F, so most papers only show EDCs at k_F

Cuprates have $d_{x^2-y^2}$ pairing symmetry



- Cuprate superconducting gap is anisotropic in momentum space
- ARPES is a momentum-resolved spectroscopic tool

Detour/disclaimer: fermi surface

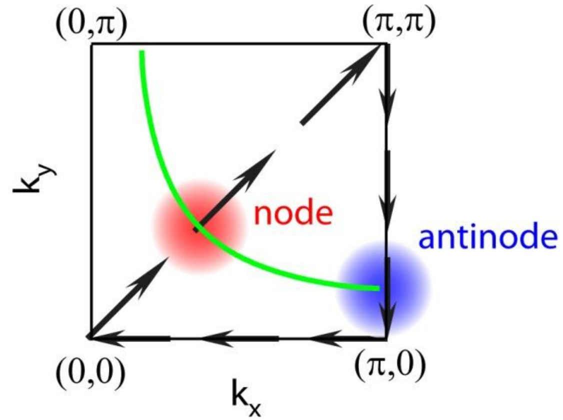


Discussion of superconducting gap and pseudogap assumes a locus in momentum space, similar to a Fermi surface, even if Fermi liquid theory may not be applicable

Detour/disclaimer: fermi surface

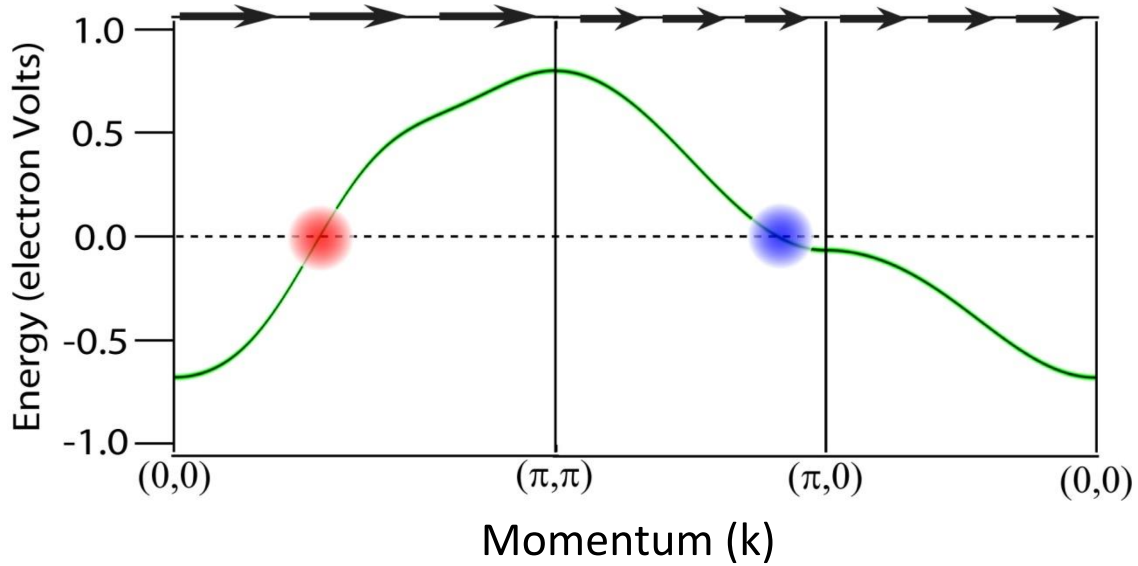
k-space: Brillouin zone

Brillouin zone and Fermi surface

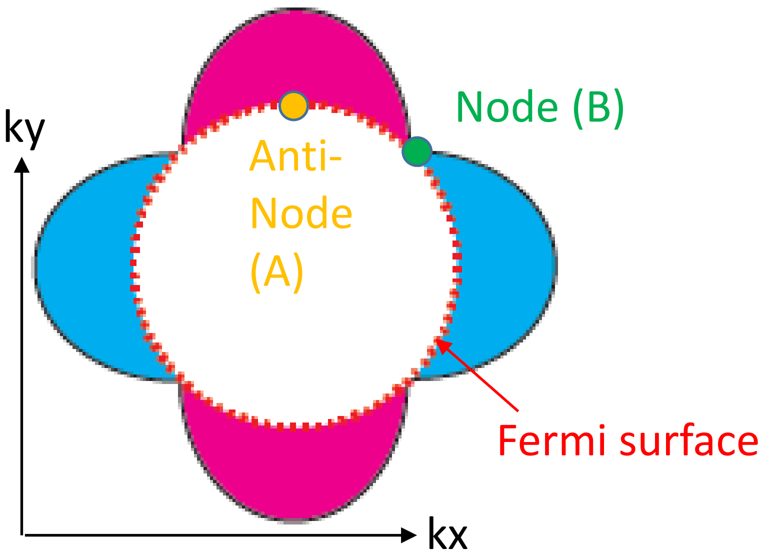


Discussion of superconducting gap and pseudogap assumes a locus in momentum space, similar to a Fermi surface, even if Fermi liquid theory may not be applicable

Band structure

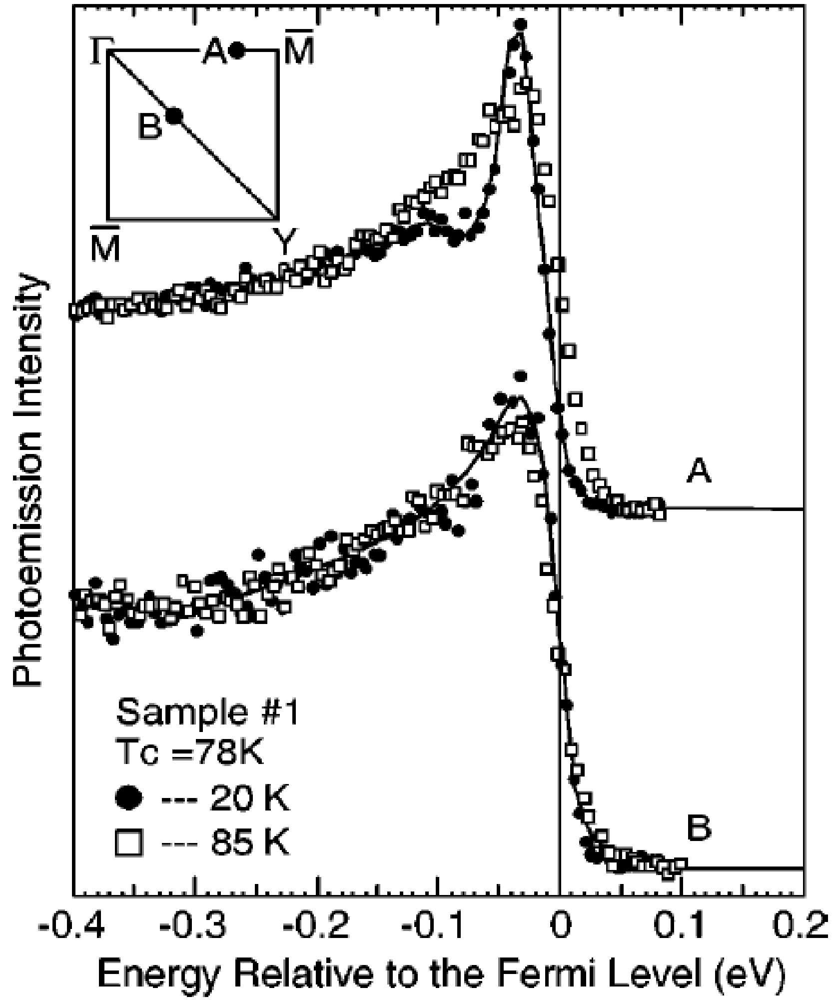


Cuprates have $d_{x^2-y^2}$ pairing symmetry



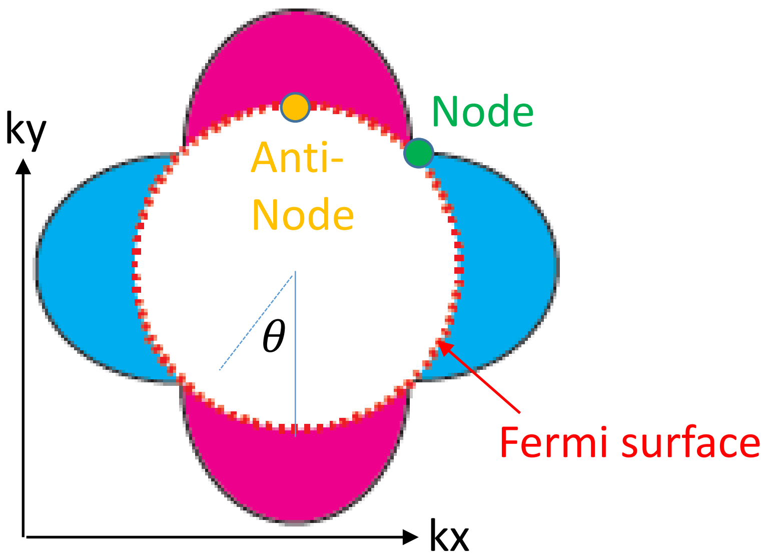
What is the evidence for a $d_{x^2-y^2}$ gap?

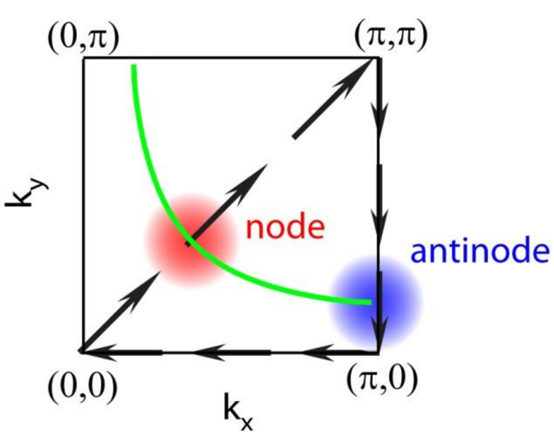
- Going across Tc: Leading-edge shift at momentum where antinode should be, none where node should be
- Spectral weight redistribution at antinode



Shen *et al.* PRL **70** (1993)

Momentum dependence of superconducting gap





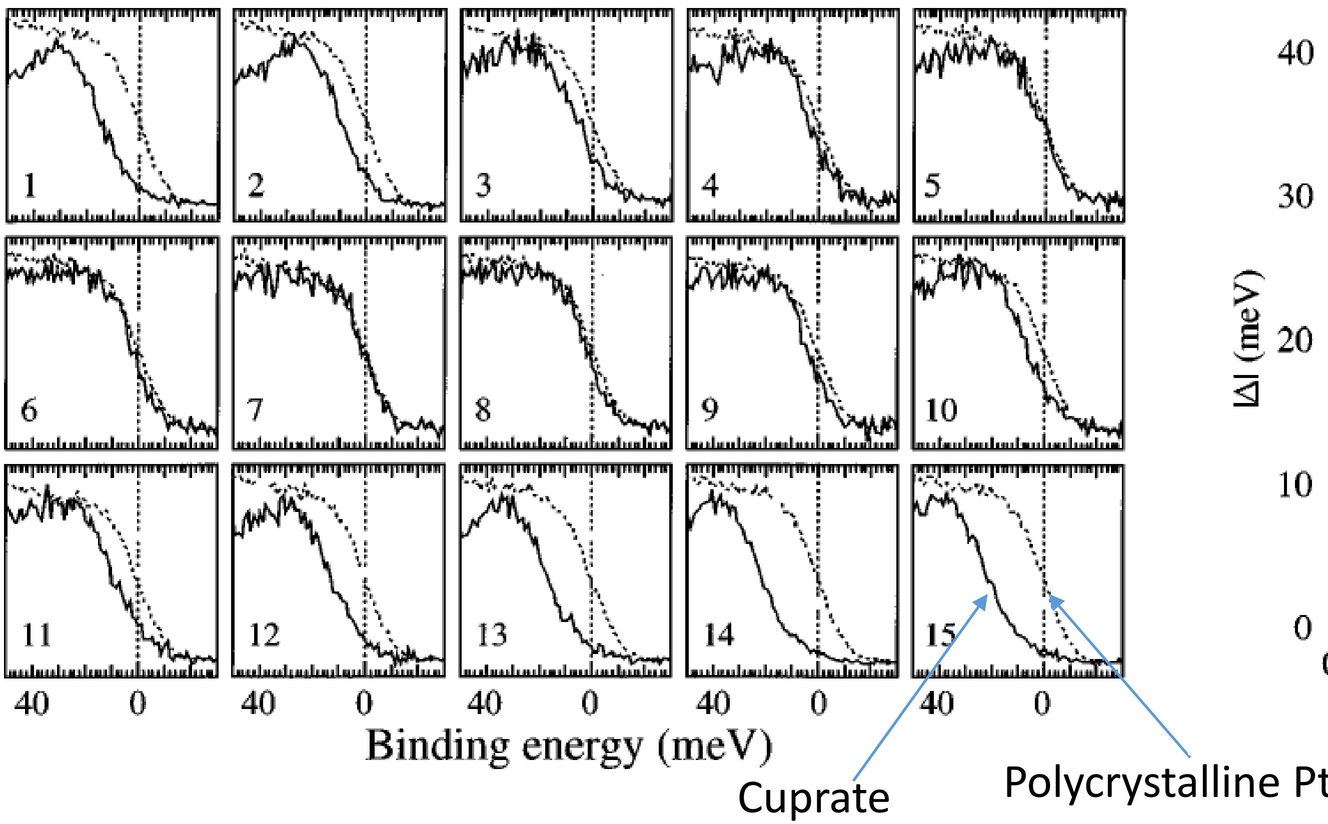
$d_{x^2-y^2}$ superconducting gap on tetragonal lattice (to leading order):

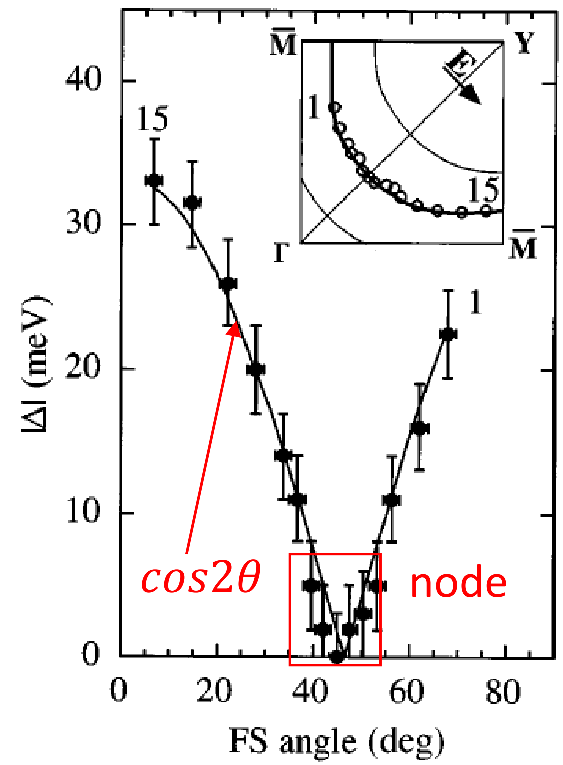
$$\Delta(k_x, k_y) = \frac{\Delta_0}{2}[cosk_x - cosk_y]$$

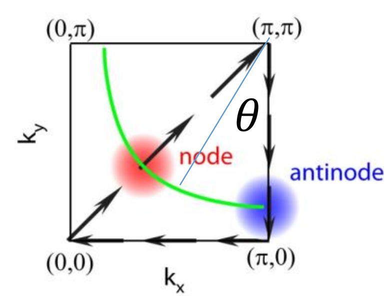
$$|\Delta(k_x, k_y)| = \frac{\Delta_0}{2}|cosk_x - cosk_y|$$

$$\Delta(\theta) = \Delta_0 cos2\theta$$

Momentum dependence of superconducting gap







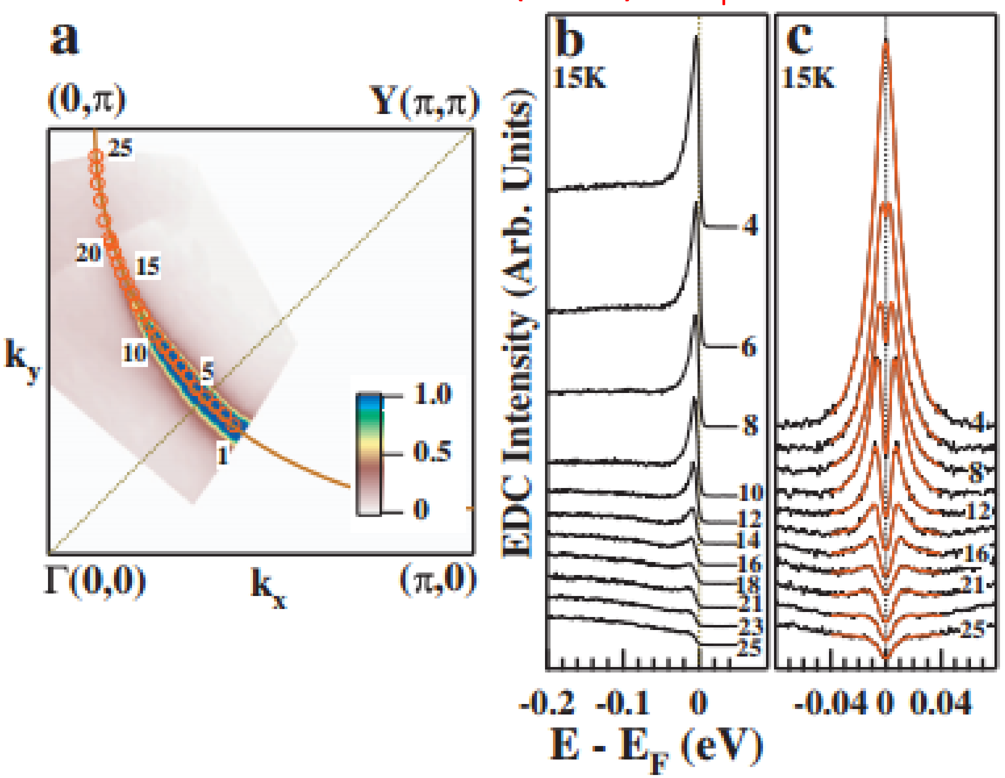
- Gap at each momentum determined from **leading edge midpoint** (distance between inflection point or ½ height and E_F)
- E_F determined from polycrystalline metal

H. Ding *et al,* PRB **54** (1996)

Momentum dependence of superconducting gap

Raw Energy distribution curves (EDCs) at k_F

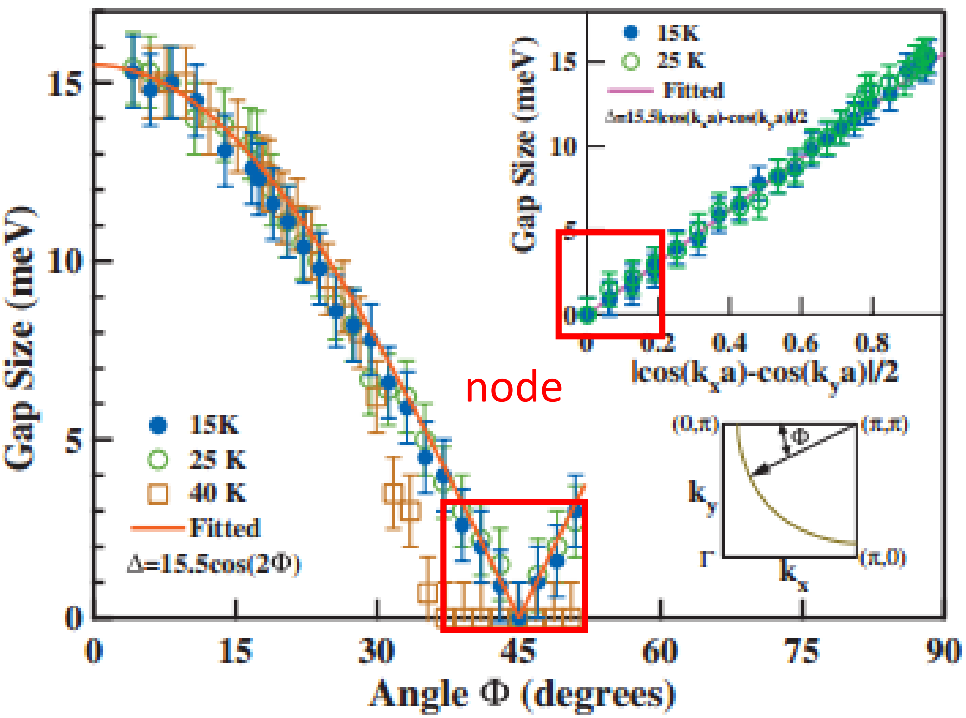
Symmetrized EDCs at k_F with model fitting



Meng *et al,* PRB **79**, 024514 (2009)

- Remove Fermi-Dirac cutoff by **symmetrizing**
  1. Flip EDC about EF: $A(k_F,\omega)f(\omega) \rightarrow A(k_F,-\omega)f(-\omega)$
  2. Add flipped EDC to original EDC: $A_{sym}(k_F,\omega) = A(k_F,\omega)f(\omega) + A(k_F,-\omega)f(-\omega)$
  3. This removes FD cutoff if there is particle-hole symmetry ($A(k,\omega) = A(k,-\omega)$), which is true at k_F for a SC
  4. Visualization tool: single peak=no gap, double peak=gap
- Extract superconducting gap at each Fermi surface point by fitting to a phenomenological model (Norman *et al*, Phys. Rev. B 57, R11093 (1998))

Momentum dependence of superconducting gap



2 ways to parametrize where you are on the Fermi surface:

1. Fermi surface angle (Φ)
   Advantage: intuitive to know where you are on Fermi surface
2. Expression for $d_{x^2-y^2}$ gap to leading order ($\frac{1}{2}|cosk_xa - cosk_ya|$)
   Advantage: easy to see if gap function has higher order terms

Meng *et al,* PRB **79**, 024514 (2009)

Summary, part 1

How do we know if there is a gap in the spectrum?

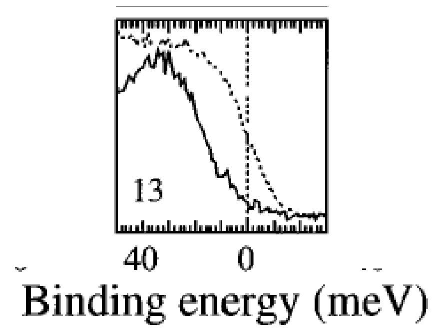
- Leading edge shifts away from Fermi level
- Quasiparticle peak (after accounting for Fermi-Dirac cutoff) is not at $\omega = 0 \; at \; k = k_F$

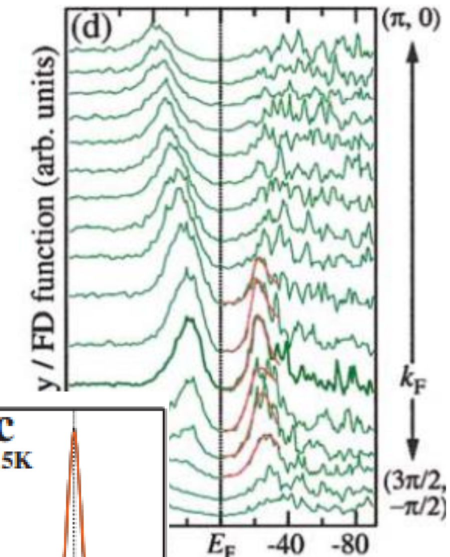
How do we account for/remove Fermi-Dirac cutoff?

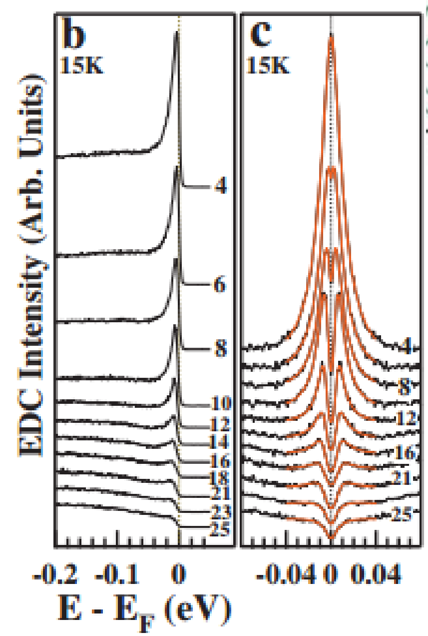
- Divide by Fermi function
- Compare measured spectrum to polycrystalline metal
- Symmetrize

How to we quantify the magnitude of the gap?

- Quasiparticle peak position
- Leading edge midpoint
- Fitting to a model







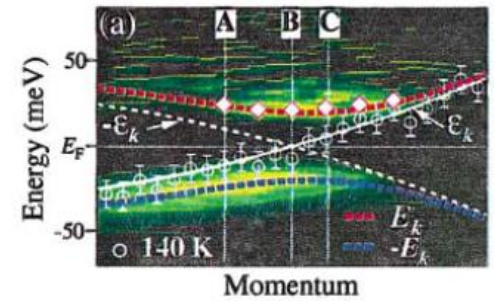
Summary, part 1

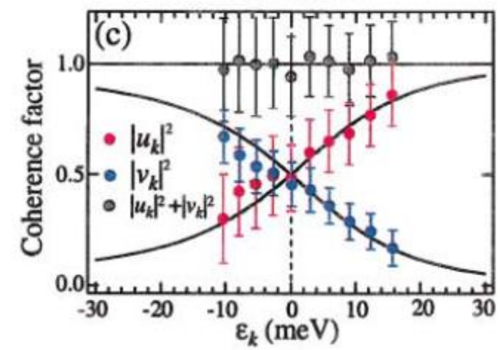
How do we know a gap has superconducting origin?

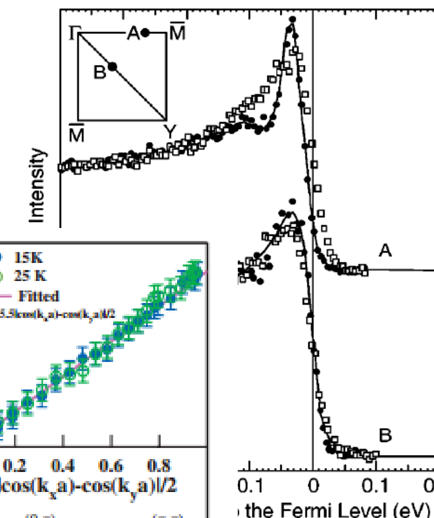
- Onsets at Tc
- Bogoliubov quasiparticle dispersion and spectral weight

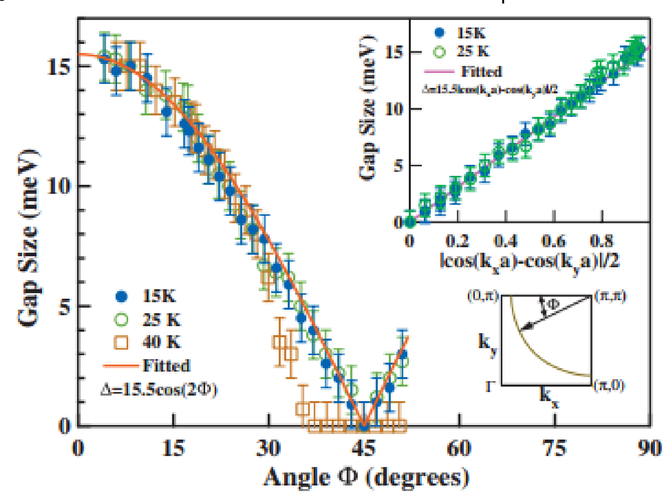
What evidence for $d_{x^2-y^2}$ pairing does ARPES provide?

- Opening of a gap at antinodal momentum but not nodal momentum below Tc
- Momentum dependence of gap magnitude consistent with $d_{x^2-y^2}$ pairing
  - $\Delta(\theta) \propto \cos(2\theta)$
  - $\Delta(\boldsymbol{k}) \propto \frac{1}{2}|cosk_x - cosk_y|$





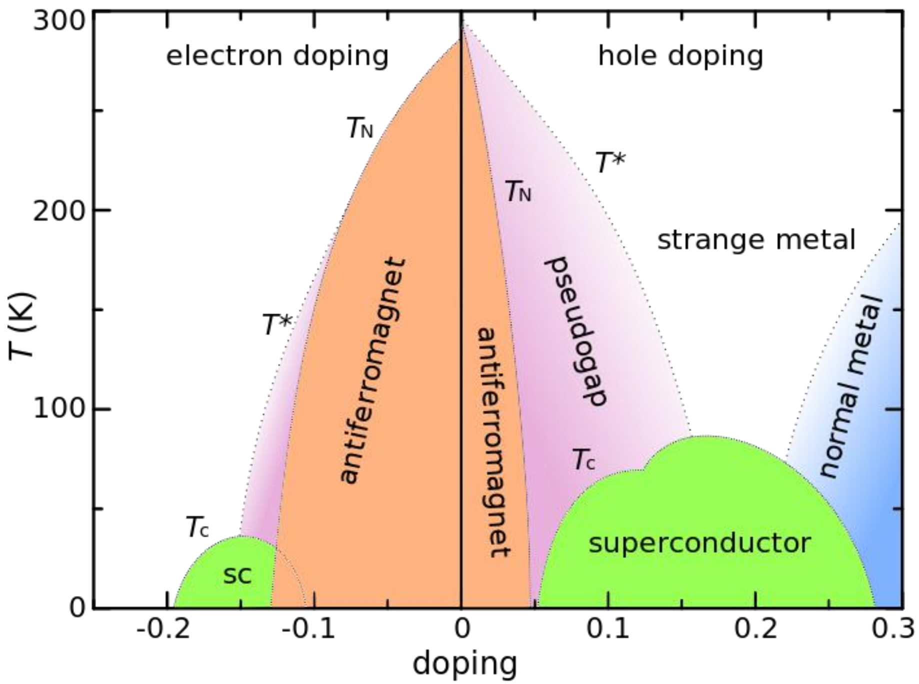




Goals of lecture

- Understand why gaps are important and various ways that gap is extracted in ARPES experiments
- Superconducting gap
  - How does one know it is a superconducting gap?
  - Momentum dependence of d-wave superconducting gap
- Pseudogap: enhance understanding of what it is exactly
- Electron-doped cuprates

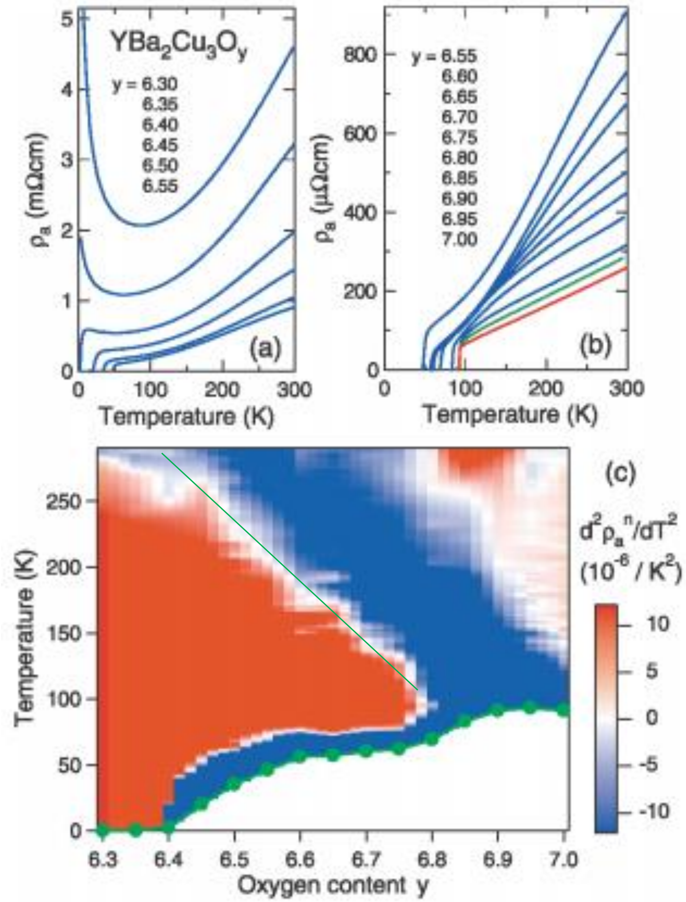
Brief pseudogap review



The pseudogap in **hole-doped** cuprates

- Is the 'normal' state accessed above T_c or in sufficiently high magnetic field
- Onsets at T*, which decreases with increasing doping
- Apparent in almost every experiment which couples to low-energy electrons

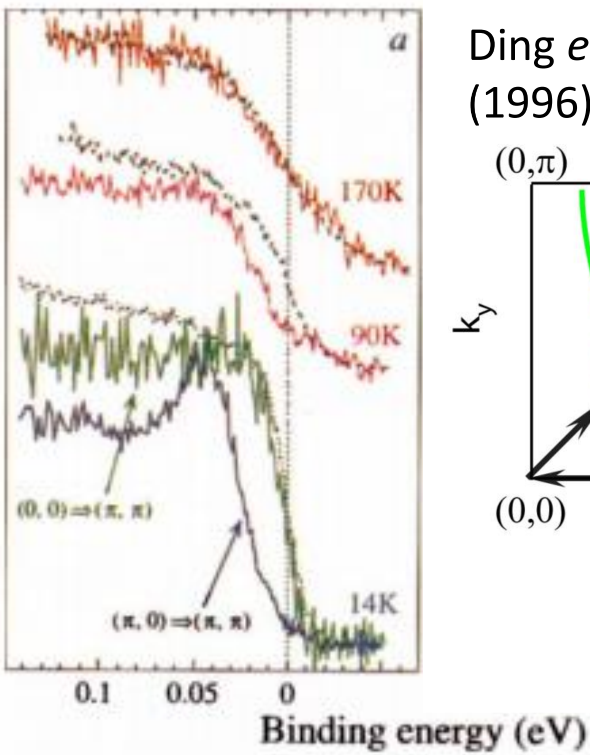
One example: in-plane resistivity



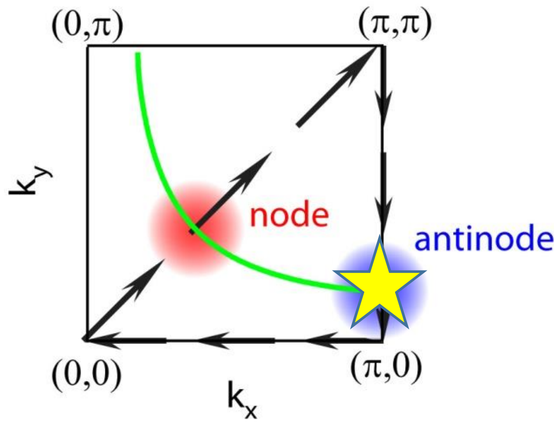
Ando et al, PRL **93** (2004)

Discovery of ARPES signatures of pseudogap

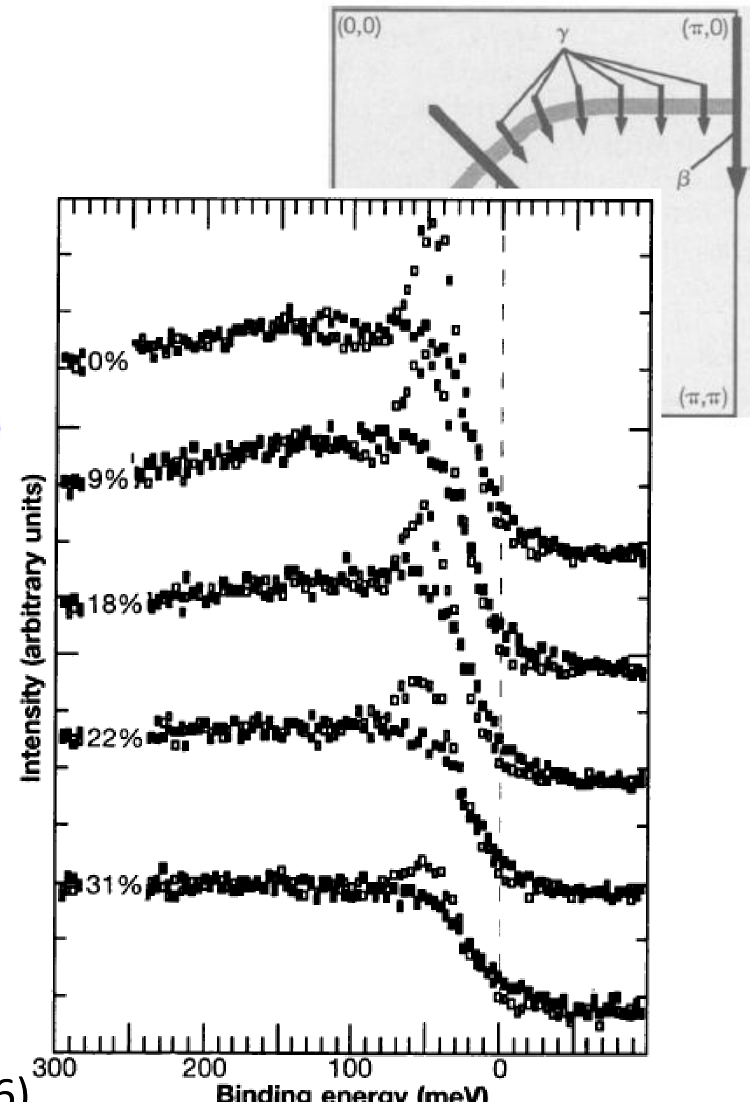
Tc=83K



Ding *et al.* Nature **382** (1996)



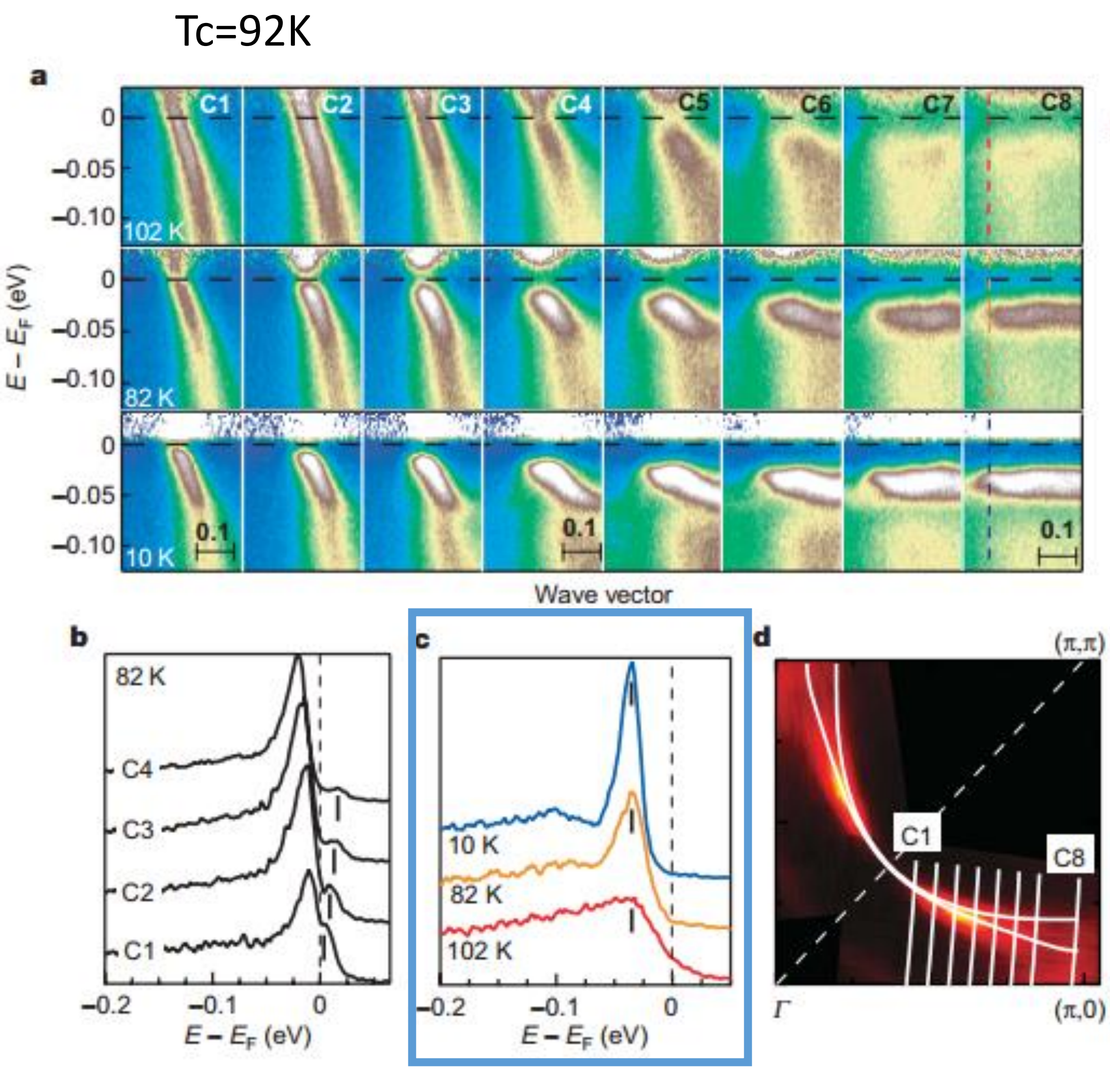
Tc=83K

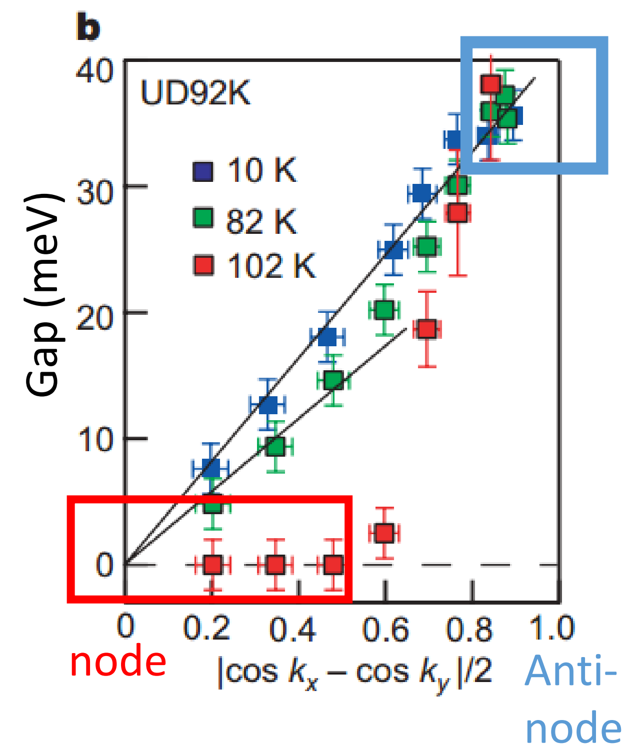


Gap at antinodal momentum remains above T_c!

Loeser *et al.* Science **273** (1996)

More modern ARPES data in pseudogap state to better visualize what is happening

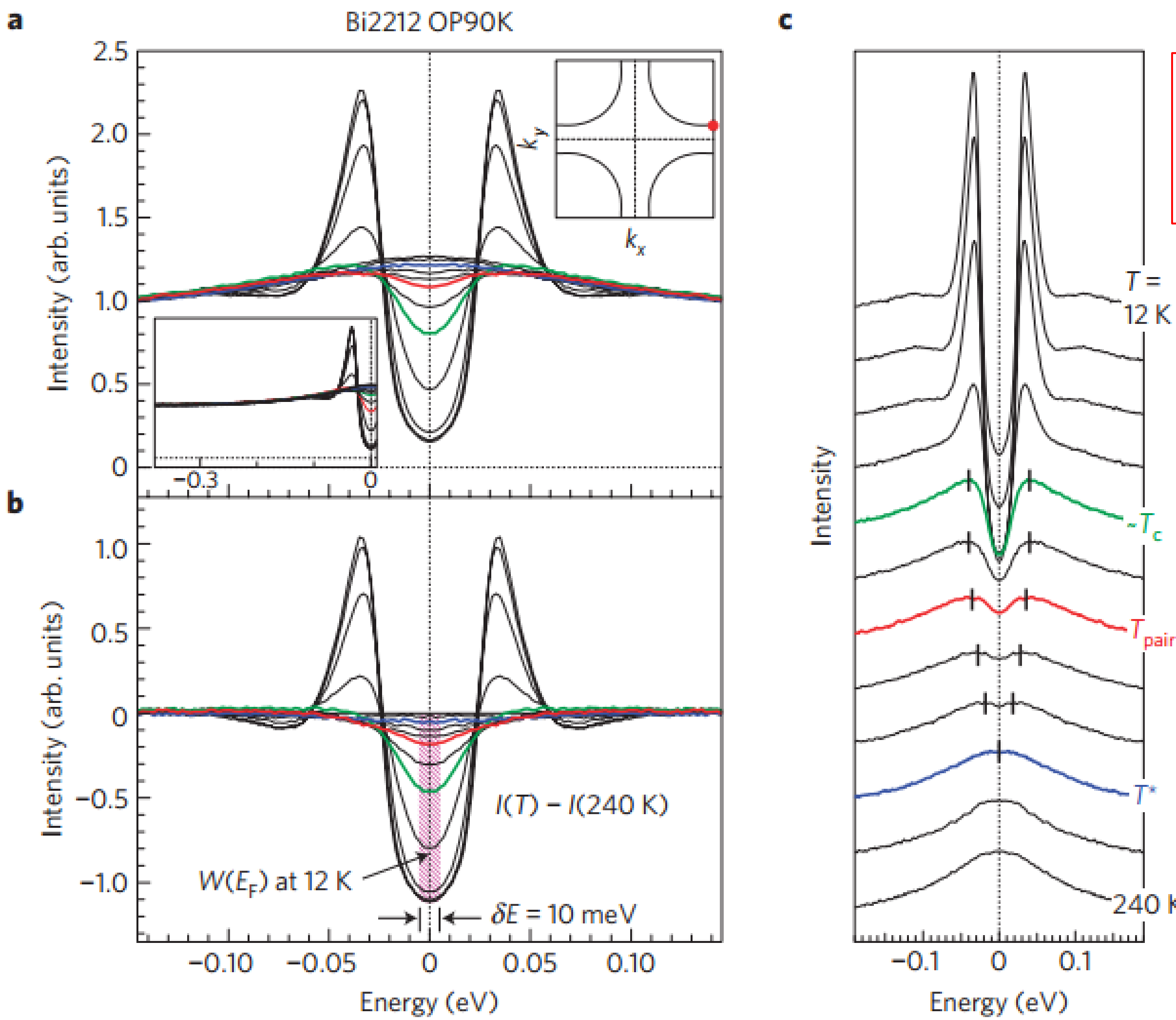




- Antinode: change in lineshape across Tc, but gap unchanged
- Node: Fermi arc above Tc
- Gap quantified by fitting symmetrized spectra to phenomenological model

Lee *et al.* Nature **450** (2007)

More modern ARPES data in pseudogap state to better visualize what is happening



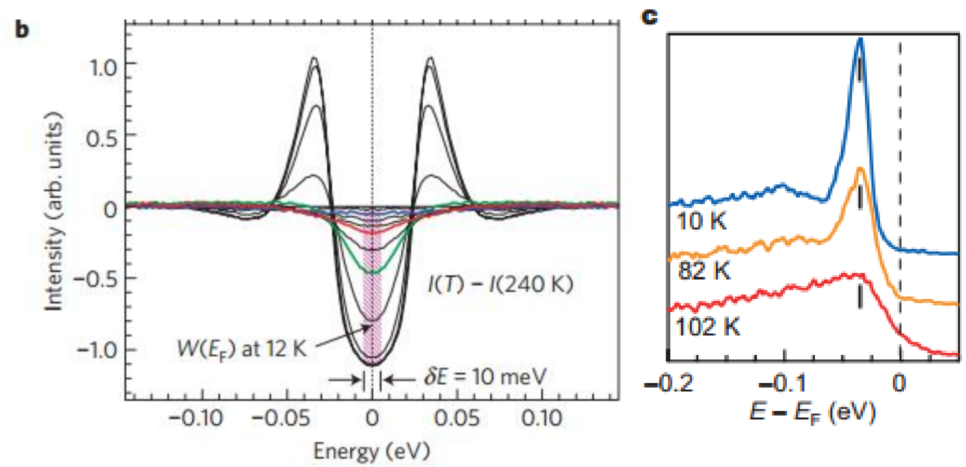
Depletion of spectral weight at E_F $T<T^*$

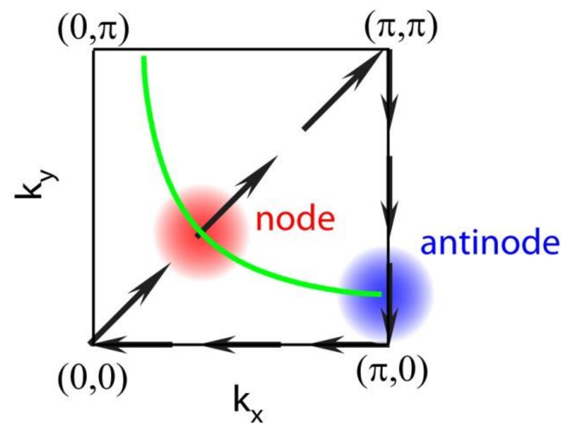
- Symmetrized EDCs at k_F at antinode
- Normalize at high energy
- Subtract highest temperature trace

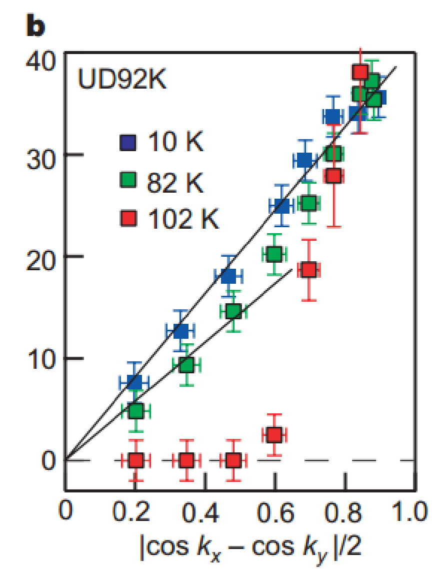
Kondo *et al.* Nat. Phys. **7** (2011)

Summary of ARPES signatures of pseudogap

- Antinode
  - Gap persists above T_c until T^*
  - Change in lineshape
  - Starting from high T: depletion of spectral weight below T^*
- Node
  - Extended region of gapless excitations (Fermi arc)

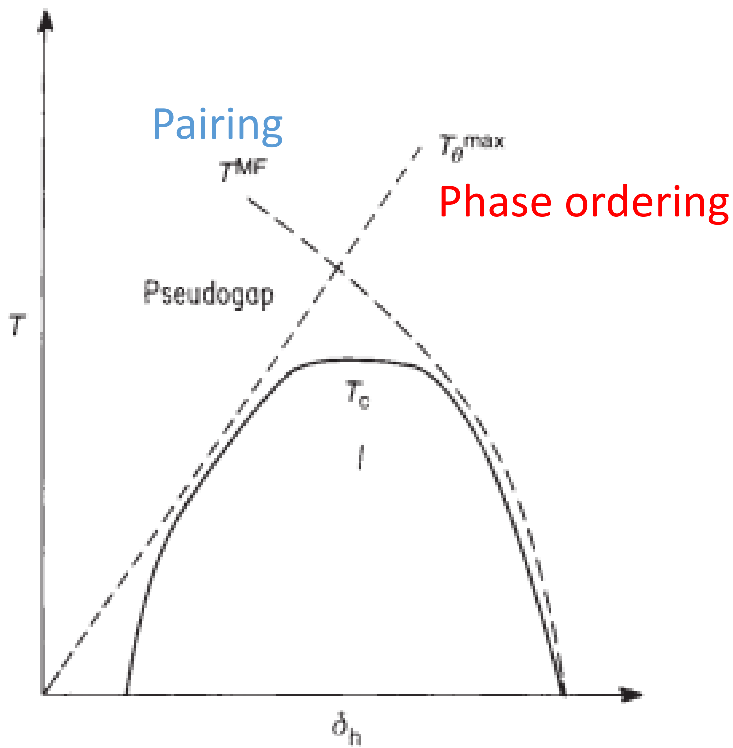






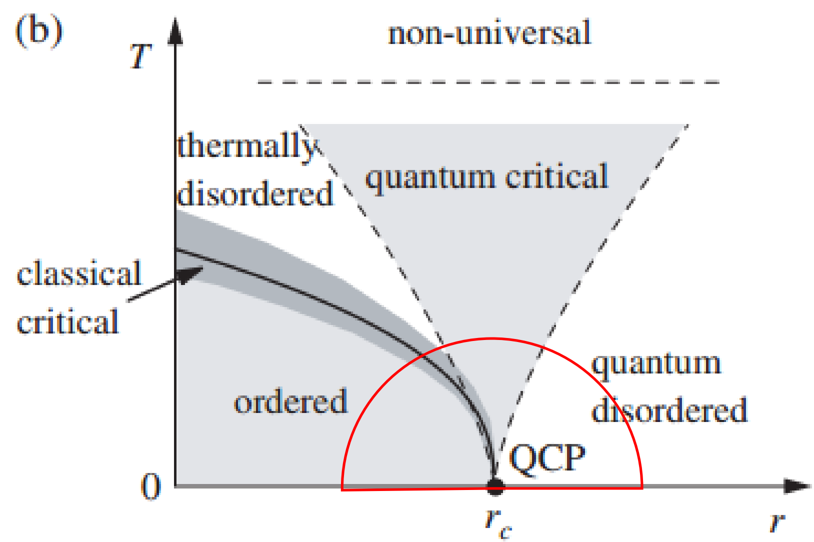
Competing explanations for pseudogap

Pseudogap is phase-disordered superconductor



Emery & Kivelson, Nature **374** (1995)

Pseudogap is distinct ordered phase

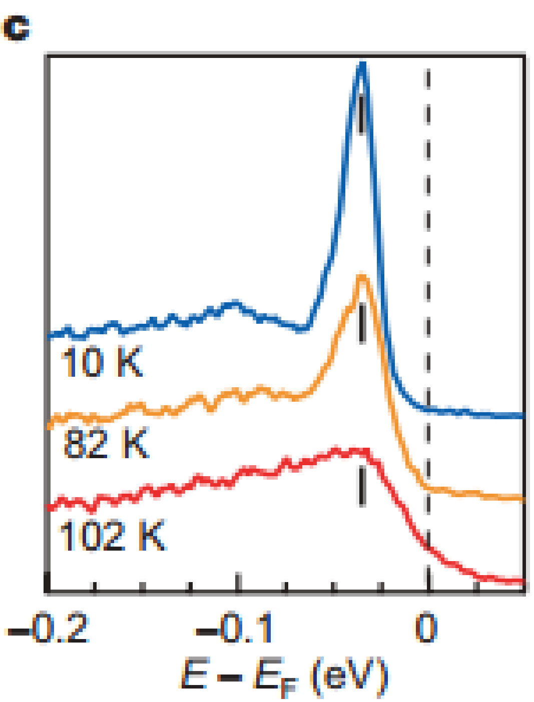


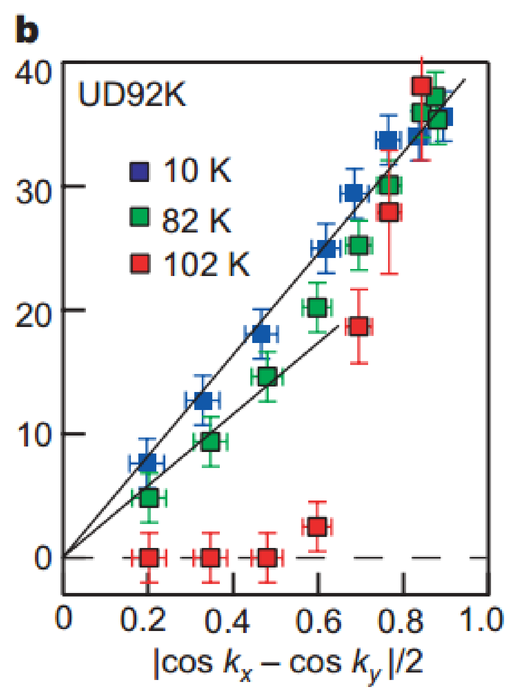
M. Vojta, Rep. Prog. Phys. **66** 2069 (2003)

Complication: evidence for both superconducting fluctuations and symmetry breaking (unrelated to SC) at T*

Evidence for ‘preformed pairs’

- Magnitude of gap unchanged across Tc



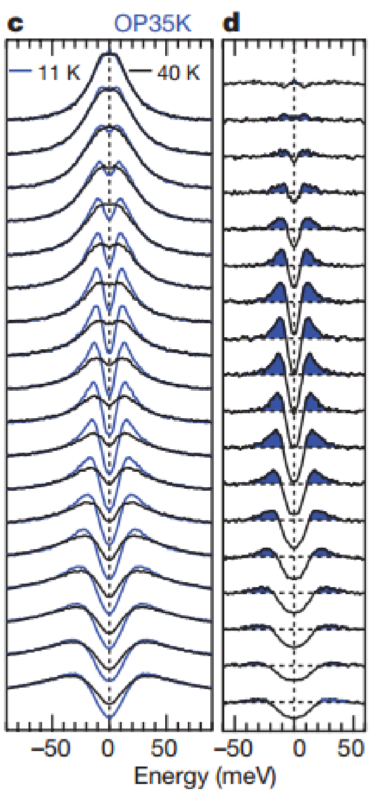


In this scenario, Fermi arc is attributed to d-wave gap which has been thermally broadened

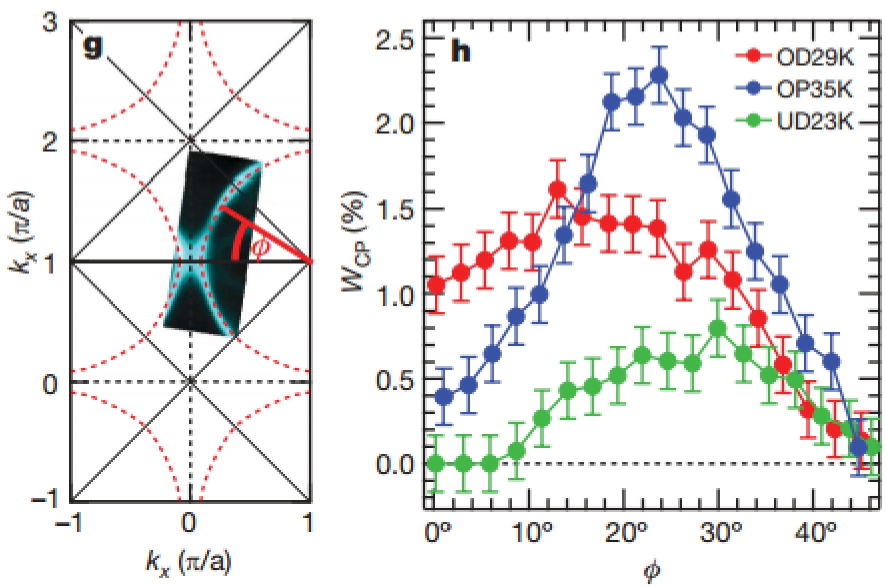
(note: the images on this slide are from a paper arguing for the opposite scenario, but they are used here for their data quality)

Evidence for ‘two-gaps’

- Distinct phenomenology in different regions of Fermi surface



Non-monotonic momentum dependence of SC spectral weight suggests another order coexists with SC below Tc



Kondo *et al.* Nature **457** (2009)

In this scenario, Fermi arc is attributed to portion of Fermi surface where superconductivity once dominated and superconducting gap closed at Tc

Summary, part 2

- Signatures of pseudogap in ARPES
  - Gap above Tc in antinodal region of Fermi surface
  - In pseudogap state, DOS at E_F does not go all the way to zero
  - Extended gapless region where node of SC gap used to be (Fermi arc)
- Competing explanations for pseudogap
  - Pre-formed pairs without phase coherence
  - A non-superconducting order which causes a gap

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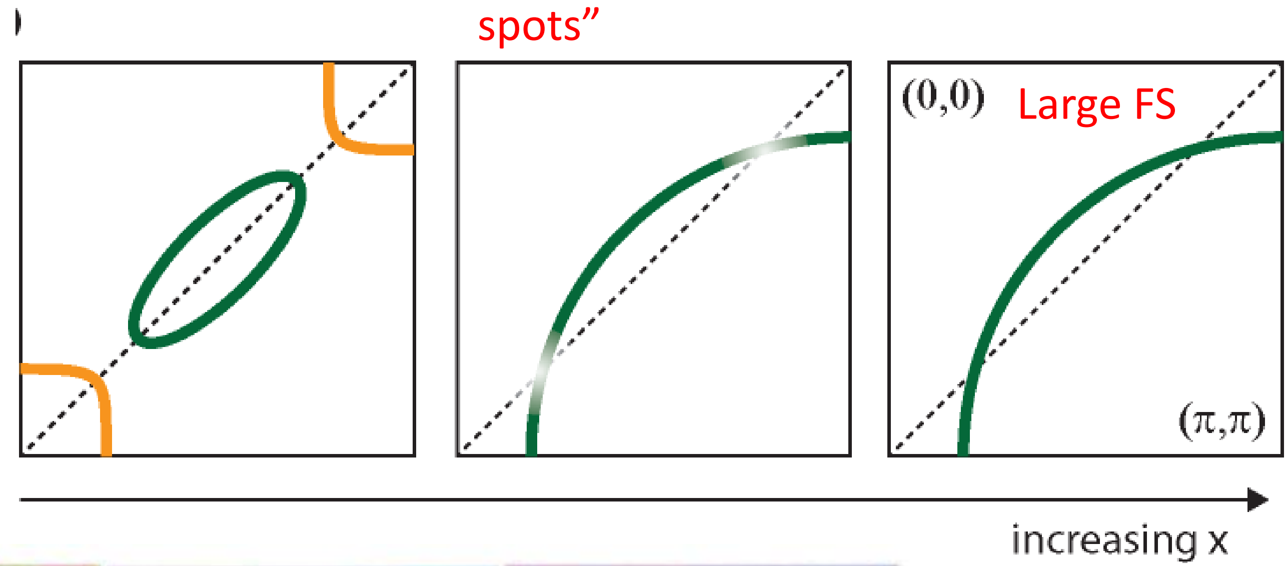
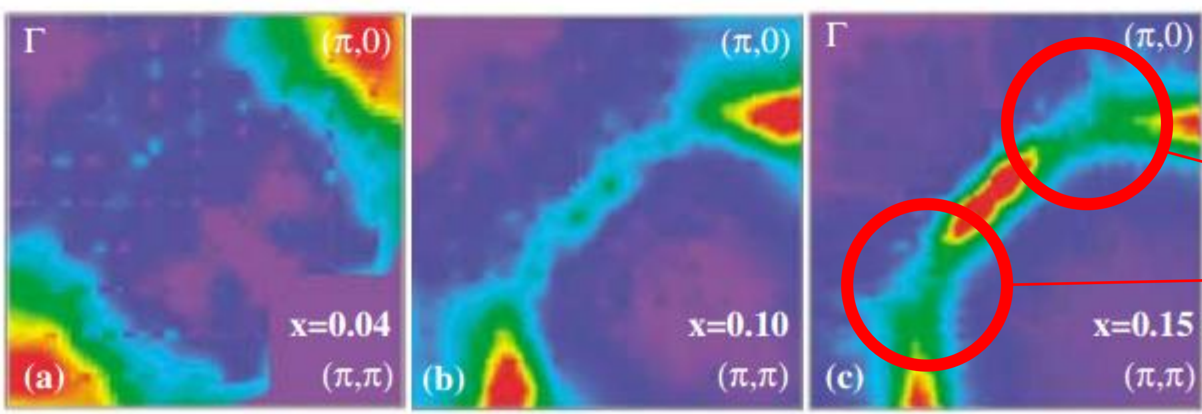
- Understand why gaps are important and various ways that gap is extracted in ARPES experiments
- Superconducting gap
  - How does one know it is a superconducting gap?
  - Momentum dependence of d-wave superconducting gap
- Pseudogap: enhance understanding of what it is exactly
- Electron-doped cuprates

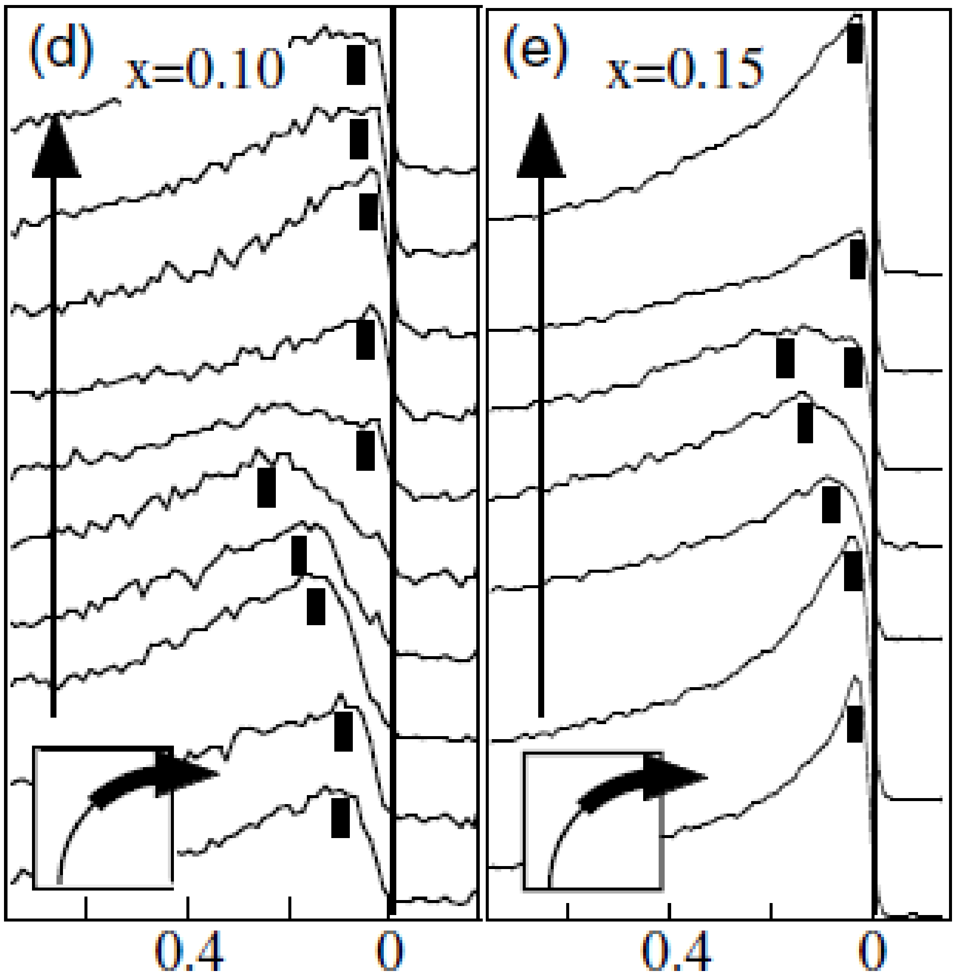
Key message: antiferromagnetism and hot spots





NCCO: Armitage *et al,* Physical Review Letters **88**, 257001 (2002)

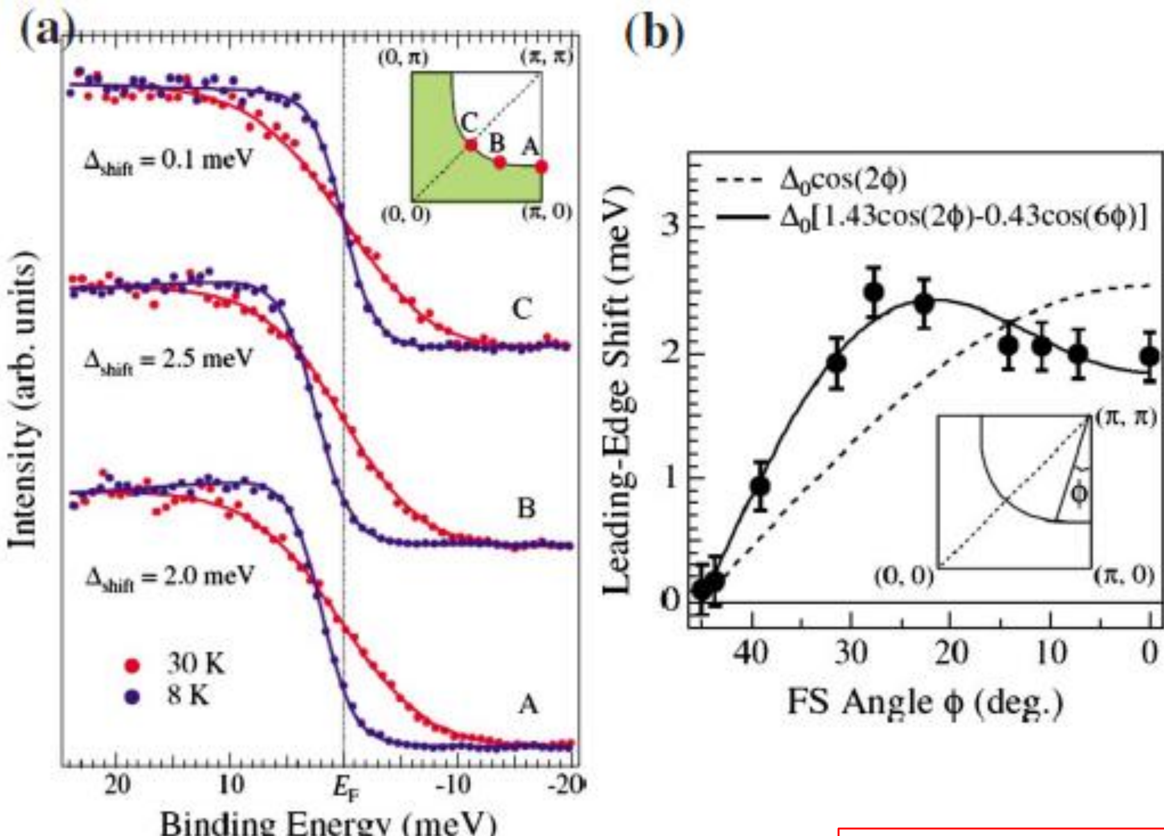
Normal state gap in electron-doped cuprates



Armitage *et al,* Physical Review Letters **88**, 257001 (2002)

- Normal-state gap in electron-doped cuprates is maximum at hotspot, not at antinodes
- Phenomenology well explained by short-range AF fluctuations

Superconducting gap in electron-doped cuprates



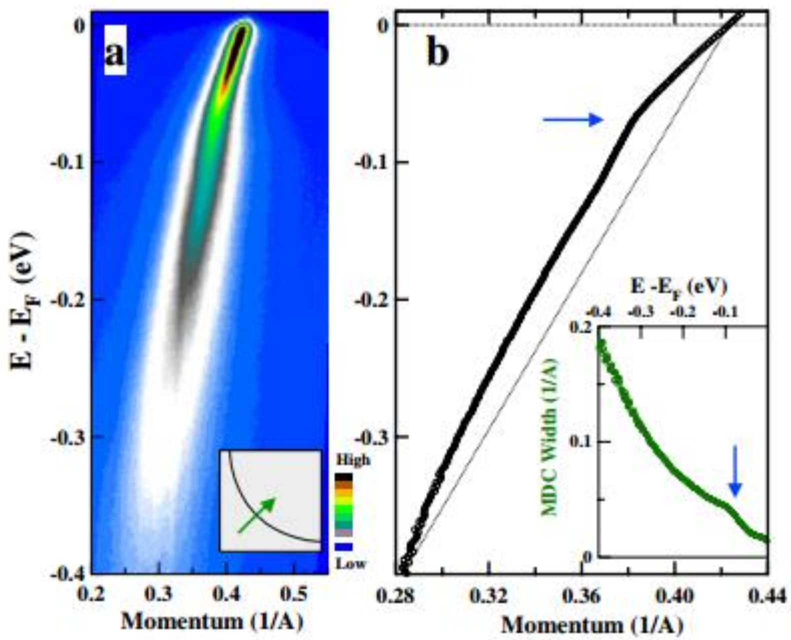
Consistent with d-wave, but gap is maximum at hot stop not at brilliouin zone boundary

Matsui *et al.* PRL **94** (2005)

How was gap assessed in this experiment?

Other misc. foci of ARPES studies of cuprates

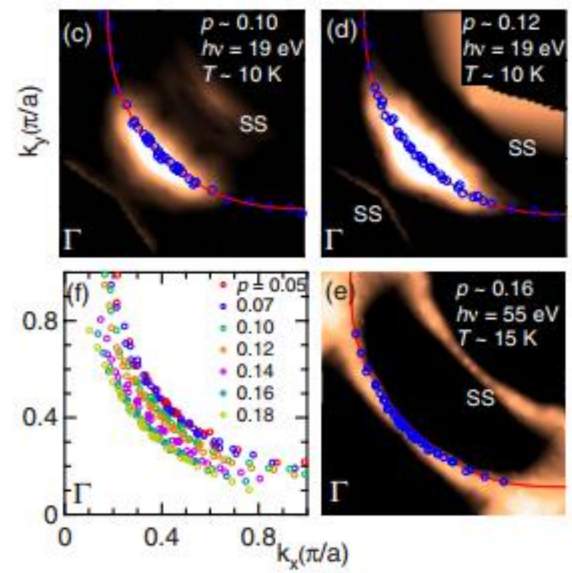
Dispersion anomalies



Zhang *et al.* PRL **100**, 107002 (2008)

Purpose: possibly related to pairing glue

Size and shape of Fermi surface



Hashimoto *et al.* PRB **77**, 094516 (2008)

Purpose:

- What is the doping, really?
- What Fermi surface instabilities are likely?

Conclusions

- ARPES has contributed to studies of superconducting gap and pseudogap because both states involve a spectral gap at E_F and are anisotropic in momentum space
- Gaps are studied via energy distribution curves (EDCs) which look at intensity vs energy at a fixed momentum
- Many ways to quantify gaps (leading edge shift, quasiparticle peak position, fitting to a model) and in the pseudogap regime, spectral weight depletion is an important metric too