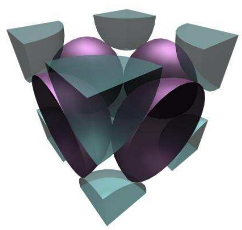
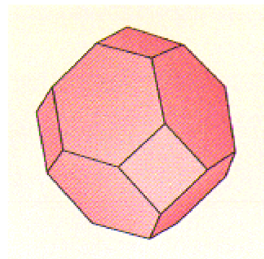
High T_c superconductors

- a view from k-space -

Mark S. Golden
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Martin Knupfer, Thomas Pichler, Timur Kim
Roland Hübel, Dieter Müller

Jörg Fink, Claus Schneider, Frank Matthes, Robert Frömter — IFF, IFW Dresden

Crystals
Helmuth Berger — EPFL Lausanne
B. Liang, A. Maliouk, C. T. Lin, Bernhard Keimer — MPI Stuttgart
Guang Yang, Stuart Abell — U. of Birmingham, UK

Experimental collaboration
Fred Schiller, Serguei Molodtsov, Clemens Laubschat — TU Dresden IOMP
Rolf Follath — BESSY
Michael Sing, Ralph Claessen — U Augsburg
Stefano Turchini, Stefano Zennaro — ELETTRA
Cesare Grazioli — CNR Rome + ELETTRA

Crystal characterisation
K. Nenkov, D. Eckert — IMW, IFW Dresden

Money
FOM, EU, BMBF, DFG, SMWK

Outline

- ARPES as k-space microscopy
- results from the $Bi_2Sr_2CaCu_2O_8$ family
  - the Fermi surface
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  - peaks, dips and humps
    - in the overdoped regime
    - in the underdoped regime

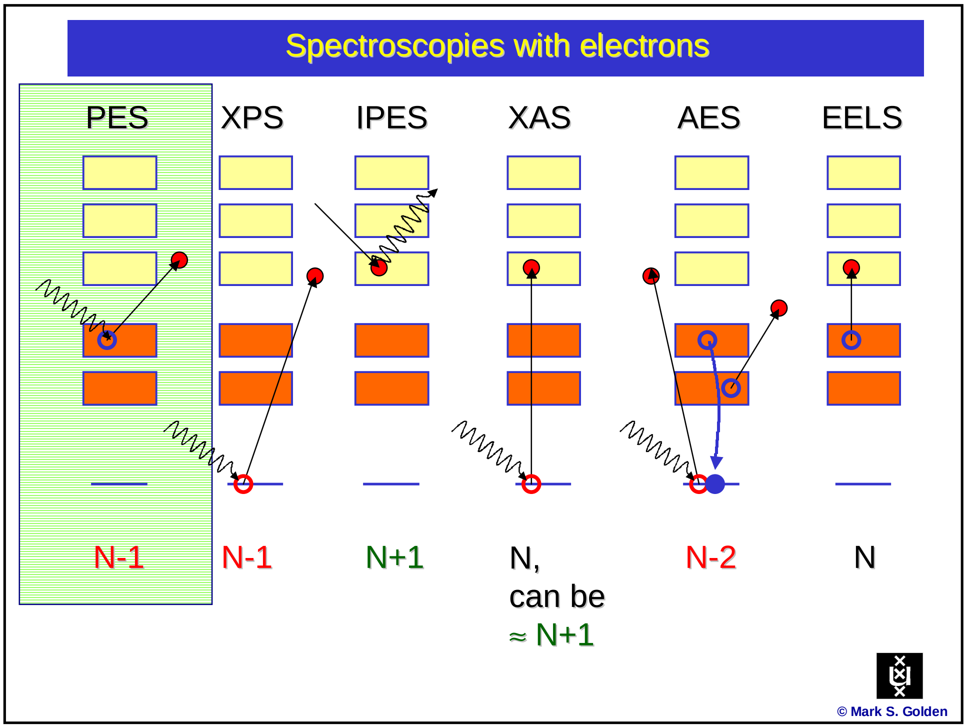
HTSC: a job for . . . . spectroscopy

- the HTSC and parents are:
  - not ordinary metals
  - not ordinary superconductors
- we need to understand the fundamentals of their electron systems

theory | experiment

s p e c t r o s c o p y

- offers a direct probe of the electronic states
- is now a 'standard' test of any aspiring theories



Angle resolved photoemission spectroscopy

A R P E S

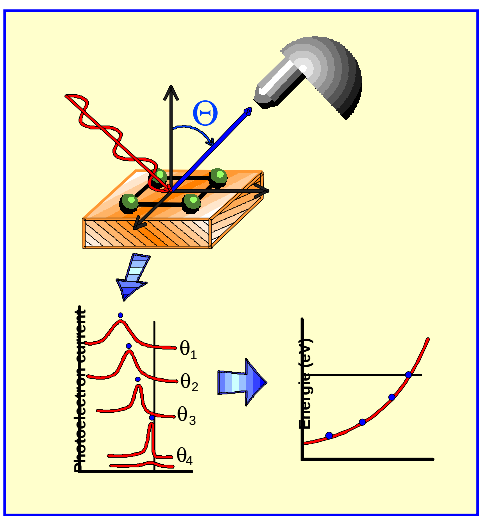
ARPES and the HTSC: a love affair with a sticky start......

at the outset:

- ARPES is somehow cranky
- measures some kind of surface stuff.....
- high energy scale

now:

⇨ powerful, k-resolved tool to provide:
  - normal state e-structure, Fermi surface
  - gaps - normal state and superconducting state
  - interactions / lifetimes
  - low energy scale
  - one of the acid tests for theories

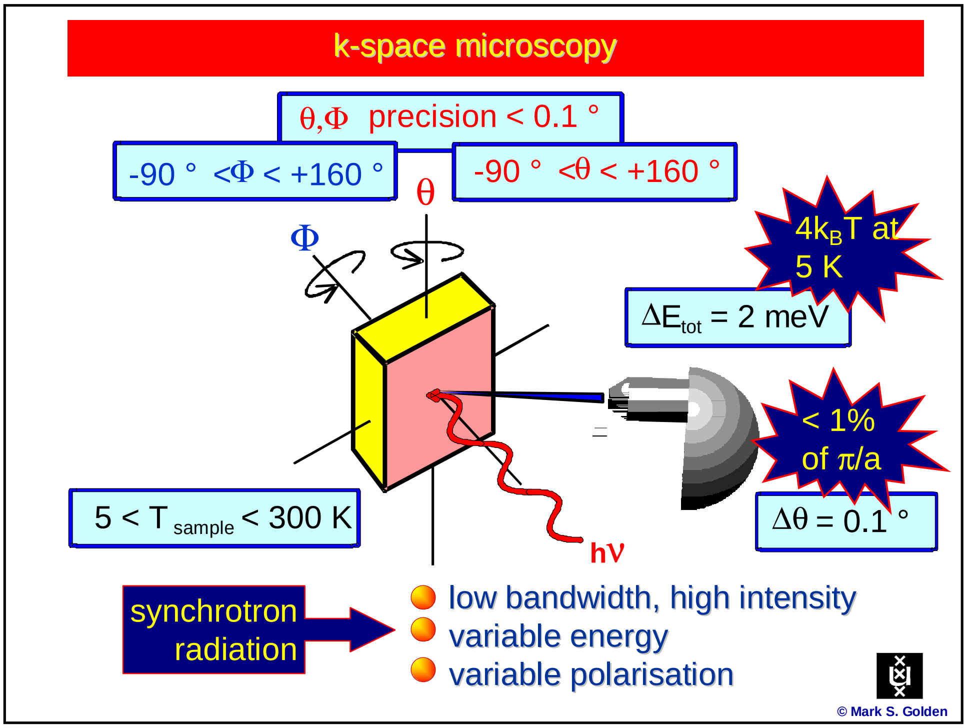


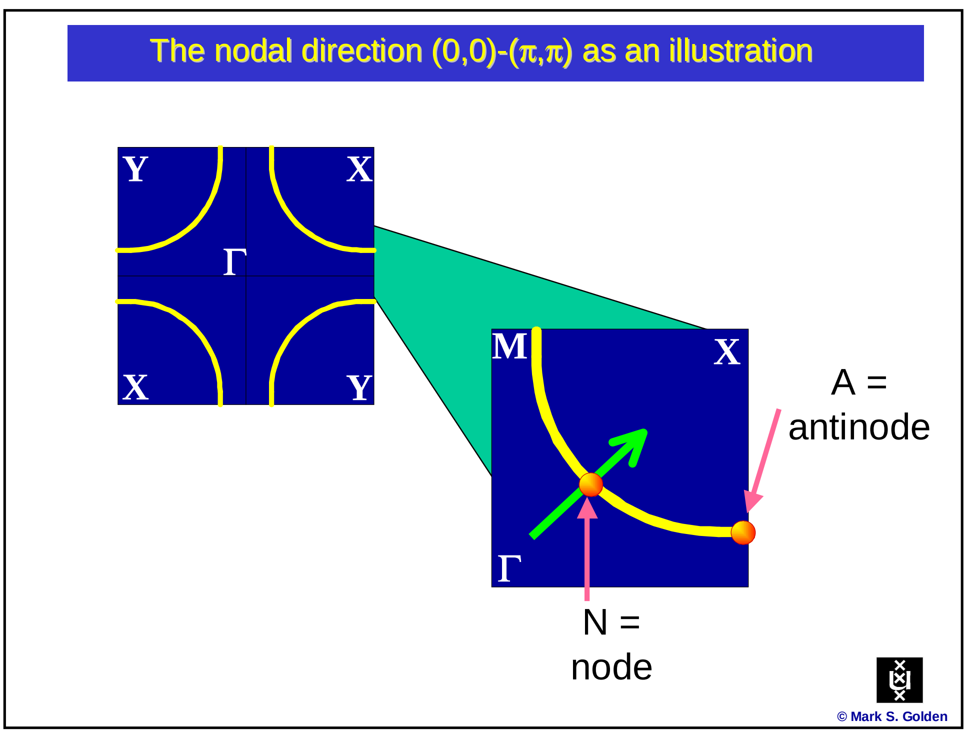
An ARPES experiment

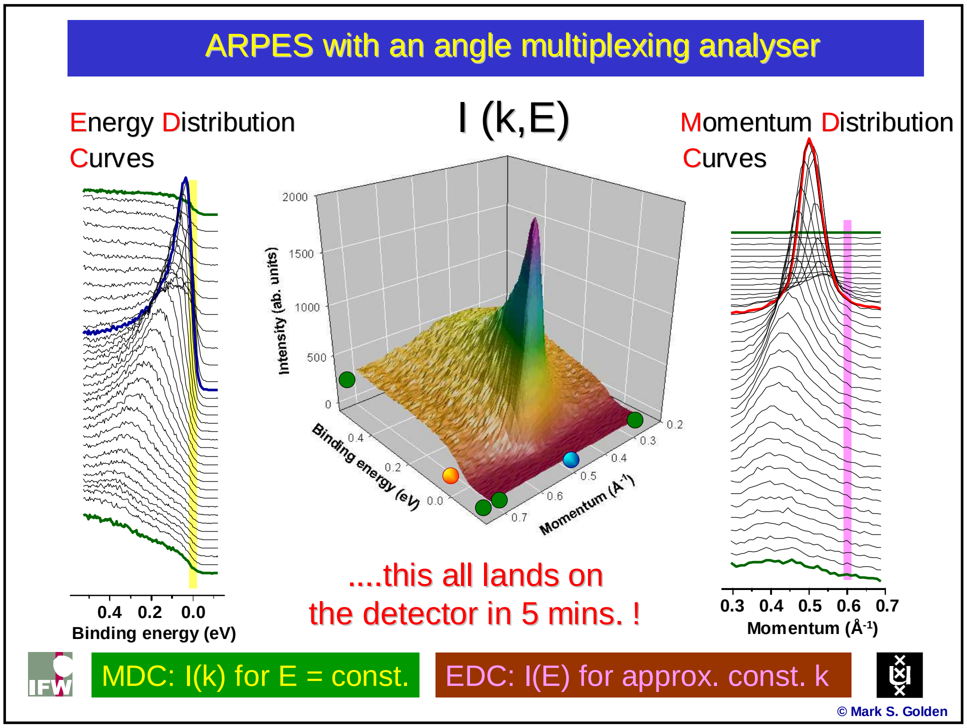
- single crystal
- monochromatic light
- ultra high vacuum
- electron energy analyser

'band mapping'

$$|k_{\parallel}| = \sqrt{\frac{2mE_{kin}}{\hbar}}\sin\theta = 0.512\sqrt{E_{kin}(eV)}\sin\theta$$


k-space microscopy
θ,Φ precision < 0.1 °
-90 ° <Φ < +160 °
-90 ° <θ < +160 °
θ
Φ
4k_BT at 5 K
ΔE_tot = 2 meV
< 1% of π/a
Δθ = 0.1 °
5 < T sample < 300 K
hν
synchrotron radiation
low bandwidth, high intensity
variable energy
variable polarisation
© Mark S. Golden


The nodal direction (0,0)-(π,π) as an illustration
Y
X
Γ
X
Y
M
X
Γ
A = antinode
N = node
© Mark S. Golden



What physical quantities are measured in photoemission ?

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

momentum (photoelectrons) — **vector potential (photons)** — **spectral function** — **Fermi function**

Spectral function:

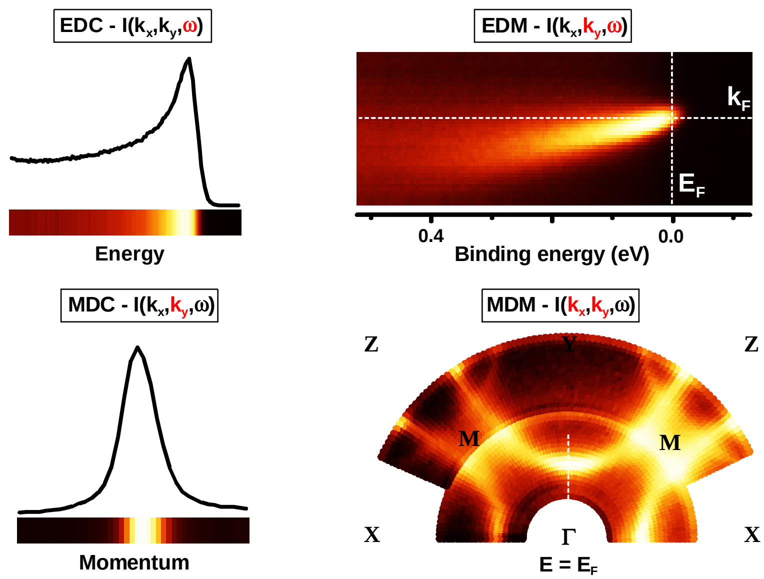
the probablility of removing an electron of energy E and wavevector k from the interacting N-electron system

BUT

the matrix element is always present:

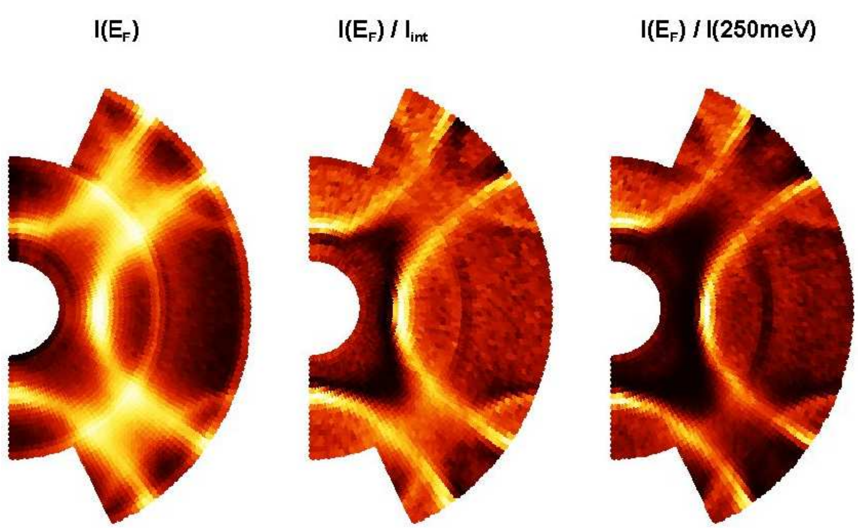
→ **dependence on photon energy, polarisation....**

Representing ARPES data in 2D



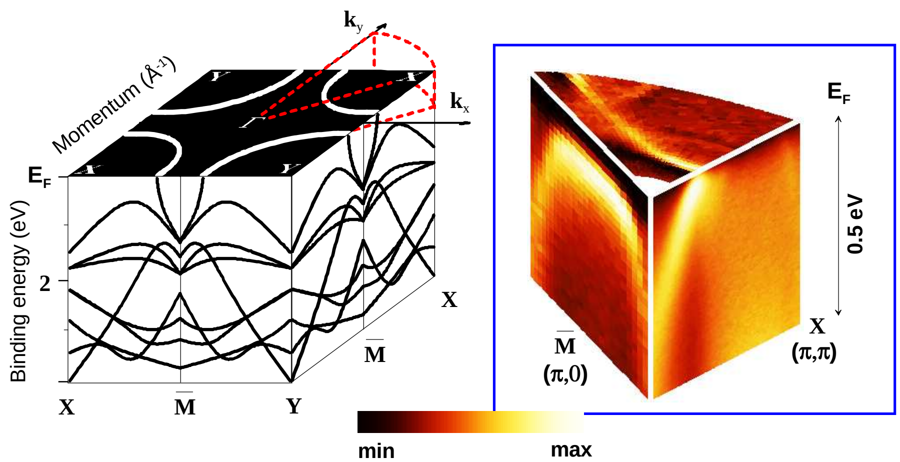
Borisenko et al., PRB**64**, 094513 (2001)

Divide raw signal



Borisenko et al., PRB**64**, 094513 (2001)

A full picture of I_{PES} vs. the 3D k_x, k_y, E_B space



Borisenko et al., PRB**64**, 094513 (2001)

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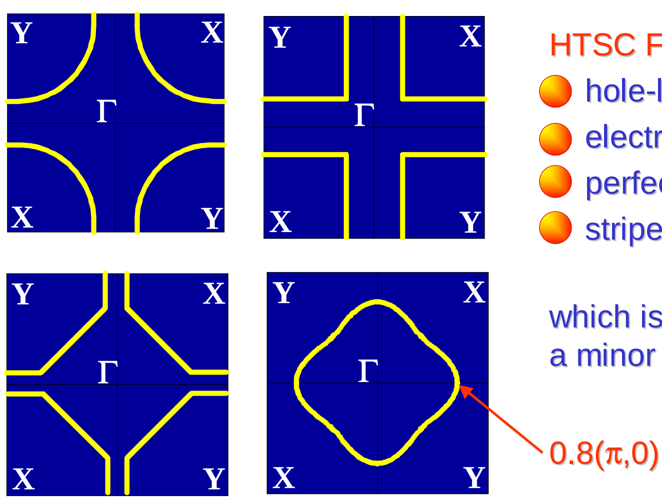
    - in the underdoped regime

Determination of the Fermi surface topology

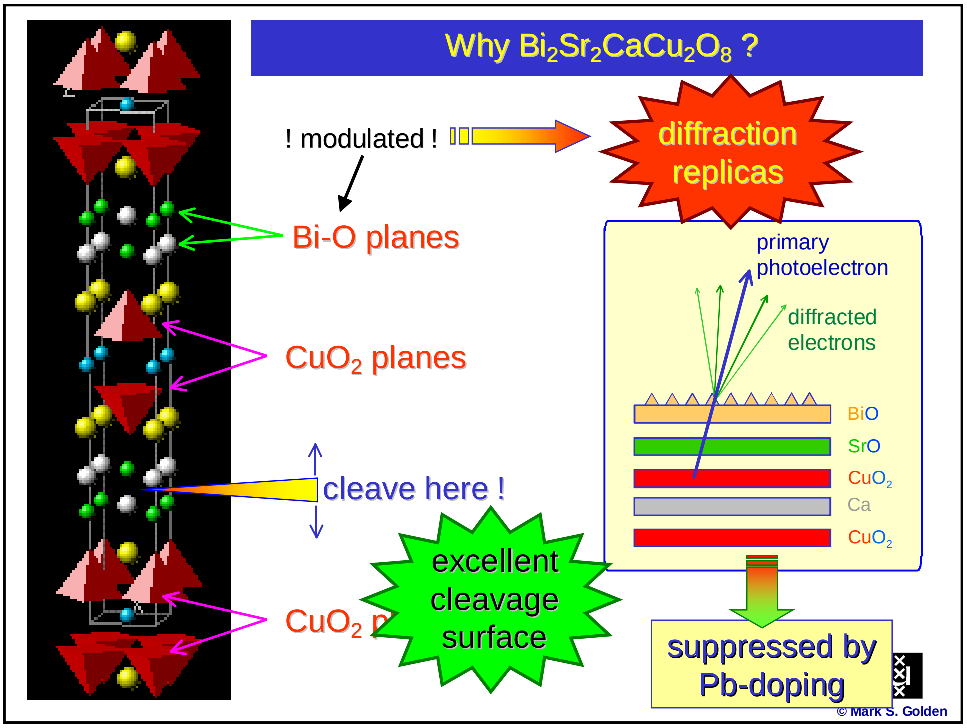
‘Experimental’ Fermi surfaces of HTSC

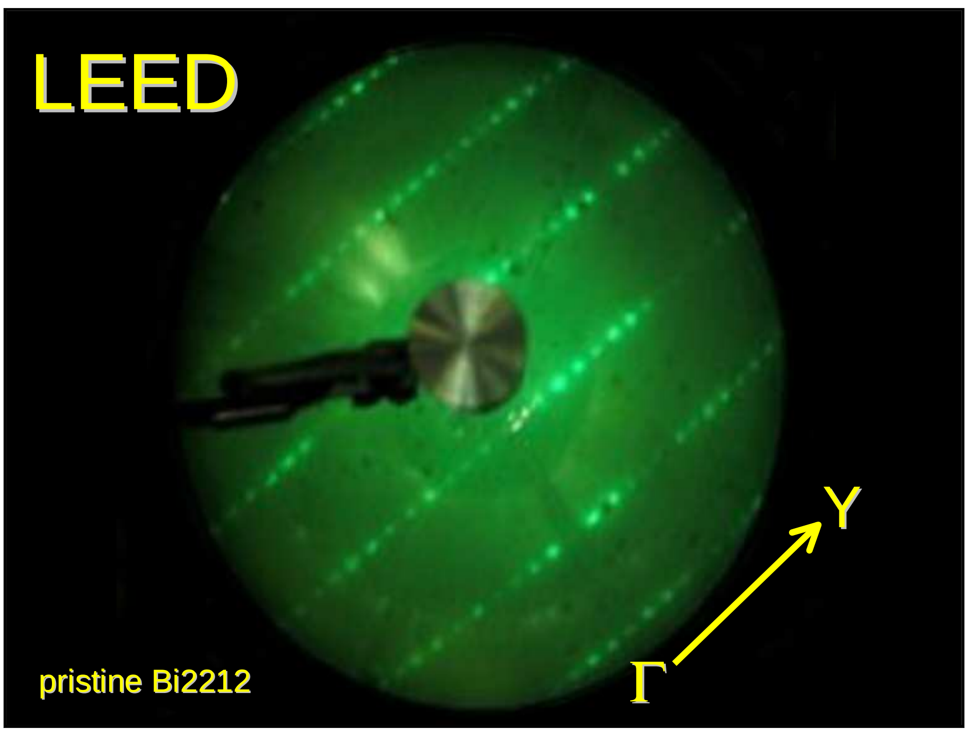


HTSC Fermi surface:

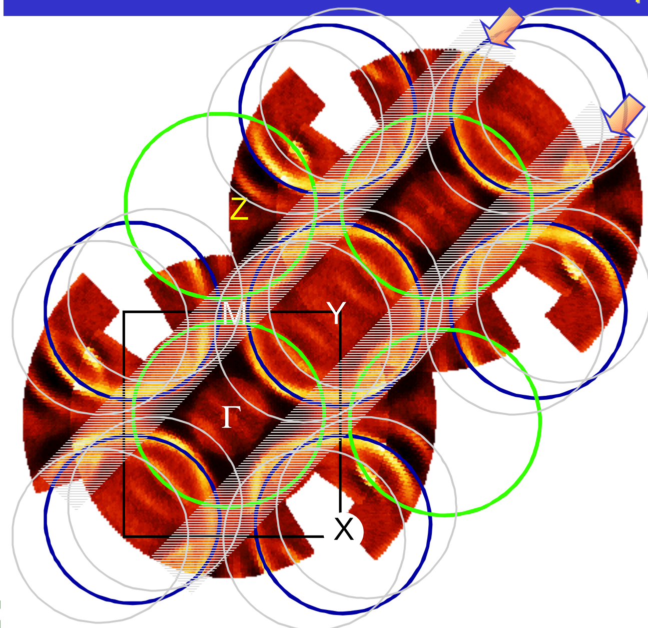
- hole-like ?
- electron-like ?
- perfect nesting ?
- stripey ?

which is correct is not a minor detail . . . . .


Why $Bi_2Sr_2CaCu_2O_8$?
! modulated !
diffraction replicas
Bi-O planes
CuO_2 planes
cleave here !
CuO_2 p
excellent cleavage surface
primary photoelectron
diffracted electrons
BiO
SrO
CuO_2
Ca
CuO_2
suppressed by Pb-doping
© Mark S. Golden


LEED
pristine Bi2212
Γ
Y

Pristine Bi-2212 Fermi surface map



main FS

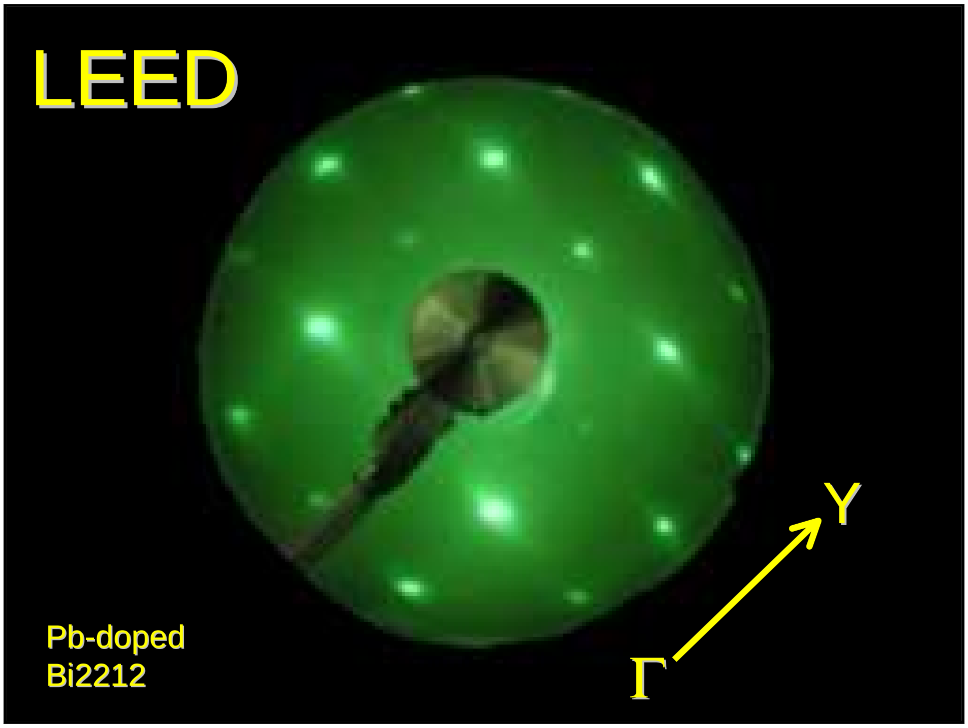
shadow FS

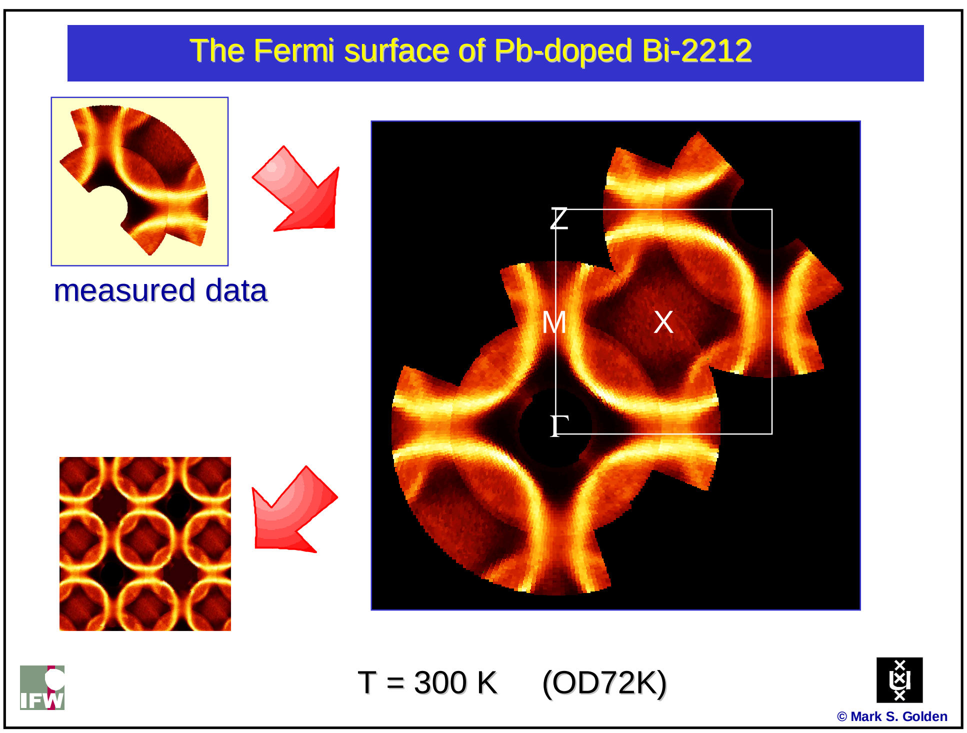
diffraction replicas

high intensity ribbons

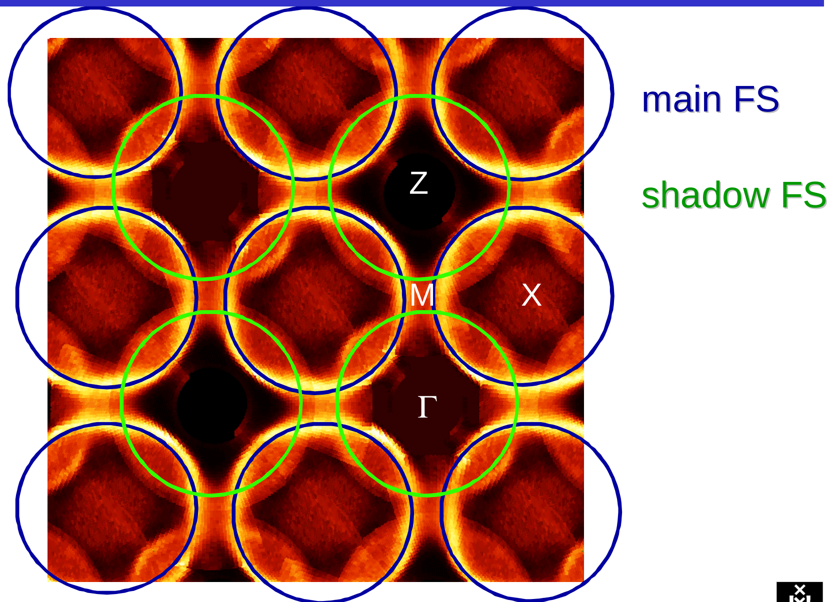
Pb-doped Bi2212:

$Bi_{2-x}Pb_xSr_2CaCu_2O_8$

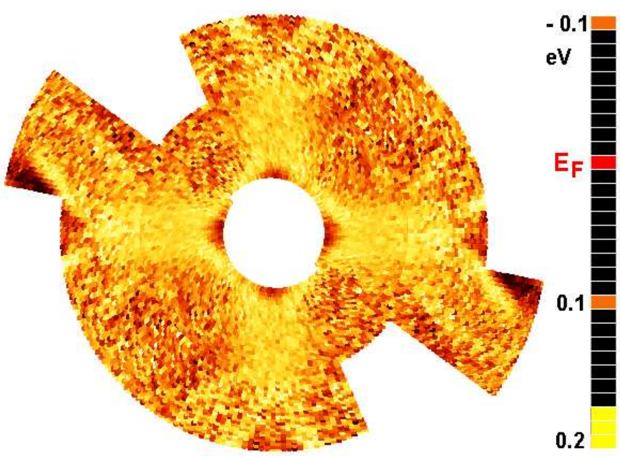

LEED
Pb-doped
Bi2212
Γ
Y


The Fermi surface of Pb-doped Bi-2212
measured data
Z
M
X
Γ
T = 300 K (OD72K)
© Mark S. Golden

The Fermi surface of Pb-doped Bi-2212



Constant energy surfaces: ω dependence (OD69K)



- symmetric 'breathing':
- FS closes around Γ only very late

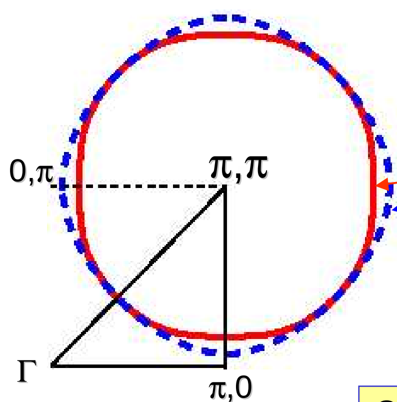
300K, hν = 21 eV

Kordyuk et al., 2000

What about the c-axis bi-layer splitting ?

……could this explain the ' sightings' of an electron-like Fermi surface in Bi2212 ?

The role of the c-axis bilayer splitting (BLS)



$(Pb,Bi)_2Sr_2CaCu_2O_8$

$2CuO_2$ planes: close together

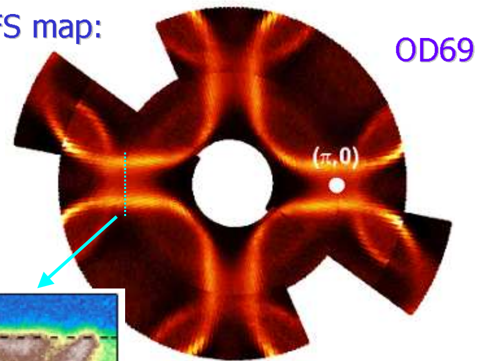
→ antibonding and bonding states due to c-axis bilayer coupling

- maximal near (π,0)
- zero along (0,0)-(π,π)

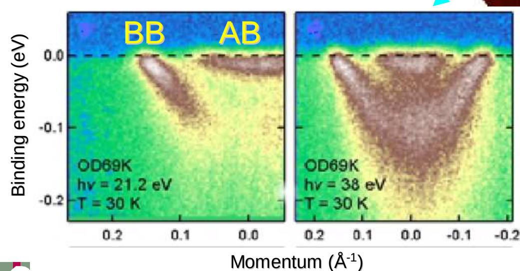
Could the antibonding band give an electron-like FS?

c-axis bi-layer splitting

- Normal state FS map: BLS 'invisible'

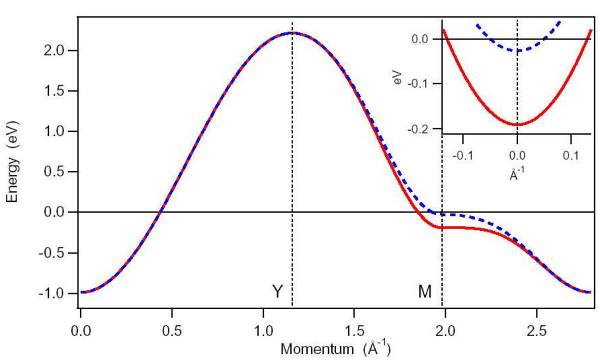


- Low T, high res. data: Both FS are hole-like



Kordyuk, Borisenko et al., 2002

Tight binding fit to the OD69K data



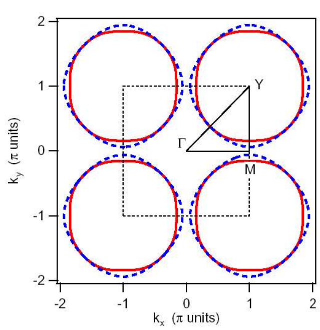


TABLE I: Tight-binding parameters of the CuO conducting band of Bi-2212.

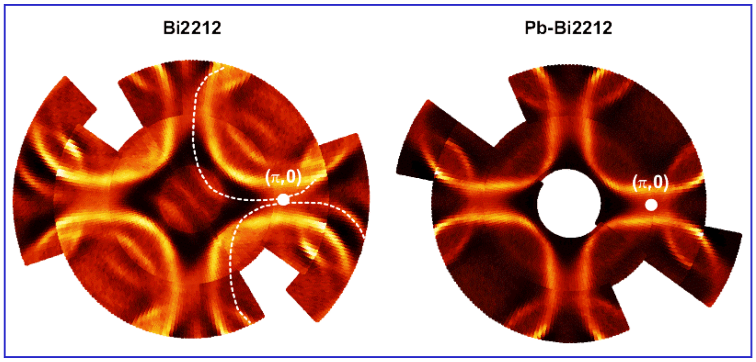
Sample	t (eV)	t' (eV)	t'' (eV)	$t_\perp$ (eV)	$\Delta\epsilon$ (eV)
OD 69 K	0.40	0.090	0.045	0.082	0.43
UD 77 K	0.39	0.078	0.039	0.082	0.29

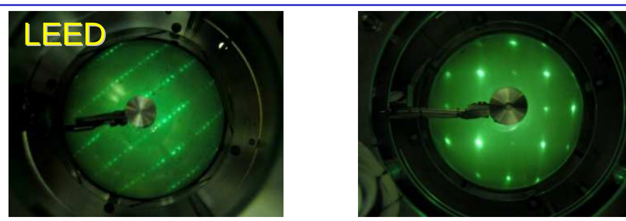
$$\begin{aligned}\epsilon_{a,b} &= \Delta\epsilon - 2t(\cos k_x + \cos k_y)\\ &+ 4t'\cos k_x \cos k_y - 2t''(\cos 2k_x + \cos 2k_y)\\ &\pm t_\perp(\cos k_x - \cos k_y)^2/4,\end{aligned}$$

Kordyuk et al., IFW Dresden, cond-mat 0208418

To Pb or not to Pb ?

$E=E_F$
300K
$h\nu$ =
21 eV





Kordyuk, Borisenko et al., 2001, IFW Dresden

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    - in the overdoped regime
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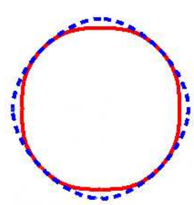
Superconducting energy gap

UD, bi-layer splitting resolved

Superconducting energy gap: revisited

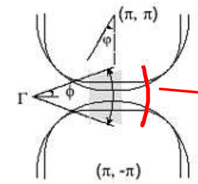
- all 'old' superconducting gap data was:
  - analysed without taking the BLS into account

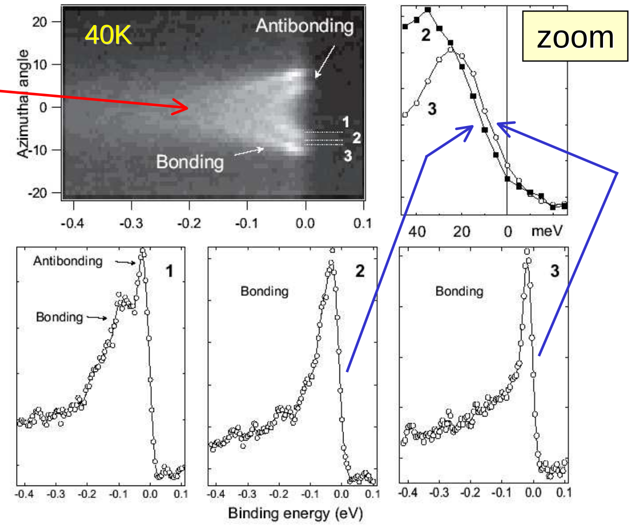


  - recorded from modulated, pristine 2212

…….a revisit is called for

EDC's *very* sensitive to k-location (UD77K)





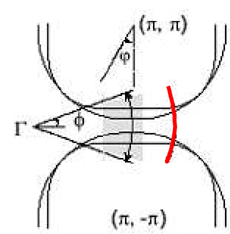
Azimuthal cut

$|k| = 1.09$ Å^{-1}

[by the way: clear BLS in UD!]

Borisenko et al., IFW Dresden, cond-mat 0208418, PRB(RC), in press

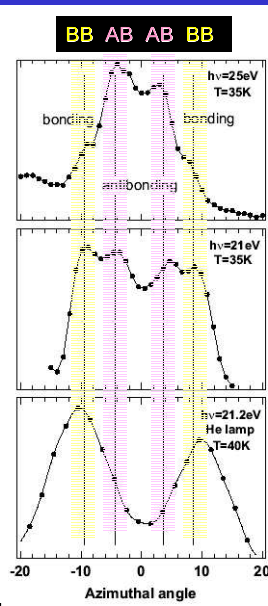
Test for the best exp. parameters.....

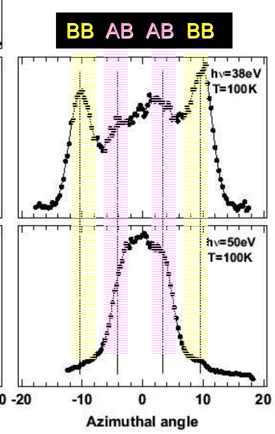


Azimuthal MDC' s

- BB vs. AB can be ' tuned' via hν :

➡ 20' s approx =
➡ 38: BB > AB
➡ 50: AB > BB

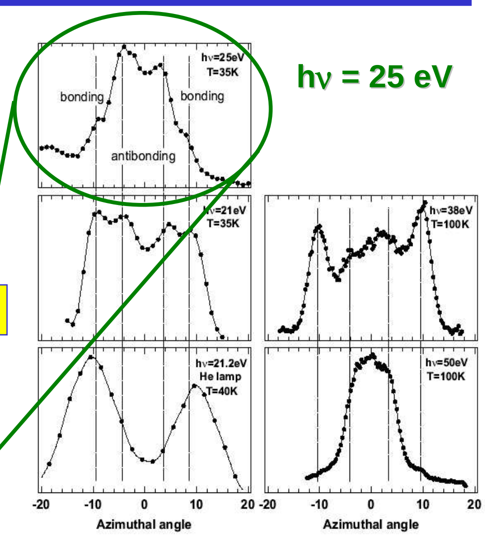




Borisenko et al., IFW Dresden, cond-mat 0208418, PRB(RC), in press

How to determine the gap

- **EDC fit**
  - \+ absolute gap
  - \- model dependent
  - ⇨ AB = BB is good
- **Leading edge gap (LEG)**
  - \- only relative gap value possible
  - \+ highly precise
  - ⇨ AB > BB is good



Borisenko et al., IFW Dresden, cond-mat 0208418, PRB(RC), in press

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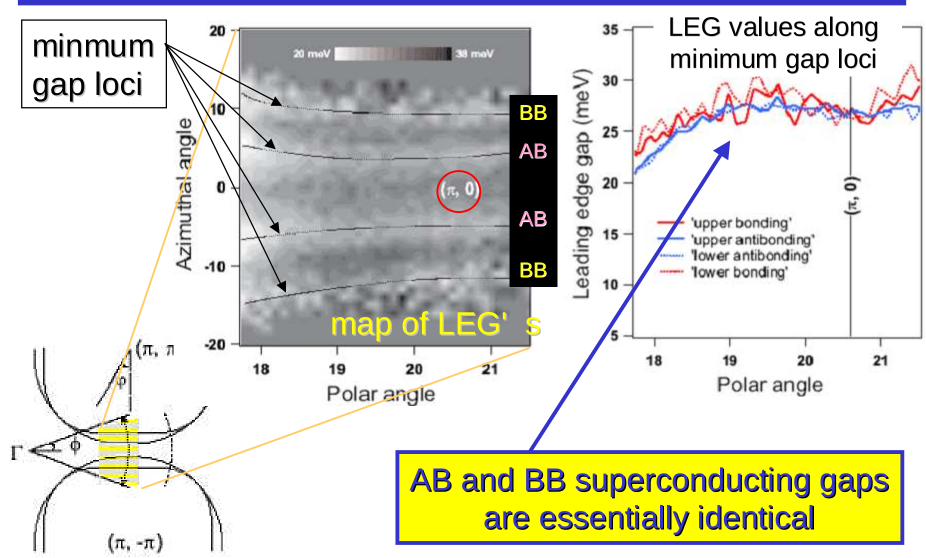
How do the gaps on the BB and AB compare ?



AB and BB superconducting gaps are essentially identical

Borisenko et al., IFW Dresden, cond-mat 0208418, PRB(RC), in press

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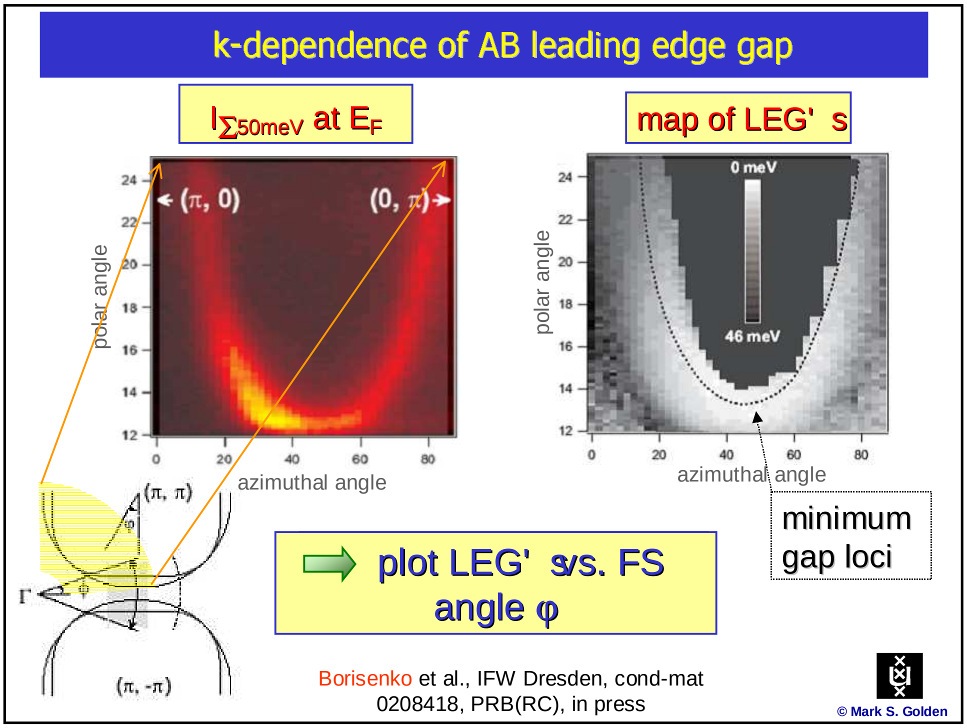
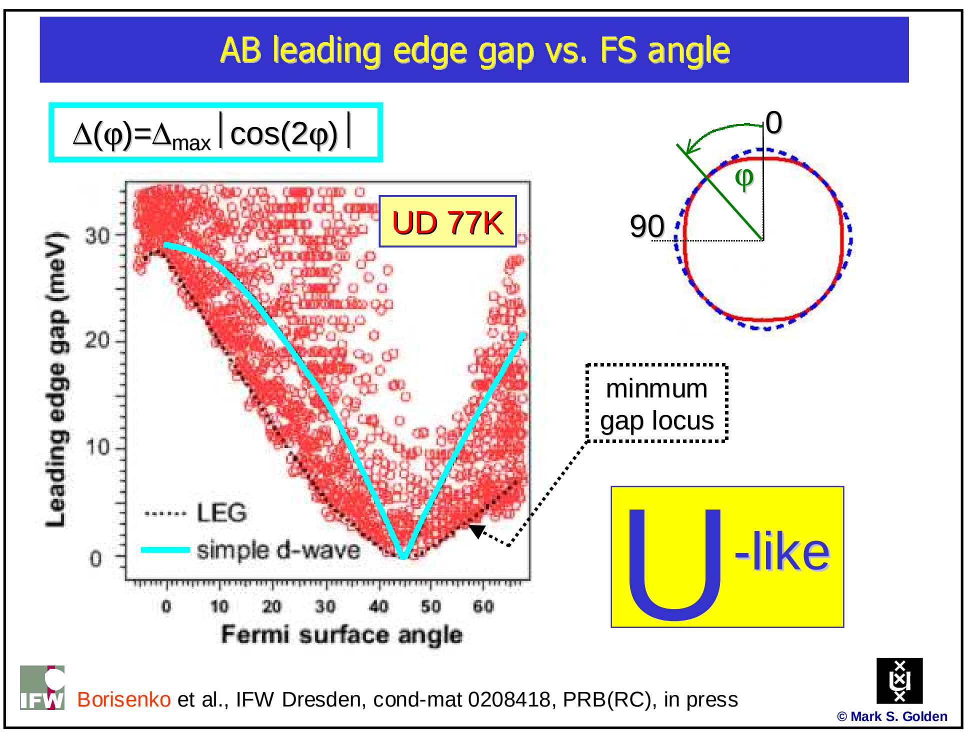

k-dependence of AB leading edge gap
I∑50meV at EF
map of LEG's
(π, 0)
(0, π)
polar angle
azimuthal angle
0 meV
46 meV
(π, π)
(π, -π)
Γ
minimum gap loci
plot LEG's vs. FS angle φ
Borisenko et al., IFW Dresden, cond-mat 0208418, PRB(RC), in press
© Mark S. Golden


AB leading edge gap vs. FS angle
Δ(φ)=Δmax|cos(2φ)|
UD 77K
Leading edge gap (meV)
Fermi surface angle
LEG
simple d-wave
0
90
φ
minmum gap locus
U-like
Borisenko et al., IFW Dresden, cond-mat 0208418, PRB(RC), in press
© Mark S. Golden

Causes of deviations from pure d-wave for UD

Flattening out of gap at nodes seen already in UD
Mesot PRL99 (pristine Bi2212, not BLS-resolved)

Causes:

? longer range pairing in UD due to ↓ screening

- standard d-wave: $\Delta(\varphi)=\Delta_{max}|\cos(2\varphi)|$
- higher gap harmonics: $\Delta(\varphi)=\Delta_1|\cos(2\varphi)| + \Delta_2|\cos(6\varphi)|$
  here = 27% $\cos(6\varphi)$

? other pairing symmetries ?
$d_{x^2-y^2}$ + is; $d_{x^2-y^2}$ + id_{xy}

IFW Borisenko et al., IFW Dresden, cond-mat 0208418, PRB(RC), in press

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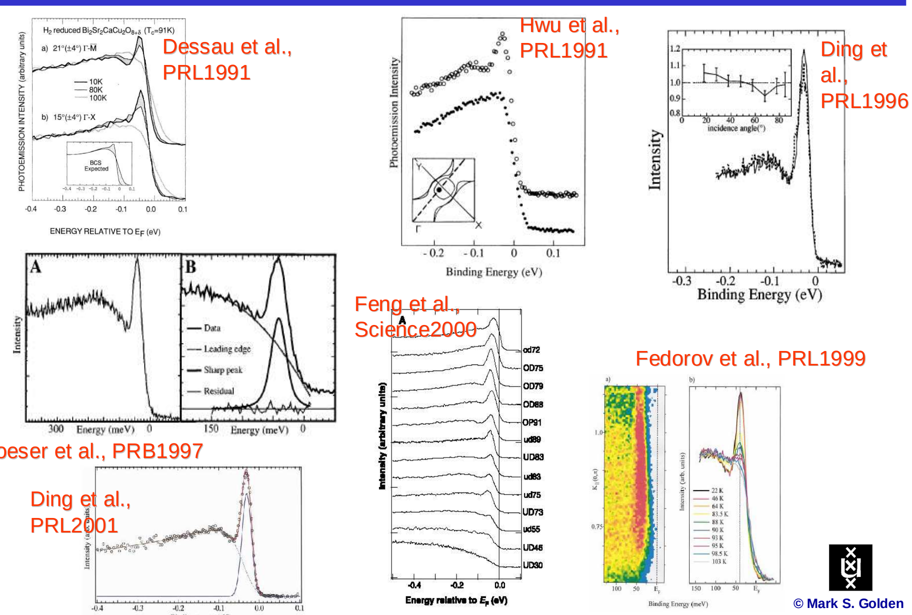
The (π,0) peak-dip-hump in overdoped Bi2212

superconducting state

The spectral function at (π,0) in the superconducting state



The $(\pi,0)$ superconducting state PDH

☆ $(\pi,0)$ peak-dip-hump lineshape in Bi2212 ☆

one of the seminal experimental results in HTSC canon

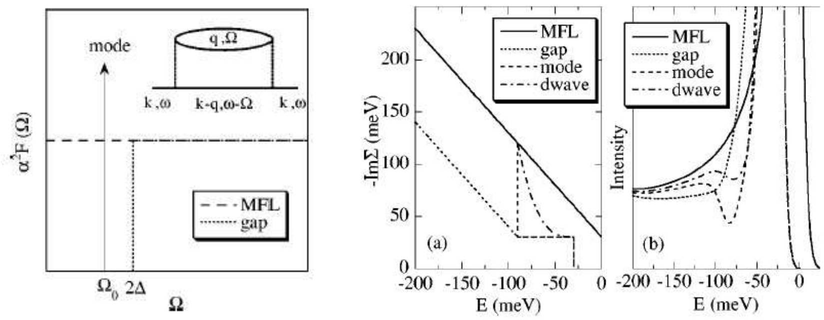
⇒ PDH lineshape in ARPES:
coupling to bosonic modes

- (π,π) resonant magnetic mode [INS]
  e.g. Campuzano PRL1999
- phonons
  e.g. Lanzara, Nature 2001

Potted history of the $(\pi,0)$ PDH in Bi2212 - I

- well developed picture for (π,π)-mode origin of 'classic' PDH
  experiment: Campuzano group
  theory: e.g. Norman, Abanov/Chubukov

Mode coupling ➔ peak-dip-hump in ARPES



Norman & Ding, PRB, 1998

coupling to (π,π) mode seen in INS results in peaked ImΣ

➔ eats away spectral weight at $\Delta_{sc} + \Omega$

➔ dip

! no BLS !

Potted history of the (π,0) PDH in Bi2212 - II

- well developed picture for (π,π)-mode origin of 'classic' PDH
  experiment: Campuzano group
  theory: e.g. Norman, Abanov/Chubukov
- 'classic' PDH becomes a cornerstone of the experimental evidence for spin fluctuation scenario
- importance of the (π,π)-mode doubted by Kee, Kivelson, Aeppli
- up till 2002 - all experimental data and models were without c-axis bilayer splitting……
- ….growing suspicion that band structure effects (bi-layer splitting) are involved Shen / Dessau / ourselves

The 'old' peak-dip-hump edifice

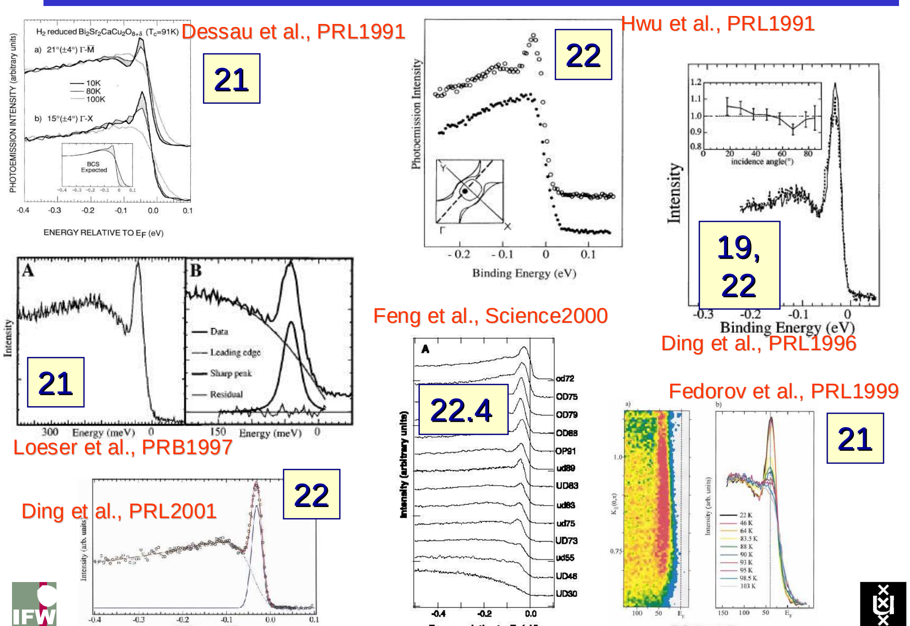
- PDH seen near (π,0) 'only' in sc state :

  $T < T_c$ (T_c ca. 90K) in Bi-2212 based materials

  - But: no PDH in sc state 1L (e.g. Bi2201) ARPES !

- PDH lineshape didn't alter on modifying **A**(z) (via incidence angle)
  - all spectra published to date are with hν 19-22 eV
- Dip position vs. doping: fits with (π,π) mode from neutrons
- Peak is non-dispersive along (0,0)-(π,0)-(2π,0)

All published PDHs are recorded with 19<hν<22.5 eV



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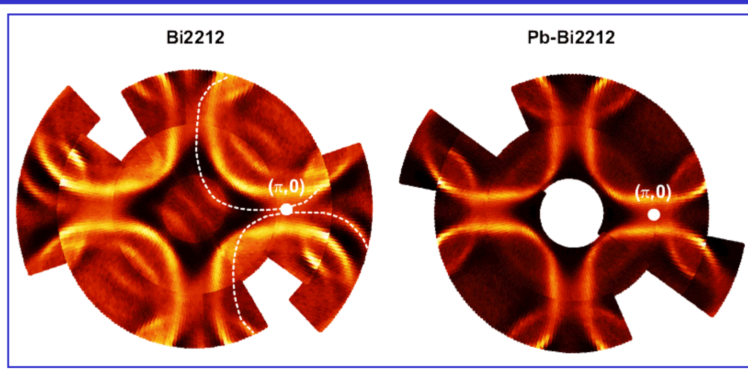
  - all spectra published to date are with hν 19-22 eV
- Dip position vs. doping: fits with (π,π) mode from neutrons
- Peak is non-dispersive along $(0,0)$-$(\pi,0)$-$(2\pi,0)$

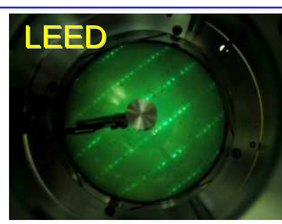
- the $(\pi,0)$ point of modulated Bi2212 is dangerous !

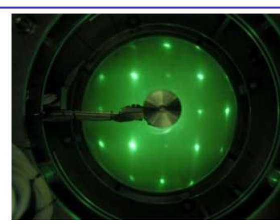
  → use modulation-free PbBi-2212

To Pb or not to Pb ?

$E=E_F$
300K
hν =
21 eV





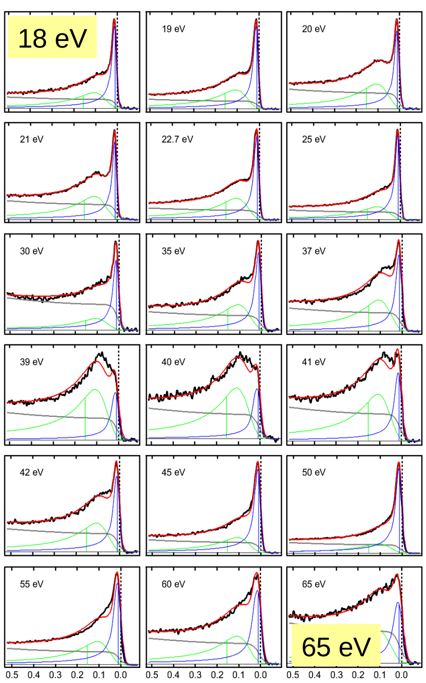


Kordyuk, Borisenko et al., 2001, IFW Dresden

The experiment

- accurately locate $(\pi,0)$ point from k-space maps
- measure $(\pi,0)$ EDC's from the s.c. state (T=25-45K) of modulation-free (Pb,Bi)2212 crystals
- use a wide hν range (without losing ΔE)
- overdoped (and underdoped) samples

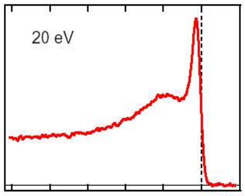
hν dependence - OD69K



let' s pick out some characteristic data…

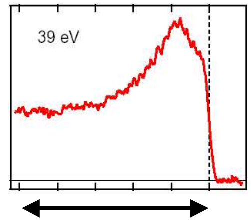
Kordyuk et al., PRL89, 077003 (2002)

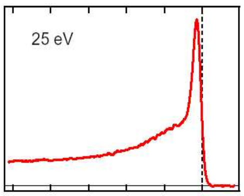
Cafeteria (self-service) lineshape - OD69K

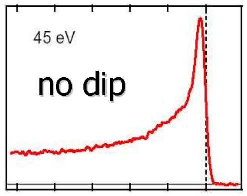


looks familiar . . .

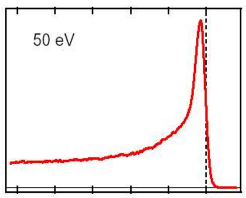
hump only







lineshape depends on photon energy



no dip, no hump

Kordyuk et al., PRL89, 077003 (2002)

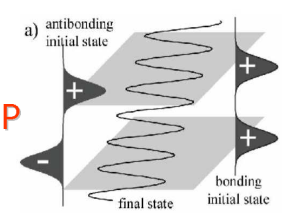
'Classic' PDH: not due to self energy effects !

- lineshape depends strongly on hν
  → it depends strongly on matrix elements
- self-energy can't depend on hν
  → reject the 'single spectral function' scenario for the 'classic' PDH

[also the 'SPR' linked to n_s or Z would be hν dependent]

Possible alternative:

two features: PEAK and HUMP which react differently to altering hν

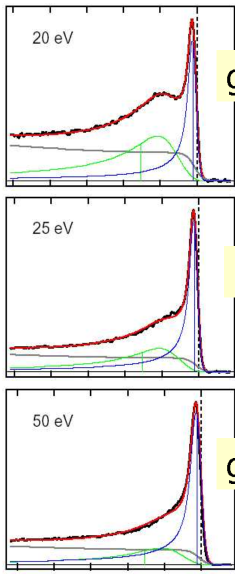


picture: © Feng et al.

Can we simulate the spectra ?

OD

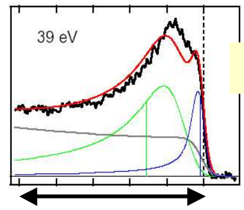
broad hν range



good !

good !

good !



poor

Toy model:

- spectral function 1
- spectral function 2
- background

Kordyuk et al., PRL89, 077003 (2002)

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Fitting function

$$I(\omega,T,h\nu) \propto [(M_a(h\nu)A(\omega,\varepsilon_a,T) + M_b(h\nu) \times A(\omega,\varepsilon_b,T))\, f(\omega,T)] \otimes R_\omega + B(\omega,T)$$

$$A(\omega,\varepsilon,T) \propto \frac{|\Sigma''(\omega,T)|}{(\omega-\varepsilon)^2 + \Sigma''(\omega,T)^2}$$

$$\Sigma''(\omega,T) = \sqrt{(\alpha\omega)^2 + (\beta T)^2}$$

$$\alpha = 1.1 \pm 0.1, \quad \beta = 2$$

Kordyuk et al., PRL89, 077003 (2002)

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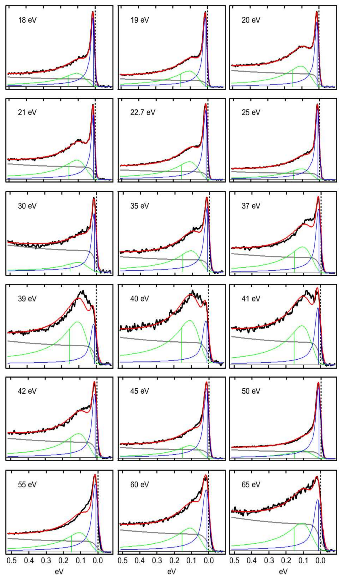
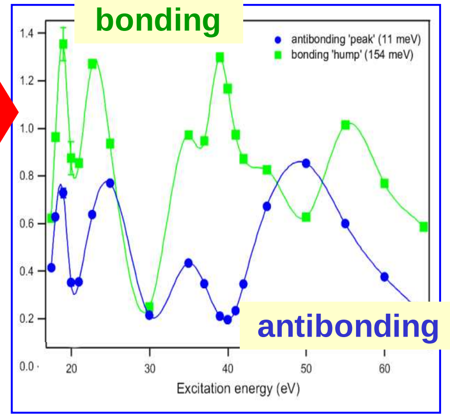
Fit vs. experiment: 'matrix elements'

OD





2 component fit

Kordyuk et al., PRL89, 077003 (2002)

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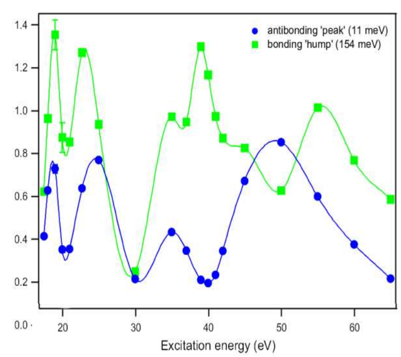
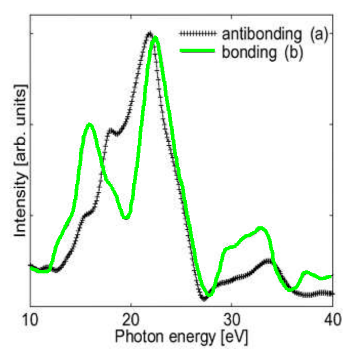
Toy model vs. one-step ARPES calculations

OD





Lindroos *et al.*,
PRB**65**, 054514 (2002)

bonding = 'hump'
antibonding = 'peak'

(π,0) OD

Kordyuk et al., PRL89, 077003 (2002)

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Consequences.....

- 'classic' PDH was a bastion as regards experimental evidence for spin fluctuation scenario

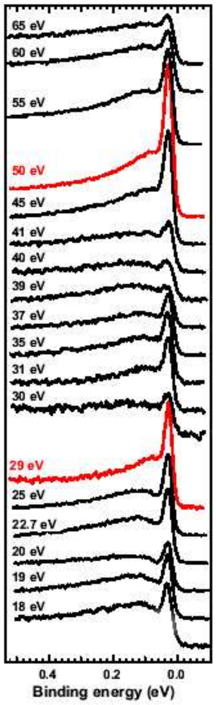
BUT:

- (π,π) mode interpretation not tenable for OD

IF in underdoped the situation is similar to OD....

Feedback effects near (π,0) in u n d e r d o p e d Bi2212

normal & superconducting state



hν dependence in UD 77K at (π,0)

- again, lineshape depends on hν

? is it the same as in overdoped ?

NO! subtle, yet crucial differences

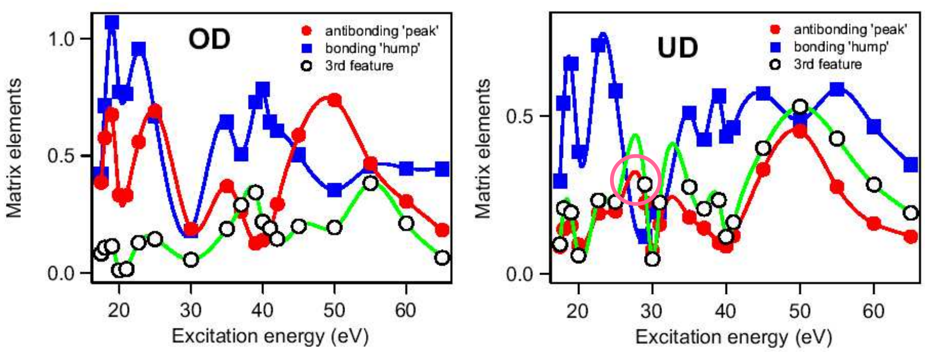
i) no spectrum without a dip or plateau

ii) details of hν dependence differ

⇨ toy model

Borisenko et al., IFW Dresden, cond-mat 0209435

Three component 'toy model' fits

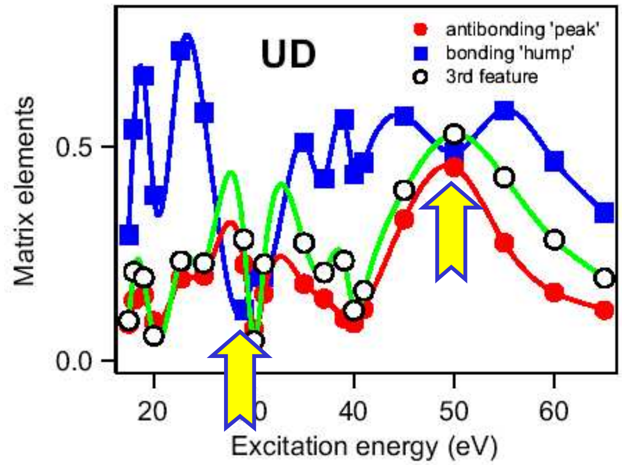


☆ Idea: ☆
select hν that shows
only AB band…..

third component clearly
follows AB band

Borisenko et al., IFW Dresden, cond-mat 0209435

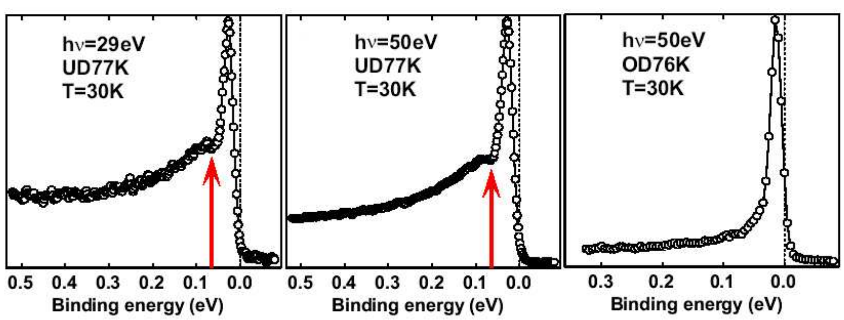
Targeting hν



Bonding band has local minima at hν 29 and 50 eV

…..these hν show 'pure' AB spectrum

(π,0) antibonding band EDC's

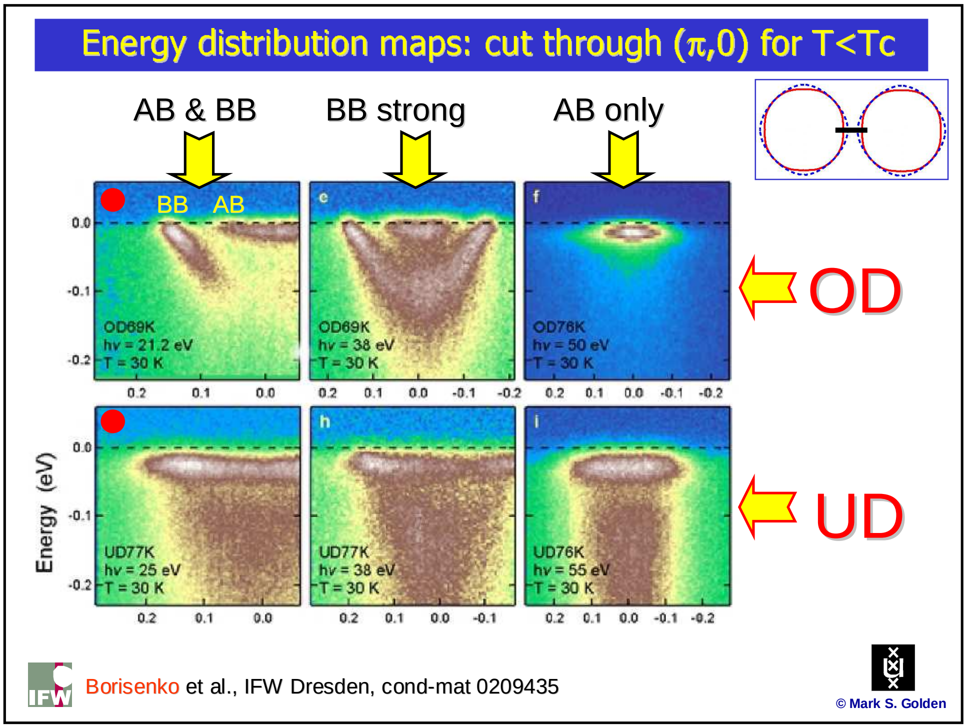


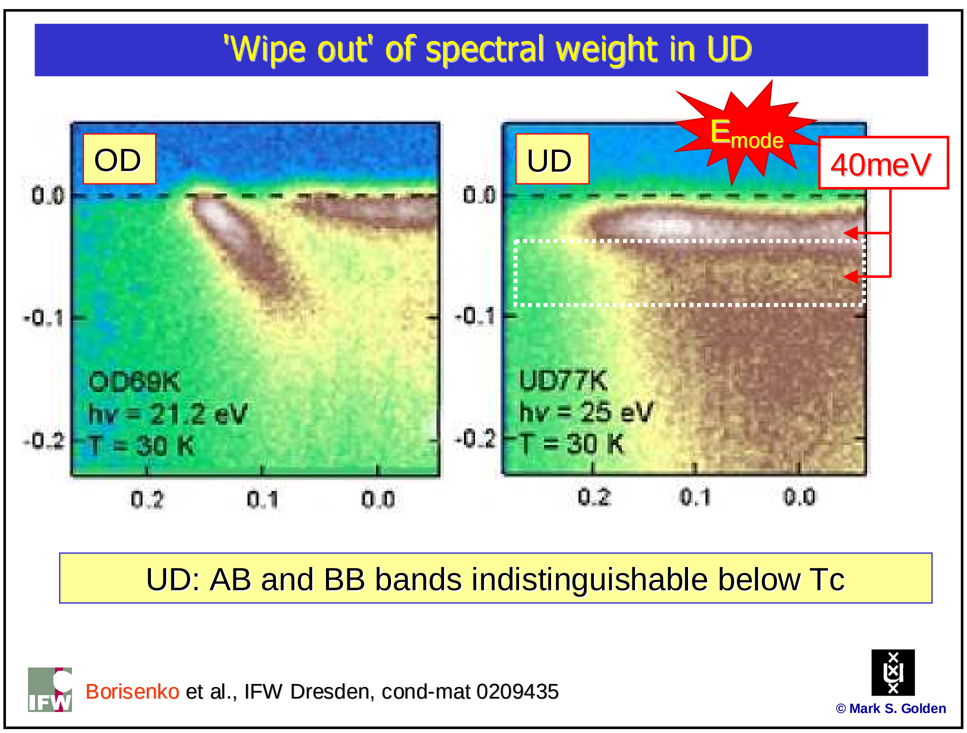
UD: dip or plateau   OD: smooth

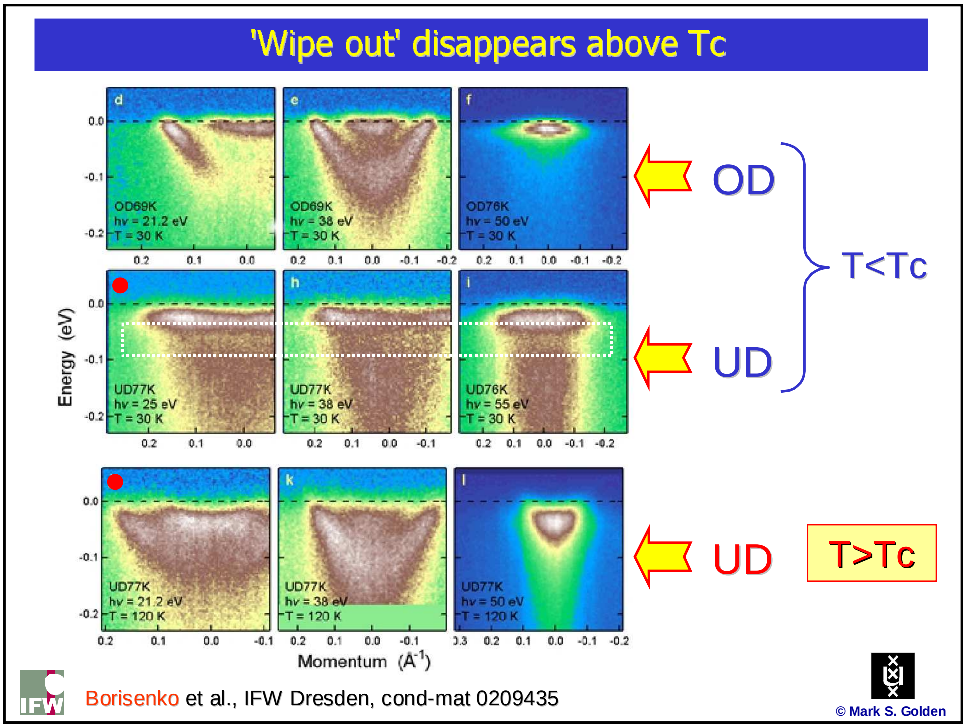
Antibonding band has an 'intrinsic' peak-dip-hump at (π,0)

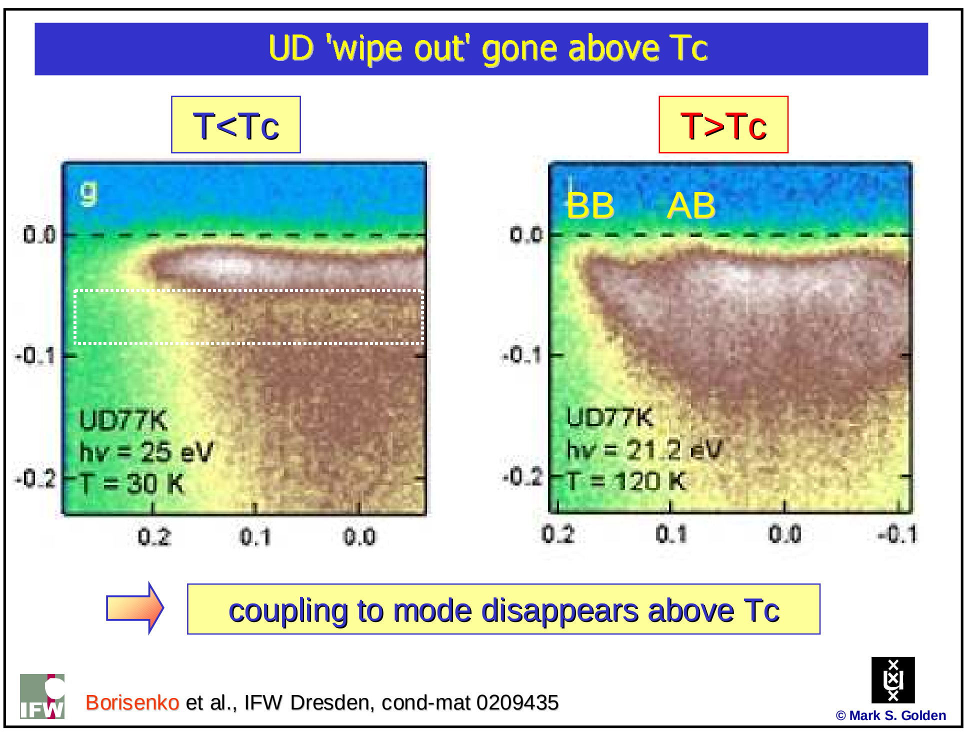
Peak ↔ dip separation = 38-40 meV E_{mode}

Borisenko et al., IFW Dresden, cond-mat 0209435


Energy distribution maps: cut through (π,0) for T<Tc
AB & BB
BB strong
AB only
BB AB
OD
UD
Energy (eV)
0.0
-0.1
-0.2
OD69K
hv = 21.2 eV
T = 30 K
OD69K
hv = 38 eV
T = 30 K
OD76K
hv = 50 eV
T = 30 K
UD77K
hv = 25 eV
T = 30 K
UD77K
hv = 38 eV
T = 30 K
UD76K
hv = 55 eV
T = 30 K
0.2 0.1 0.0 -0.1 -0.2
Borisenko et al., IFW Dresden, cond-mat 0209435
© Mark S. Golden

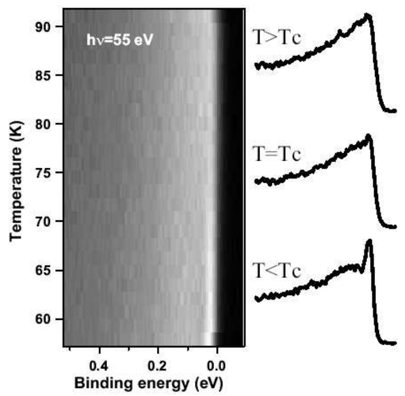

'Wipe out' of spectral weight in UD
OD
UD
E mode
40meV
0.0
-0.1
-0.2
OD69K
hv = 21.2 eV
T = 30 K
UD77K
hv = 25 eV
T = 30 K
0.2 0.1 0.0
UD: AB and BB bands indistinguishable below Tc
Borisenko et al., IFW Dresden, cond-mat 0209435
© Mark S. Golden


'Wipe out' disappears above Tc
OD
T<Tc
UD
UD
T>Tc
Energy (eV)
Momentum (Å^{-1})
Borisenko et al., IFW Dresden, cond-mat 0209435
© Mark S. Golden


UD 'wipe out' gone above Tc
T<Tc
T>Tc
BB AB
UD77K
hν = 25 eV
T = 30 K
UD77K
hν = 21.2 eV
T = 120 K
coupling to mode disappears above Tc
Borisenko et al., IFW Dresden, cond-mat 0209435
© Mark S. Golden

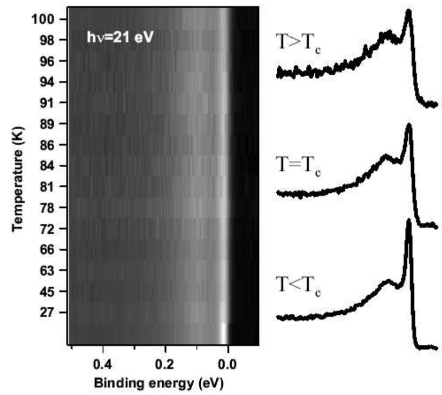
T-dependence of (π,0) PDH

UD



many body PDH gone above Tc

OD



band structure PDH remains above Tc

Borisenko et al., IFW Dresden, cond-mat 0209435

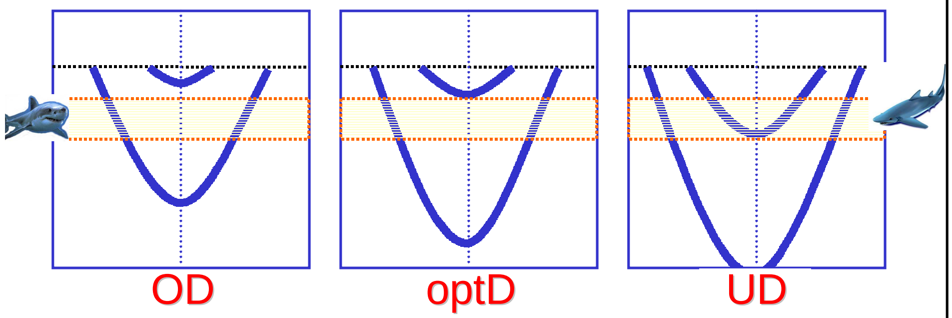
Fingerprints of the mode......

(π,π) mode

- lives at ca. 38-40 meV energy ✓
- strongest effects closer to (π,0) ✓
- only significant effects for T < Tc ✓
- coupling in UD much stronger than OD ✓
- odd symmetry w.r.t. bilayer (interband scattering) → data: Feng/Chuang, theory: Eschrig&Norman

Rehabilitation of the bi-layer splitting *

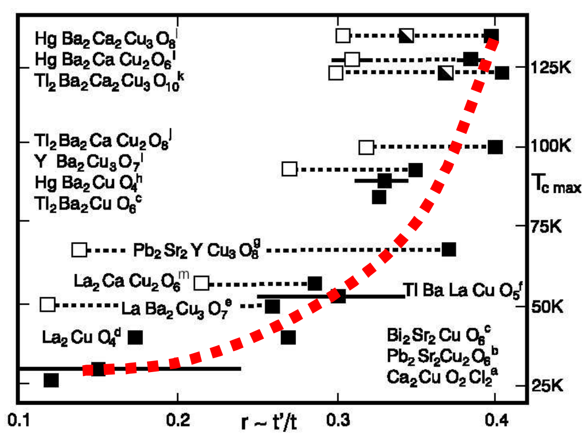
- multilayer splitting becomes an advantage:



materials' dependence of band structure + doping dependence of ε_{AB} and ε_{BB} + odd (interband) character of feedback =

* trying to make amends for the bashing the LDA-men got….

Correlation between T_c^{max} and r parameter

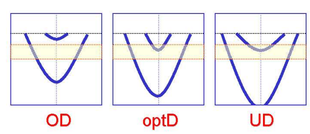


Pavarini et al., PRL **87** 047003 (2001)

r ~ t' /t of bonding band of multilayer HTSC

T_c^{max}

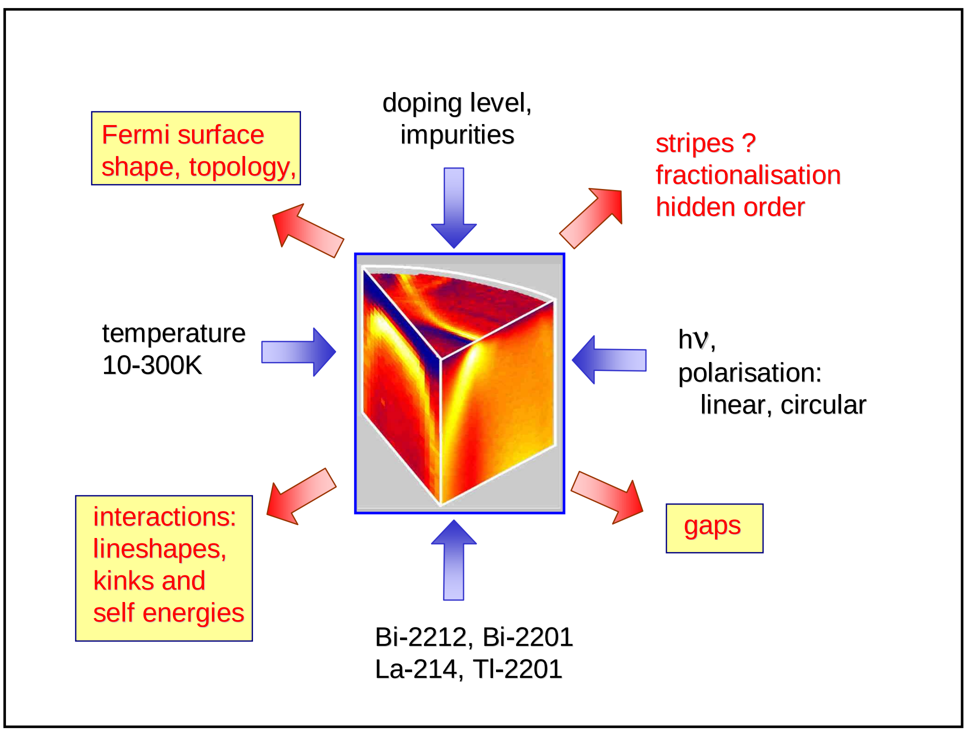
?



Outline

- ARPES as k-space microscopy
- results from the $Bi_2Sr_2CaCu_2O_8$ family
  - the Fermi surface
    - topology, or: *"to Pb or not to Pb"*
    - doping dependence
  - superconducting energy gap
  - peaks, dips and humps
    - in the overdoped regime
    - in the und… …oped regime
  - the shad… …mi surface

next workshop….



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Martin Knupfer	Thomas Pichler	Timur Kim
Roland Hübel	Dieter Müller	

Jörg Fink, Claus Schneider, Frank Matthes, Robert Frömter — IFF, IFW Dresden

Crystals

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B. Liang, A. Maliouk, C. T. Lin, Bernhard Keimer	MPI Stuttgart
Guang Yang Stuart Abell	U. of Birmingham, UK

Experimental collaboration

Fred Schiller, Serguei Molodtsov, Clemens Laubschat	TU Dresden IOMP
Rolf Follath	BESSY
Michael Sing, Ralph Claessen	U Augsburg
Stefano Turchini, Stefano Zennaro	ELETTRA
Cesare Grazioli	CNR Rome + ELETTRA

Crystal characterisation
K. Nenkov, D. Eckert — IMW, IFW Dresden

Money
FOM, EU, BMBF, DFG, SMWK