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SMR 1232 - 5

XII WORKSHOP ON
STRONGLY CORRELATED ELECTRON SYSTEMS

17 - 28 July 2000

THE ELECTRONIC STRUCTURE AND FERMI SURFACE OF Bi-2212 BASED HTSC FROM HIGH RESOLUTION ANGLE-SCANNED PHOTOEMISSION

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The electronic structure and Fermi surface of of Bi-2212 based HTSC from high resolution angle-scanned photoemission

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Outline of the talk

- The ARPES Holy Grail: A(**k**,ω) - what stands in our way ?
- 3D ARPES data-sets: Intensity (k_x, k_y, B.E.)
  - high (E,**k**)-resolved angle-scanned photoemission with full EDC's
- Some technical (but still important) points
  - correctly defining: E(k) dispersion and k_F
  - normalisation
- Data from pristine Bi-2212 and Pb/Bi-2212:
  - Fermi surface topology
  - shadow Fermi surfaces
  - diffraction replicas (only Bi-2212 !!)
  - doping dependence
  - ......
-

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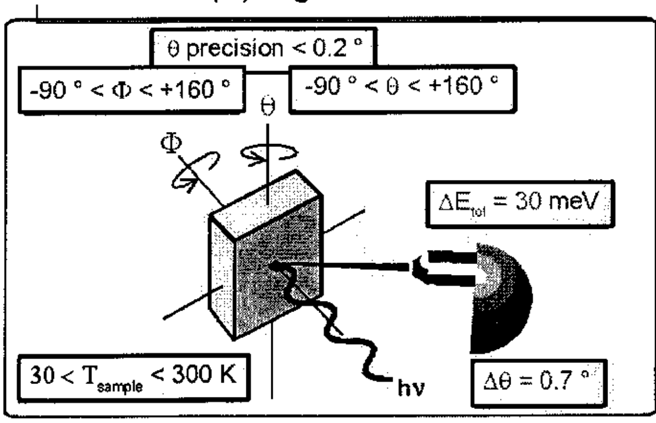
Experimental details

- **Single crystals:**
  - Bi-2212 - T_C = 87 K, ΔT_c = 2 K (Uni. Birmingham)
  - Pb/Bi2212 - T_C = 72 K, ΔT_c = 2 K (EPFL)
- **ARPES:**
  - VUV5000 light source (+TGM) + SCIENTA SES200 analyser
  - angle multiplexing mode Θ range = ±7 °; $\Delta\Theta$ = 0.7 °
  - purpose-built cryo-manipulator for angular scanning of polar (θ) and azimuthal (Φ) angles.



! unpolarised radiation !

- a big advantage for FS mapping as no states 'disappear' merely due to polarisation dependence of the ARPES matrix element.

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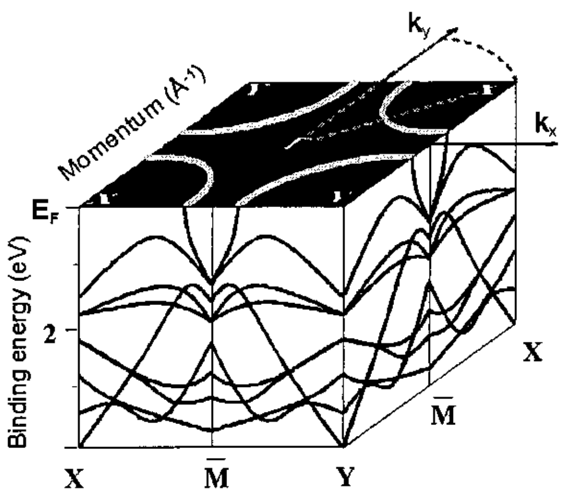
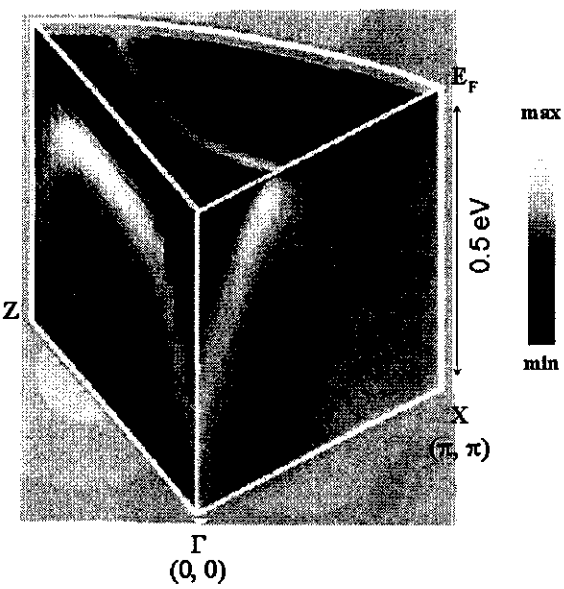
ARPES from quasi-2D systems:

photoemission intensity versus three variables - k_x, k_y, E_B





$(Pb,Bi)_2Sr_2CaCu_2O_{8+\delta}$

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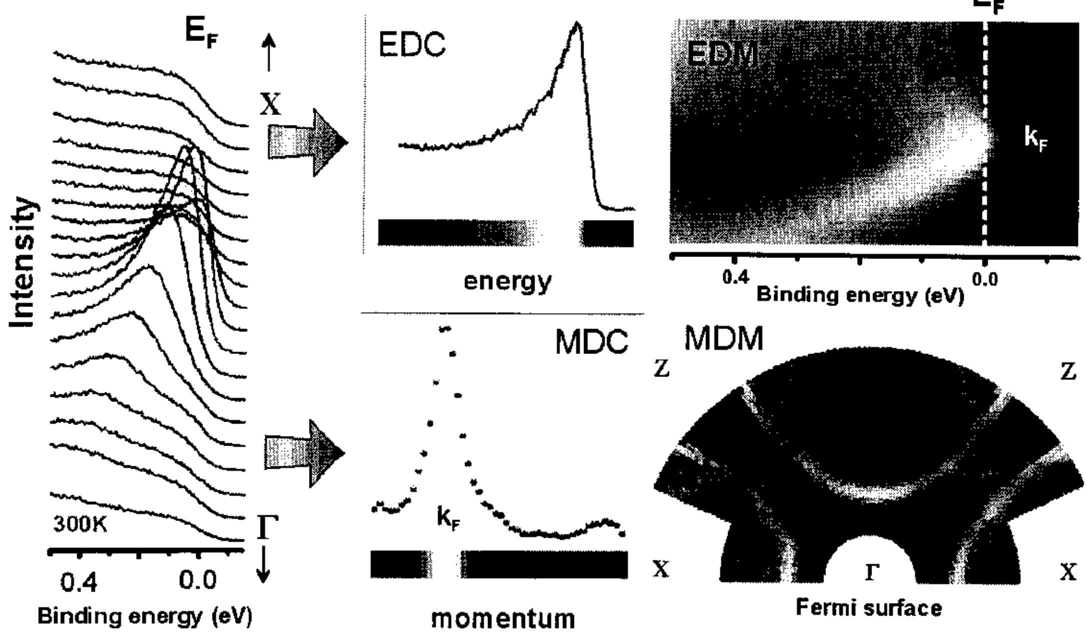
Energy and momentum distributions from ARPES



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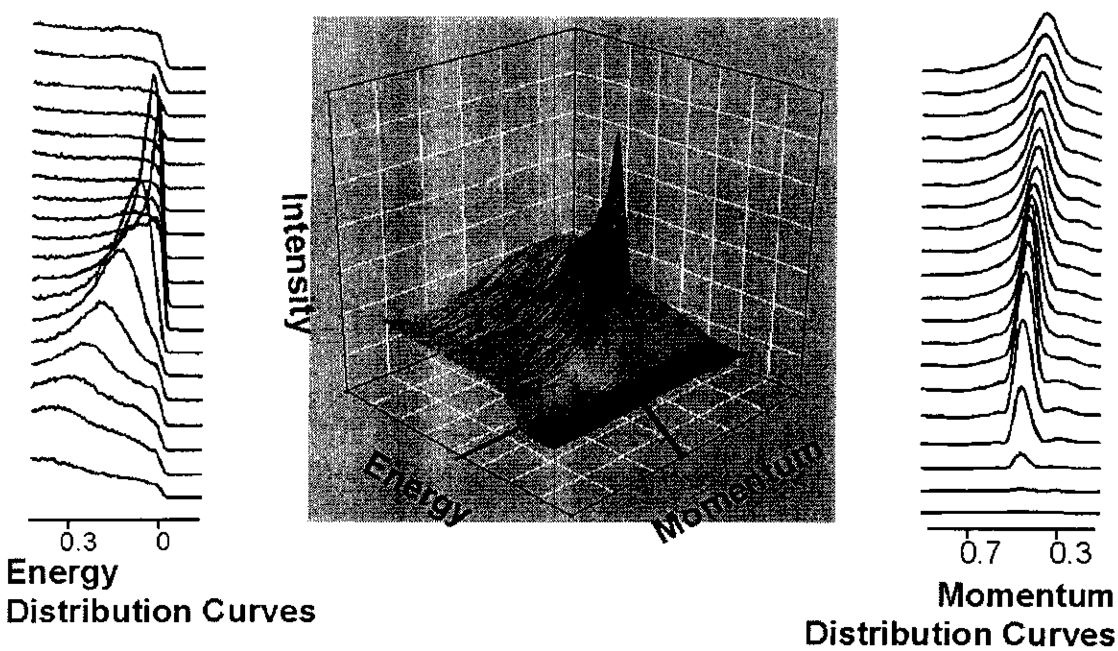
EDC's and MDC's



Pb/Bi-2212 along the nodal line (T=30K)

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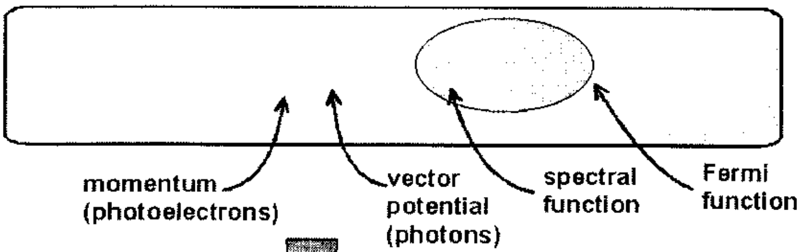
The ARPES Holy Grail - the spectral function A(**k**,ω)



$$I_{real}(\vec{k},\omega)=I_0\sum_{\vec{k}'}\int_{-\infty}^{+\infty}R(\omega-\omega')f(\omega')A(\vec{k}',\omega')d\omega'$$

matrix elements

momentum resolution

energy resolution

temperature

$$I_{obs}(\vec{k},\omega)=C_{extrinsic}\cdot I_{real}(\vec{k},\omega)$$

extrinsic parameters

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What stands between us and A(**k**,ω) ?

Intrinsic factors

- **Matrix elements:**
  - photon energy
  - polarisation conditions
  - emission angle → absolute $k_{||}$ value (e.g. which Brillouin zone?)
- **momentum resolution**
- **energy resolution**

Extrinsic factors

- **time-dependent photon flux (synchrotron only)**
- **geometric effects: hν vs. analysed spot as function of angle**
- **analyser effects: transmission vs KE; parallel detector calibration**
- **surface flatness/quality: not just dirt - also limits effective $\Delta k_{||}$!**

.....measure with favourable conditions and use a good normalisation

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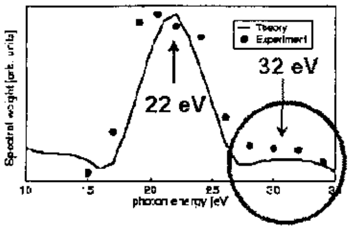
Matrix elements

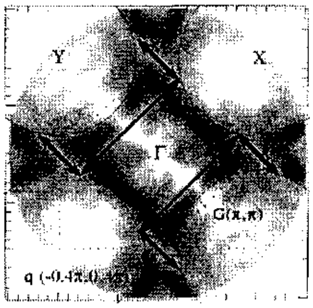
- **value of the photon energy**



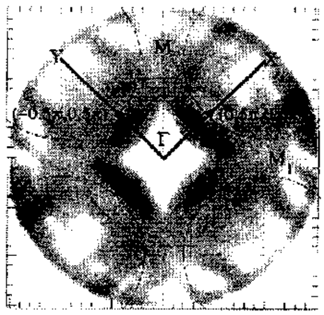
Spectral weight around the (π, 0) point versus photon energy.

A. Bansil and M. Lindroos
PRL 83, 5154 (1999)

- **polarisation of light**
  e.g. Bi-2212, optimal doping, T_{exp} = 300K
  ARPES intensity $E=E_F$, recorded with linearly polarised light (32eV)



'even'



'odd'

A. Bianconi *et al.*,
Physica C, 317–318, 304 (1999)

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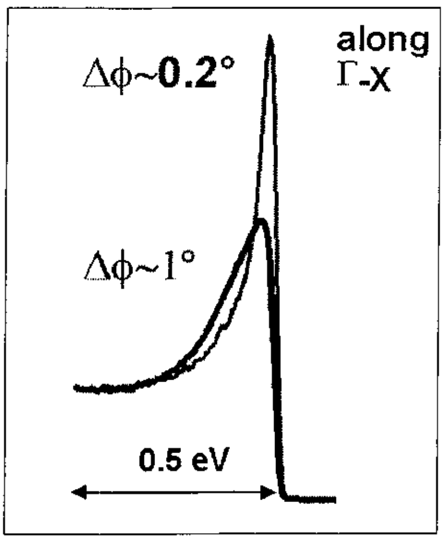
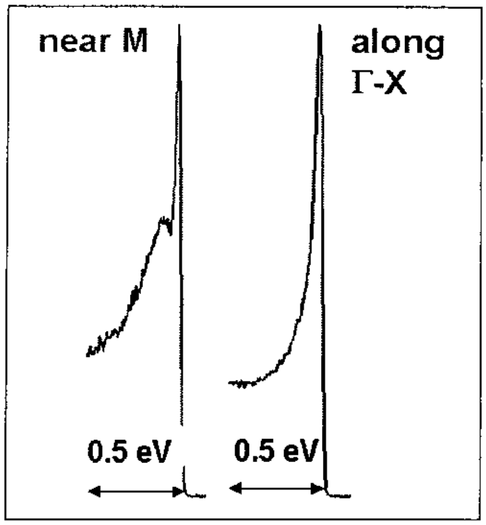
Matrix elements continued....

- **momentum resolution**



- **energy resolution (ΔE<25 meV)**



Pb/Bi-2212
$h\nu$ = 21.22 eV

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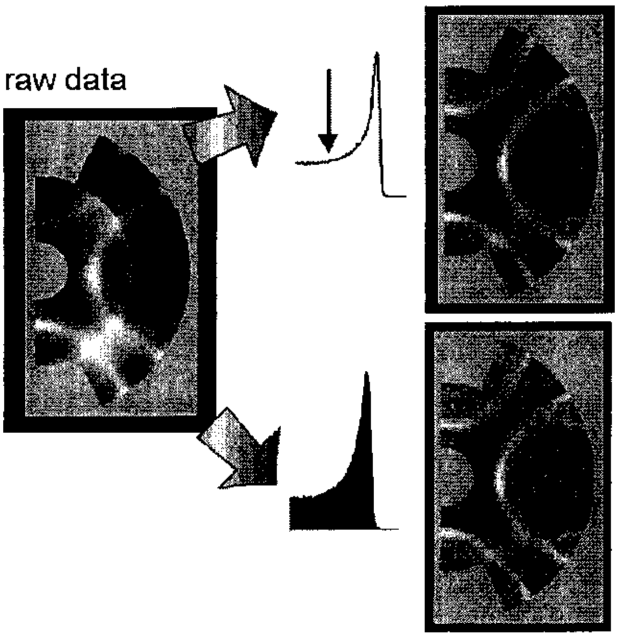
Normalisation

- Pb/Bi-2212 - ARPES intensity, $E=E_F$, $h\nu=21$ eV, T_{exp} = 300K



A good normalisation doesn't change the FS topology !!

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How should one extract k_F from ARPES data ?

- 'Older' methods:
  - extrapolate the peak dispersion in EDCs
  - intensity method

- Newer:
  - leading edge
  - symmetrisation
  - integrated ARPES intensity: "n(k)"
  - steepest descent of integrated ARPES intensity: del "n(k)"
  - delta T
  - maximum in momentum distribution curve

A good k_F method applied to well-normalised data
is maximally impervious to matrix elements

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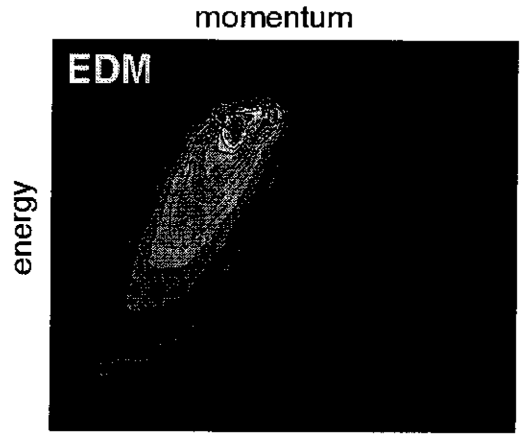
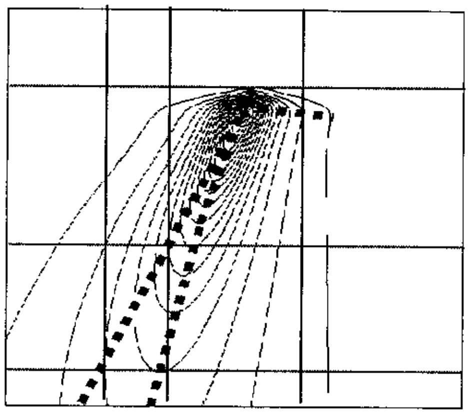
k_F determination continued...

- Extrapolation of EDC's





FS crossing along nodal line
Pb/Bi-2212

EDC dispersion
MDC dispersion

Are methods based on EDC dispersion still trustworthy ?

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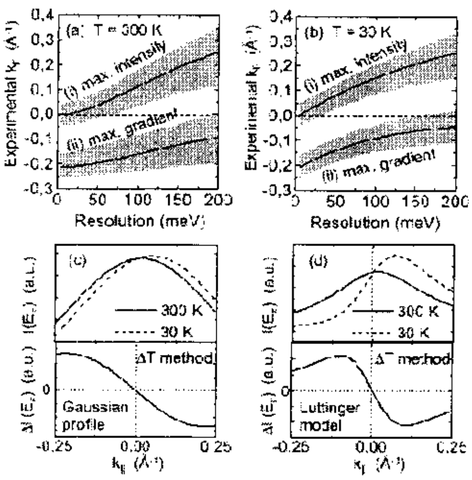
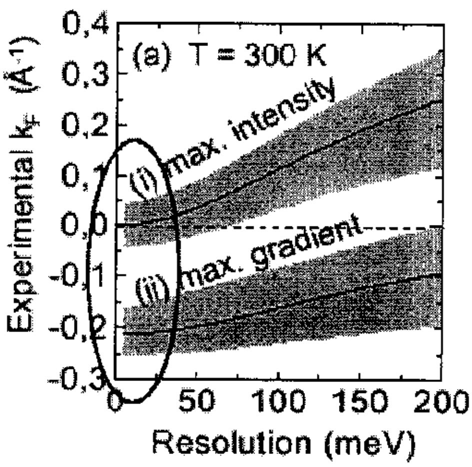
k_F determination continued...

- delta T vs. max. intensity vs. max. gradient





L. Kipp et al.,
PRL 83, 5551 (1999)

even if we *could* measure del_n(k), it's not accurate

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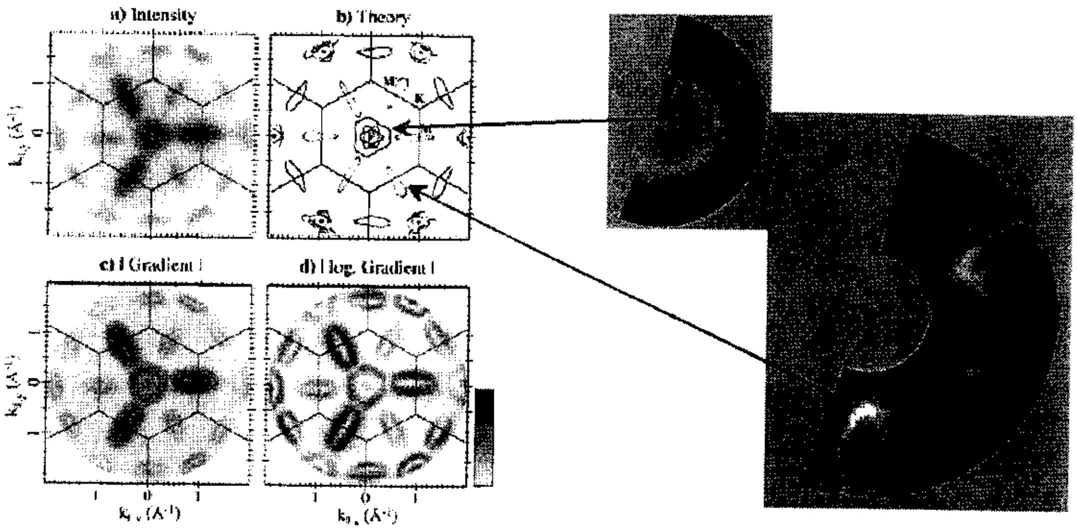
A test of the max_MDC method: $TiTe_2$

- systems with flat bands can be dealt with: e.g. $TiTe_2$



Th. Straub *et al.* PRB, 55, 13473 (1997)

- no need for |gradient|
- FS loop already hollow using max MDC

The maximum of a sharply peaked, normalised MDC = k_F

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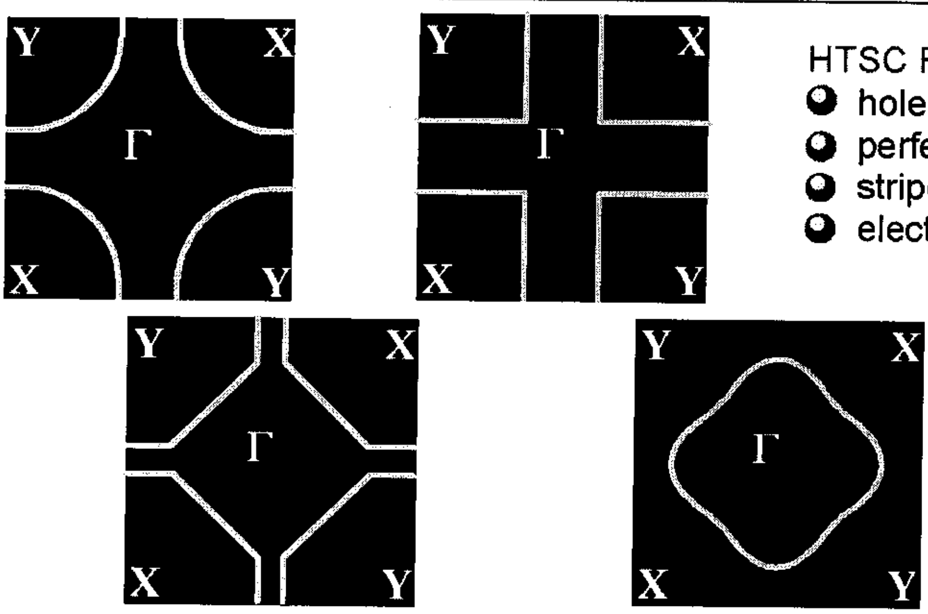
The context



HTSC Fermi surface:

- hole-like ?
- perfect nesting ?
- stripes ?
- electron-like ?

!! These are vital questions that need to be cleared up !!

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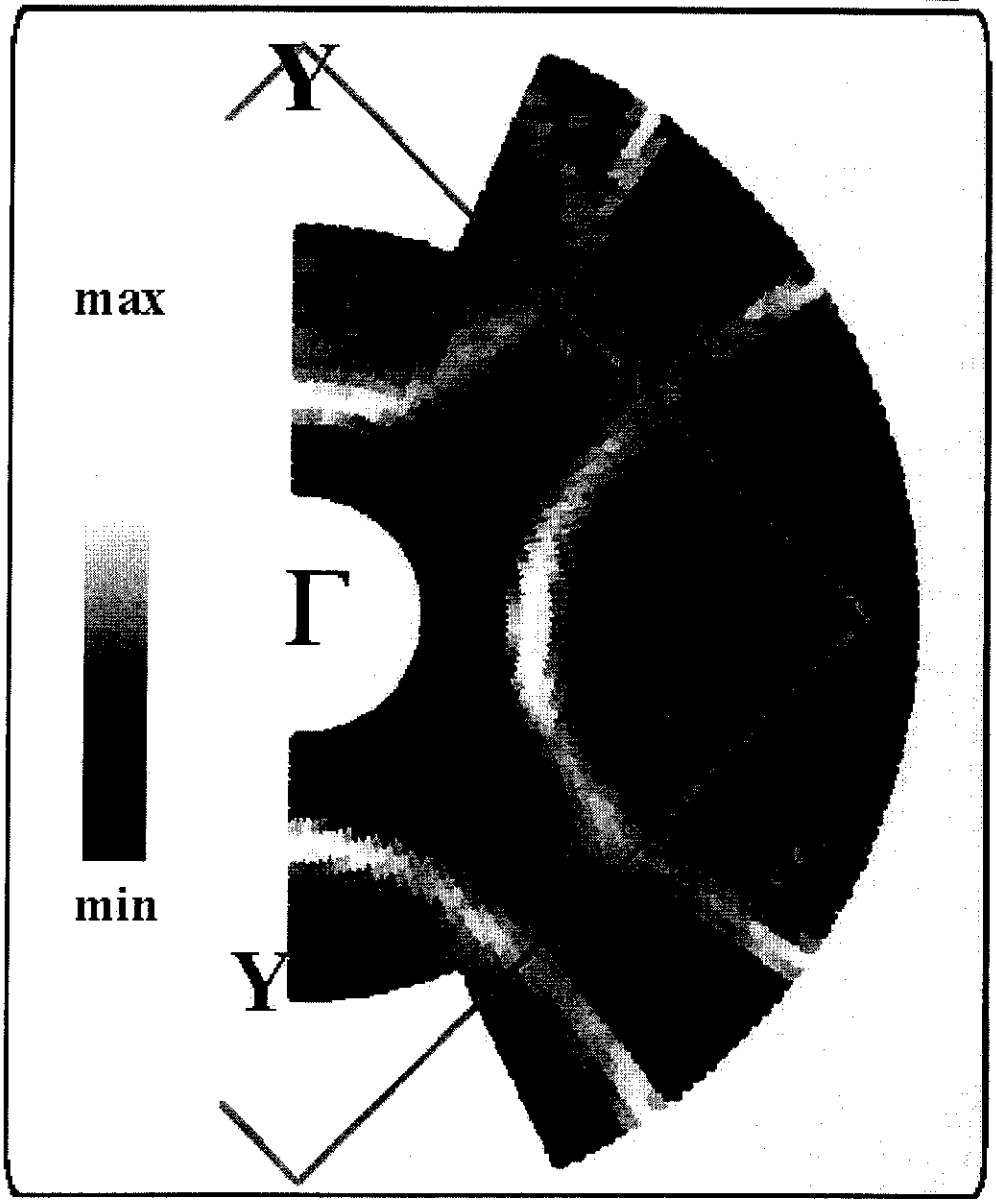
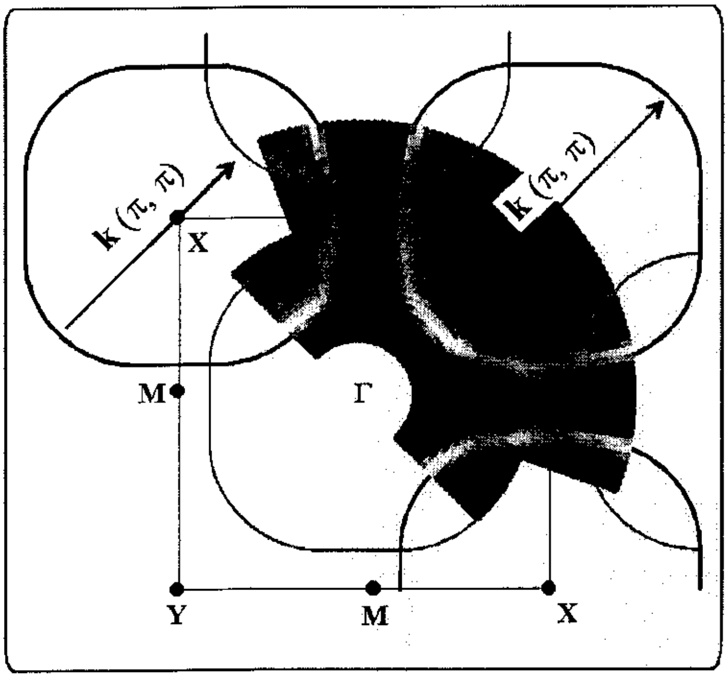
Pb/Bi-2212 Fermi surface map   T = 300 K



Golden et al., Adv. Solid State Physics 2000

Fermi surface features: Pb/Bi-2212



T = 300 K

- clear main FS:
  barrels centred at X,Y
- clear shadow FS:
  (π,π) shifted versions
  of the main FS

...every pixel
hides an EDC

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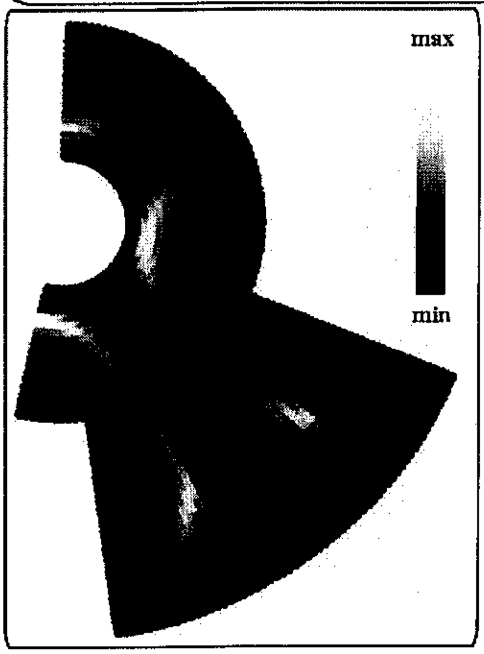
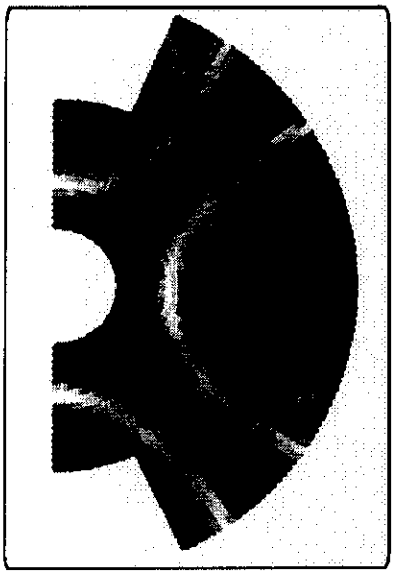
Temperature dependence of the FS of Pb/Bi-2212



T = 120 K



T = 300K

Borisenko *et al.*, Phys. Rev. Lett. **84**, 4453 (2000)

Golden *et al.*, Adv. in Solid State Physics 2000

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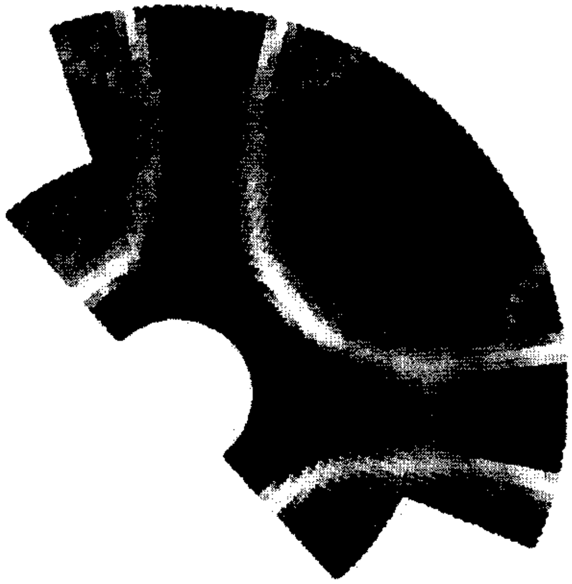
Stripes in Pb/Bi-2212 ? (OD 72K)



- no extended straight sections of FS around $(\pi,0)$

  > perfect nesting only for small areas of the FS

- FS robust along (0,0) - (π,π)
- little similarity to Nd-stabilised LSCO (Zhou et al. Science 1999)

incompatible with stripes for overdoped Pb/Bi-2212

...remember - every pixel hides an EDC

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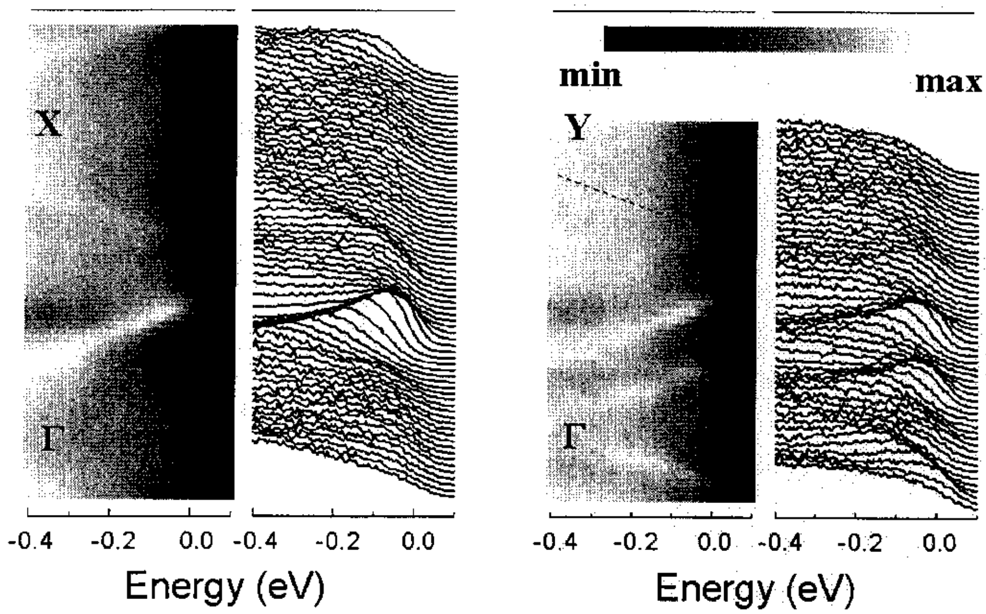
EDCs - Bi-2212 T=300K



Borisenko et al., Phys. Rev. Lett. **84**, 4453 (2000)

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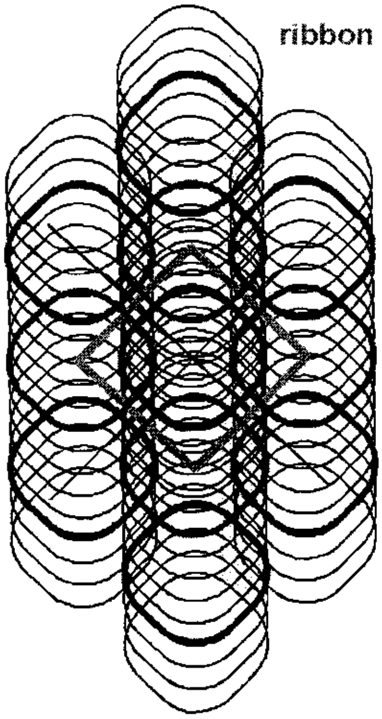
The role of the *diffraction replica* features in Bi-2212



- diffraction replicas of the main FS shifted by ca. 0.21(π,π)
- DR's add up to give bright ribbons along (0,-π)-(π,0)

The picture around (π,0) is complex:

- main FS
- shadow FS
- DR's

. . . *take care !*

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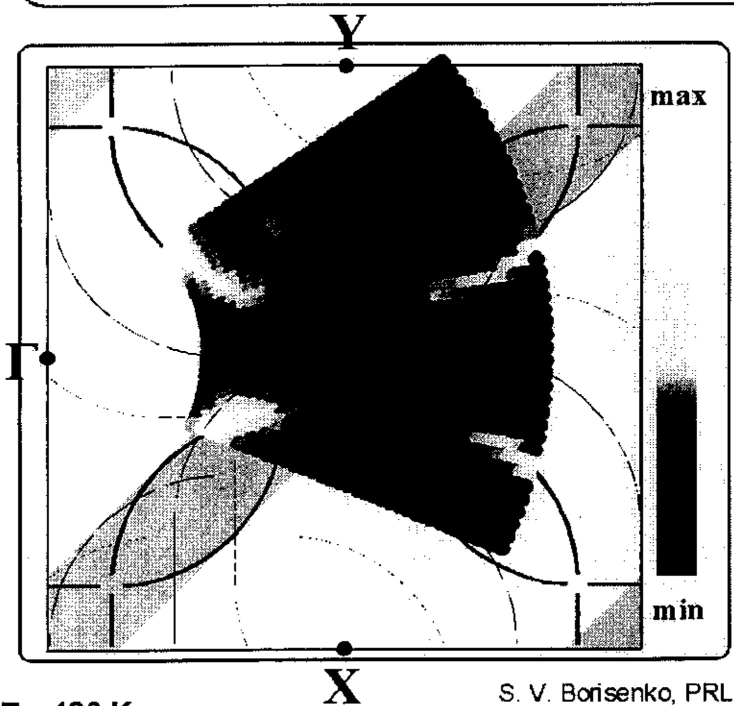
Bi-2212 - the situation around (π,0)



- **main FS**
- **shadow FS**
- **DR's**

- **the overlap of all these features gives rise to a high intensity ribbon (grey shading)**

situation around (π,0) is highly complex !

T = 120 K

S. V. Borisenko, PRL, in press
cond-mat /9912289

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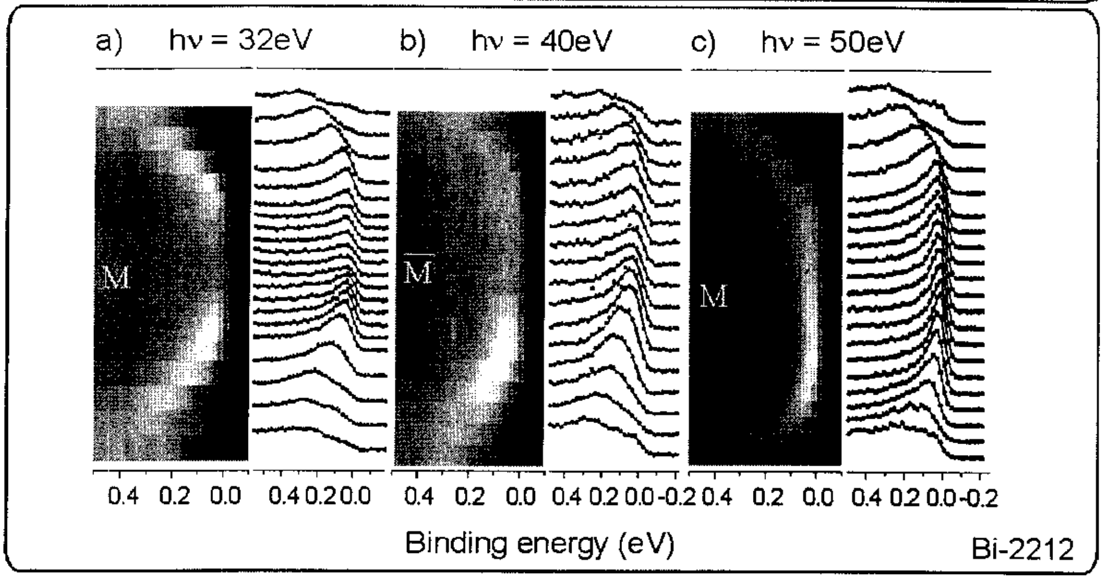
EDCs along (0,0)-(2π,0) versus photon energy



- ☆ Spectral weight aroung (π,0) reduced for hν = 32 eV and hν = 40 eV
- ☆ BUT: clear extended saddle point behaviour for hν = 50 eV (as for 21.2 eV)
- ☆ Is the spectral weight reduction at (π,0) from a main FS crossing ?

Legner et al., PRB**62**, 1 July 2000

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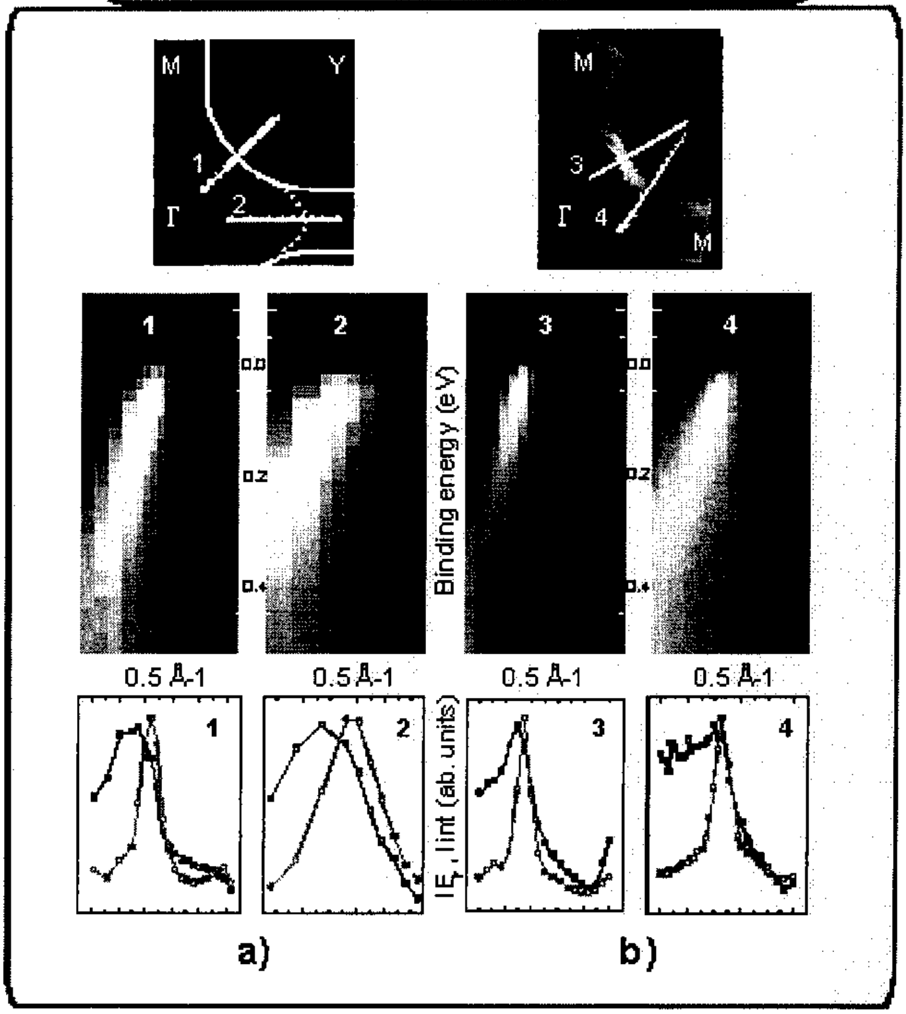
Analysis of the Γ-M-Z spectra

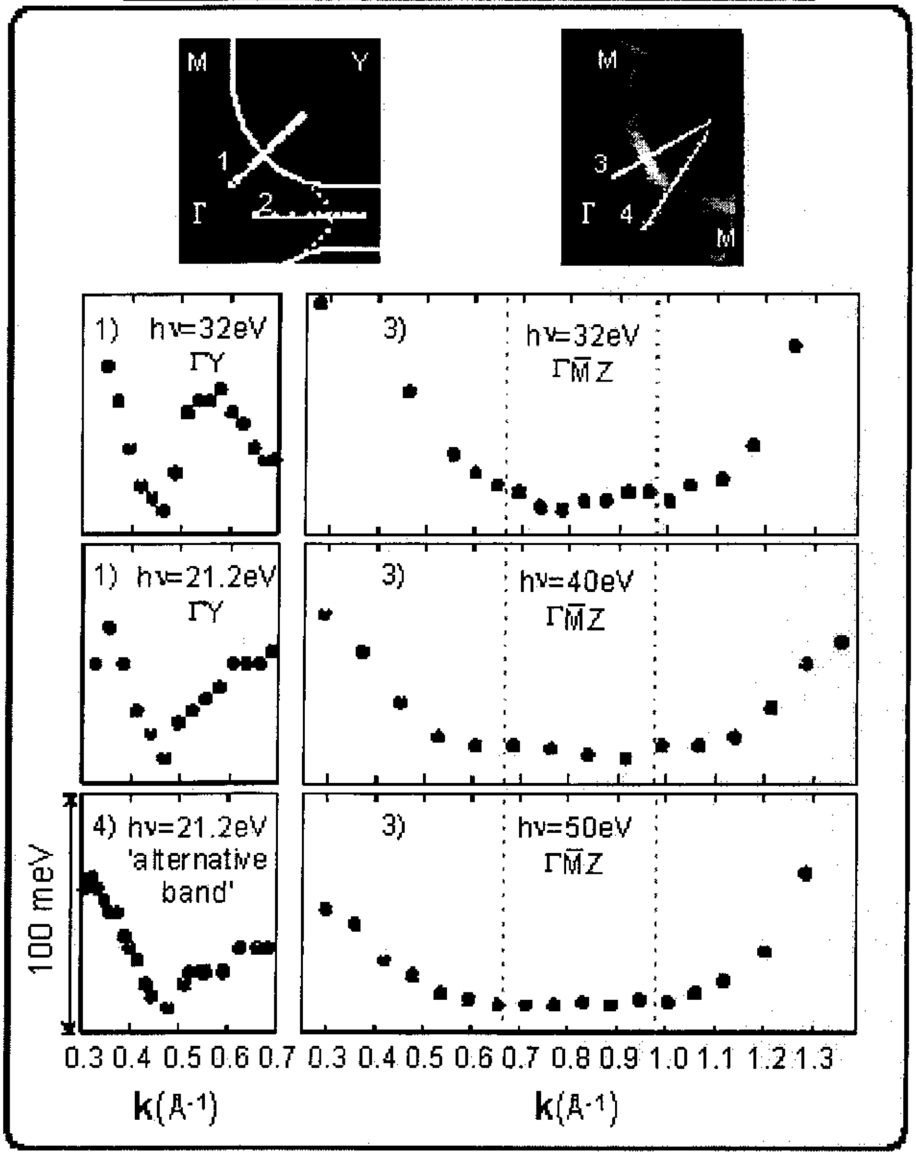


ARPES of:
(a) Bi2212 hν =32 eV
(b) Pb-Bi2212 hν =21.2eV

Legner et al., IFW
cond-mat /0002302

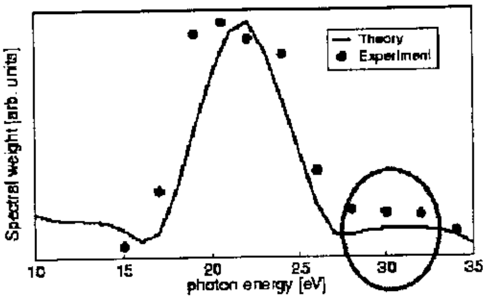
★ Bands 1, 3 & 4 are main FS crossings
Band 2 is the 'odd one out'

Analysis of the leading edge BE



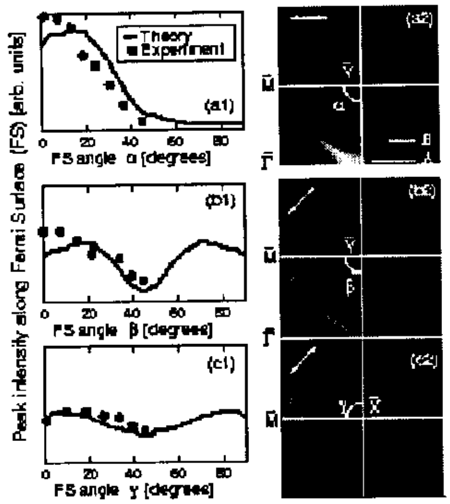
S. Legner et al, IFW
cond-mat / 002302

Strong effects of matrix elements



Spectral weight around the (π, 0) point versus photon energy.

A. Bansil and M. Lindroos
PRL 83, 5154 (1999)



Intensity distribution along the Fermi surface + simulated ARPES FS maps for different polarizations.

- Flat band (π,0) spectral weight suppressed for $h\nu \sim$ 28-35 eV
- FS maps depend on polarisation conditions (ARPES with SR)

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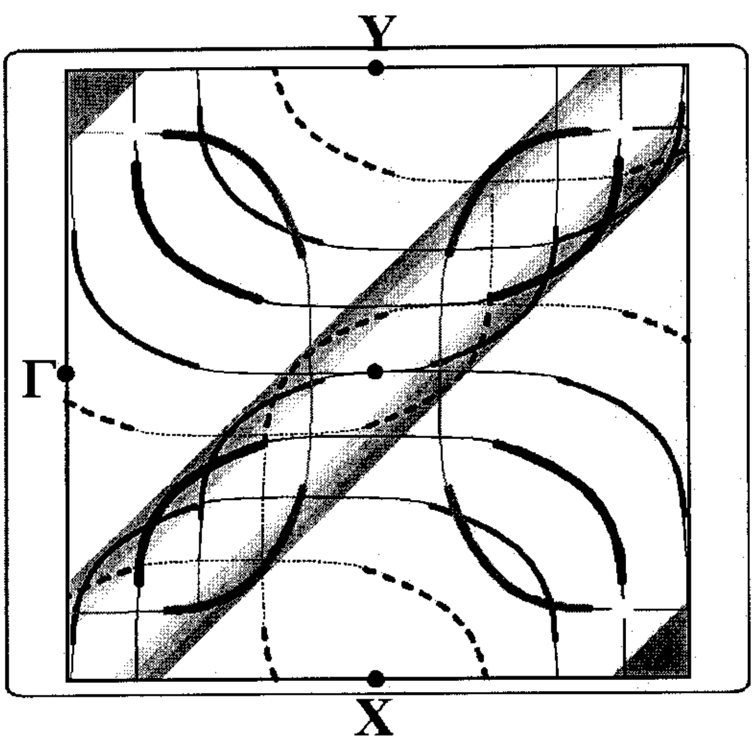
Bi-2212 - the situation around (π,0) for $h\nu$ = 32 eV



- matrix elements suppress ESPS emission for $h\nu$ = 32 eV
- hollows out ribbon

⇩

- two lines
- *appear* like FS crossings as one goes from (0,0) to (2π,0)

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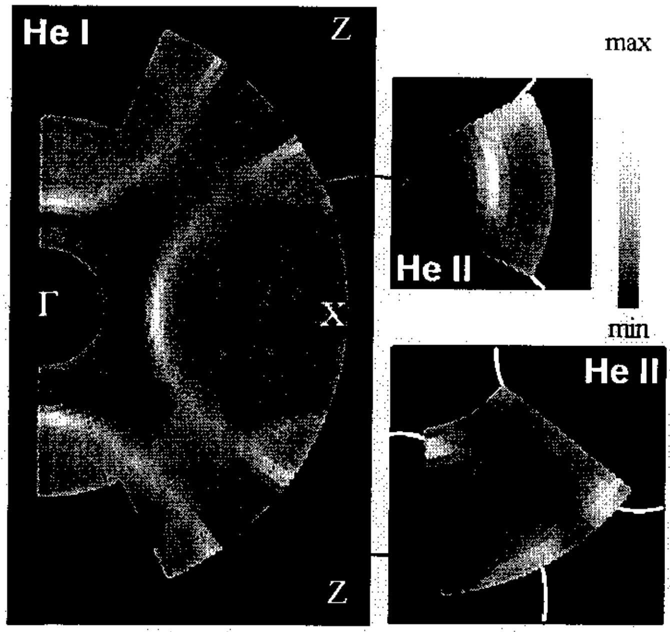
FS topology as a function of photon energy



- hν = 40 eV appears to be in the 'doubtful' hν range

however

- FS topology for He I and He II radiation is identical.

- Thus, the thue FS topology is:

hole-like barrels centred at the X,Y points

no FS crossing along ΓMZ

Pb/Bi-2212 Legner et al., PRB**62**, 1 July 2000

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Conclusions

- Angle-scanned photoemission with full, high E,**k** resolved EDCs is a powerful route towards attaining A(**k**,ω)
  BUT:
  - be aware of polarisation
  - use a fine k-mesh (100% real data)
  - normalise MDCs (divide out extrinsics, minimise $|M|^2$)

- the sharp maximum of a normalised MDC for $E=E_F$ gives k_F and thus the Fermi surface topology

- Pb-doped Bi-2212 (no incommensurate Bi-O plane modulation!) is *the* substance for studying FS topology, lineshapes, ...

- All our data fit naturally into a picture of a **hole-like, X/Y-centred** normal state Fermi surface

- Very clear shadow Fermi surface: appears not to be a pi,pi shifted version of the main FS -> lenses centred at (pi/2,pi/2)

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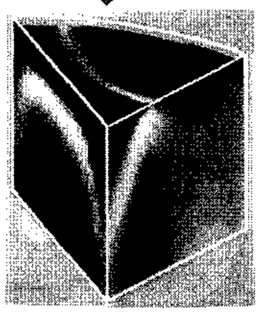
Angle-scanned ARPES with EDC's:
a self-consistent and coherent picture of HTSC from ARPES

Fermi surface topology

Doping

Superconducting and pseudo gaps

Temperature (30 to 300 K)



Photon energies, polarisation

Line shape, QP spectral weight, self-energy

Dispersion, Fermi velocity, scattering rate

Systems: BSCCO, LSCO, YBCO...?

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With essential input from :

- Dr. Sergey Borisenko (Spectroscopy Group)
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  Sibylle Legner
  Dr. Thomas Pichler
  Dr. Martin Knupfer
  Dr. Roland Hübel
  Dieter Müller
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