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I.C.T.P., P.O. BOX 586, 34100 TRIESTE, ITALY, CABLE CENTRATOM TRIESTE

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MINIWORKSHOP ON STRONG ELECTRON CORRELATIONS
"Disorder and Interaction in Quantum Systems and Their Classical Analogs"

(1 - 19 July 1996)

"High T_c Superconductors"

Mohit Randeria
Tata Institute of Fundamental Research
Theoretical Physics Group
Bombay - Mumbai 400 005
India

These are preliminary lecture notes, intended only for distribution to participants.

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HIGH T_c SUPERCONDUCTORS

NEW INSIGHTS FROM ANGLE-RESOLVED PHOTOEMISSION (ARPES)

MOHIT RANDERIA, TIFR, Bombay

collaborators:

HONG DING
JUAN CARLOS CAMPUZANO } ANL, UIC

MIKE NORMAN ANL

Samples: K. KADOWAKI, T. MOCHIKU
T. TAKAHASHI, T. YOKOYA

References:

- $n(\mathbf{k})$, sum rules:
  M. Randeria et al., PRL 74, 4951 (1995)
- dispersion; FS; bilayer splitting etc.:
  H. Ding et al., PRL 76, 1533 (1996)
- SC gap:
  H. Ding et al., PRL 74, 2784 (1995)
  PRL 75, 1425 (E) (1995)
  cond-mat/9603044
- gap, SL + selection rules:
  M. Norman, M. Randeria, H. Ding & J.C. Campuzano
  PRB 52, 615 (1995)
  PRB 52, 15107 (1995)
- p-h mixing in SC:
  J.C. Campuzano et al, PRB 53, RC 14737 (1996)
- pseudo gap:
  H. Ding et al, Nature July 4th (1996)

Why has ARPES played a major role in high T_c SC?

* improved resolution:

ω : FWHM $\gtrsim$ 15 meV

$\vec{k}$: $\pm 1°$

* large gaps, high T_c's

* quasi 2D → $\vec{k}$ determined uniquely

but: short escape depth
⇒ surface sensitive probe!

Bi 2212

- Bi-O bilayer → natural cleavage plane
  van der Waals bonds
- quasi 2D — no "surface states"
- compare w/. bulk probes

Outline:

* what does ARPES measure?

* $A(\vec{k}, \omega)$ interpretation
  - sum rules
  - new probe of $n(\vec{k})$

* electronic excitations in Bi 2212
  - dispersion
  - Fermi surfaces

  } band-like features

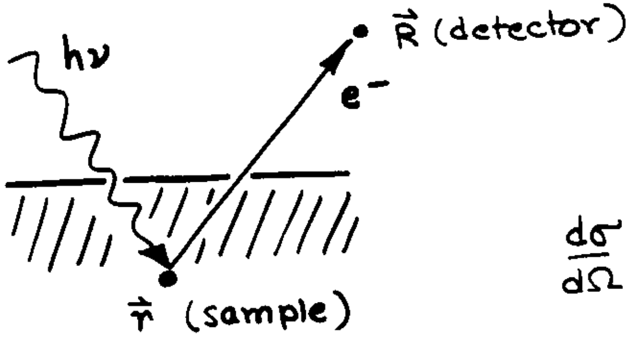
  - linewidth
  - dip (below T_c)
  - absence of bilayer splitting

  } many-body features

* SC gap anisotropy $|\Delta(\vec{k})|$ in Bi 2212
  - spectral fn. fits
  - polarization selection rules

* pseudo-gap: $T > T_c$, underdoped

What does photoemission measure ?



$$\frac{d\sigma}{d\Omega} \sim \langle J(\vec{R}t) \rangle$$

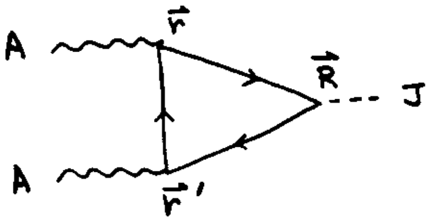
$$\langle J(\vec{R}t) \rangle = \underbrace{\langle 0 | J(\vec{R}t) | 0 \rangle}_{=0}$$

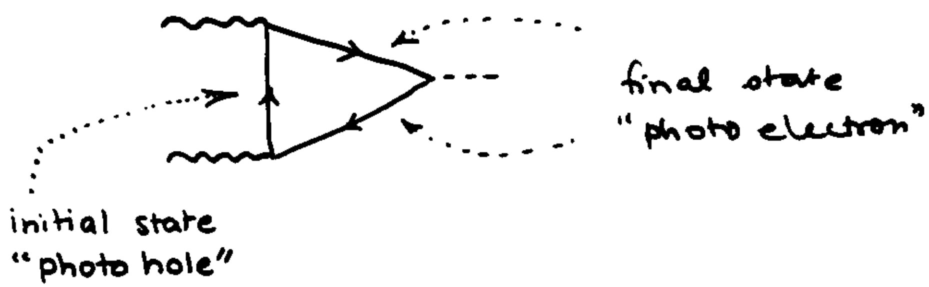
$$+ \int_{\vec{r}\tau} \underbrace{\langle 0 | J(\vec{R}t)}_{=0} J(\vec{r}\tau) | 0 \rangle \, A(\vec{r}\tau)$$

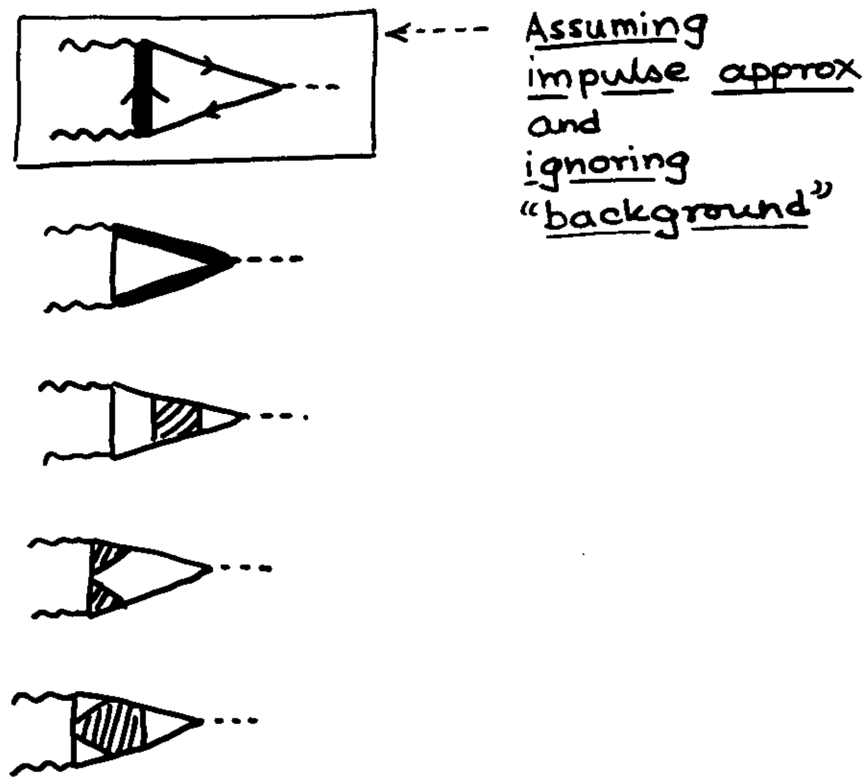
$$+ \int_{\substack{\vec{r}\tau \\ \vec{r}'\tau'}} \langle 0 | J(\vec{r}\tau) J(\vec{R}t) J(\vec{r}'\tau') | 0 \rangle \times A(\vec{r}\tau) A(\vec{r}'\tau')$$

quadratic response [Ashcroft & Shaich 1970]

Caroli et al. (1973) :







ω : initial state energy relative to μ

↳ from Pt reference

$\vec{k}$: in-plane momentum

↳ conserved

$$I(\vec{k},\omega) = \underbrace{I_0(\vec{k};\vec{A};h\nu)}\ \underbrace{f(\omega)A(\vec{k},\omega)}$$

depends on
- $\vec{k}$
- polarization
- incident $h\nu$

* selection rules

depends on
- $\vec{k}$
- ω
- T

* sum rules

$$A(\vec{k},\omega) = -\frac{1}{\pi}\,\mathrm{Im}\,G(\vec{k},\omega+i0^+)$$

initial state spectral function

$$f(\omega) = \frac{1}{e^{\beta\omega}+1}$$ Fermi fn.

one-particle spectral function:

$$A(\vec{k},\omega) = A_+(\vec{k},\omega) + A_-(\vec{k},\omega)$$

add a particle (BIS):

$$A_+(\vec{k},\omega) = \sum_{m,n}\frac{e^{-\beta\varepsilon_m}}{Z}\left|\langle n|c_k^+|m\rangle\right|^2 \times \delta(\omega+\varepsilon_m-\varepsilon_n)$$

$$= [1-f(\omega)]\,A(\vec{k},\omega)$$

remove a particle (ARPES):

$$A_-(\vec{k},\omega) = \sum_{m,n}\frac{e^{-\beta\varepsilon_m}}{Z}\left|\langle n|c_k|m\rangle\right|^2 \times \delta(\omega+\varepsilon_n-\varepsilon_m)$$

$$= f(\omega)\,A(\vec{k},\omega)$$

sum-rules:

- $\int_{-\infty}^{\infty} d\omega\, A(\vec{k},\omega) = 1$ BIS + ARPES
- $\sum_{\vec{k}} A(\vec{k},\omega) = N(\omega)$ tunneling; angle-integr. PES (?)
- $\boxed{\int_{-\infty}^{\infty} d\omega\, f(\omega)\,A(\vec{k},\omega) = n(\vec{k})}$

Approximate sum rule:

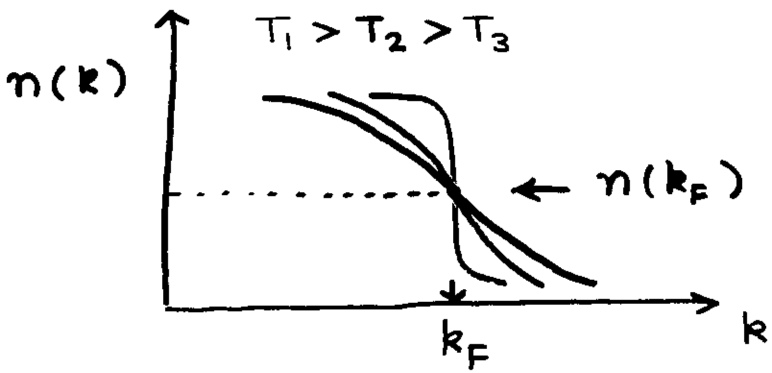
Integrated intensity [$\propto n(\vec{k}_F)$] is T-independent at $\vec{k}_F$

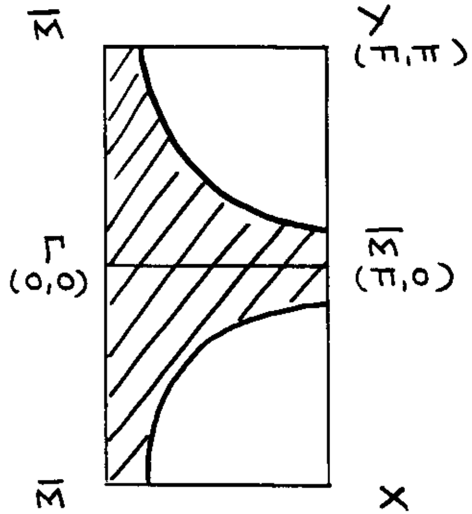
$$n(\vec{k}_F) = \frac{1}{2} - \int_0^\infty \frac{d\omega}{2} \tanh\left(\frac{\beta\omega}{2}\right) \times \left[A(\vec{k}_F,\omega) - A(k_F,-\omega)\right]$$

"p-h symmetry" (weak)

$A(\vec{k}_F,\omega) = A(\vec{k}_F,-\omega)$ for "small" ω

$$\Rightarrow \quad \frac{\partial n(k_F)}{\partial \beta} \approx 0$$

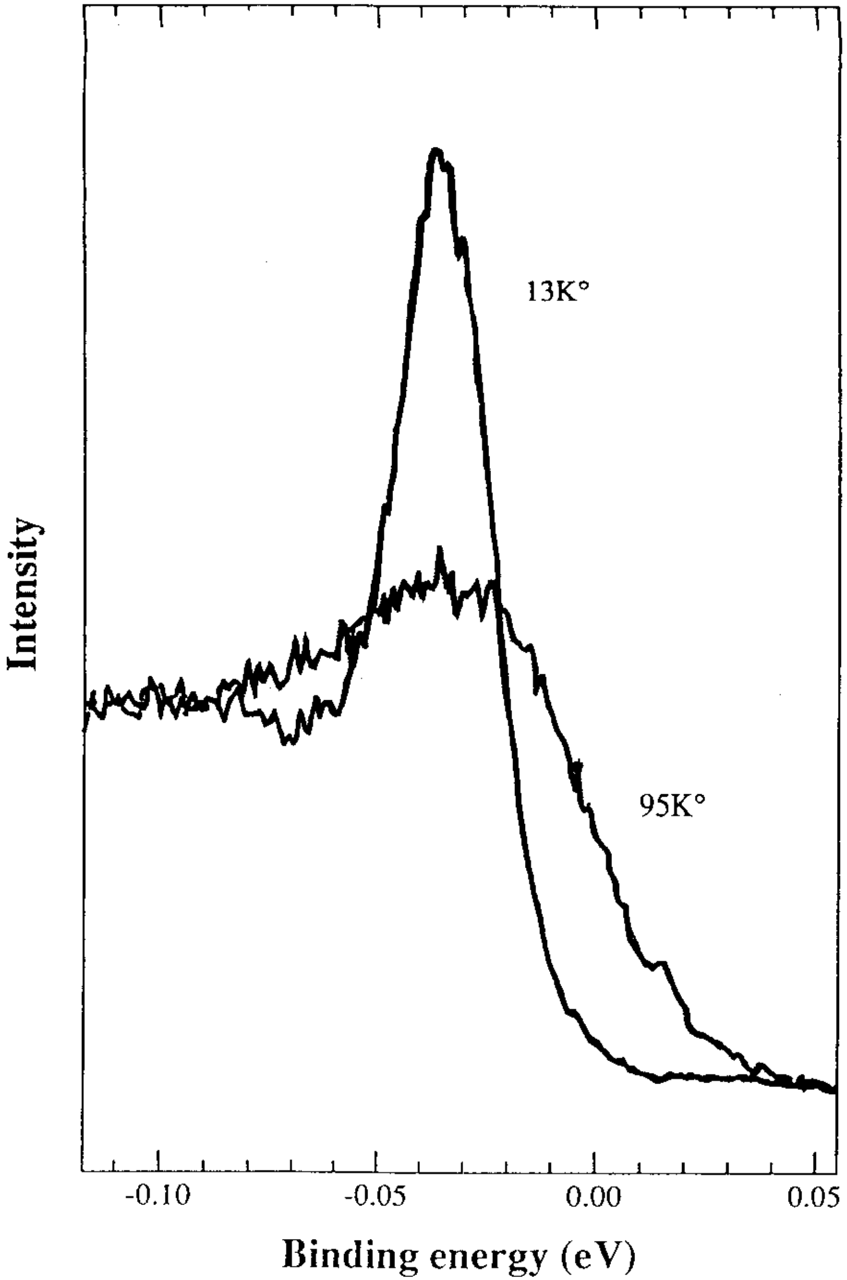




BISCO
Bi 2212

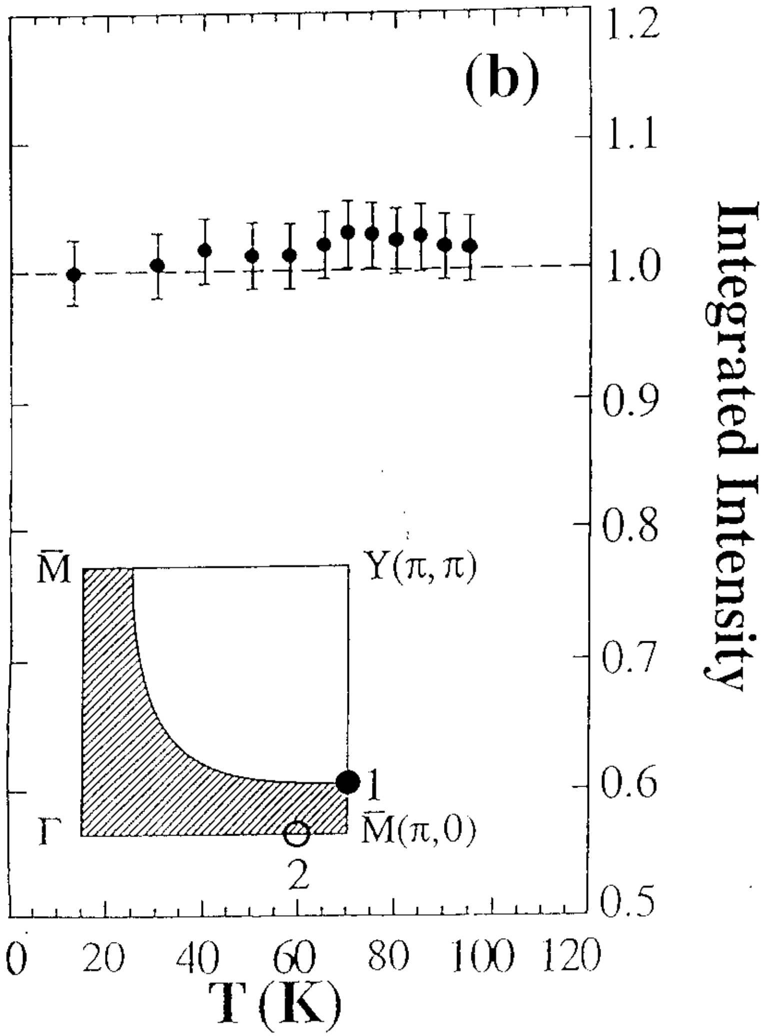
→ Cu-O bond

$T_c = 87\,K$ Bi 2212 $\bar{M} \to Y$ F.S. crossing



SUM RULE CHECK ON VALIDITY OF $f(\omega) A(\vec{k}, \omega)$ INTERPRETATION OF ARPES

M. Randeria et al, PRL (1995)



Qualitative Features of $A(\vec{k},\omega)$:

$T > T_c$

- anomalously broad even as $\vec{k} \to \vec{k}_F$

$T < T_c$

- shift : sc gap opens up
- resolution limited line ($T \ll T_c$)

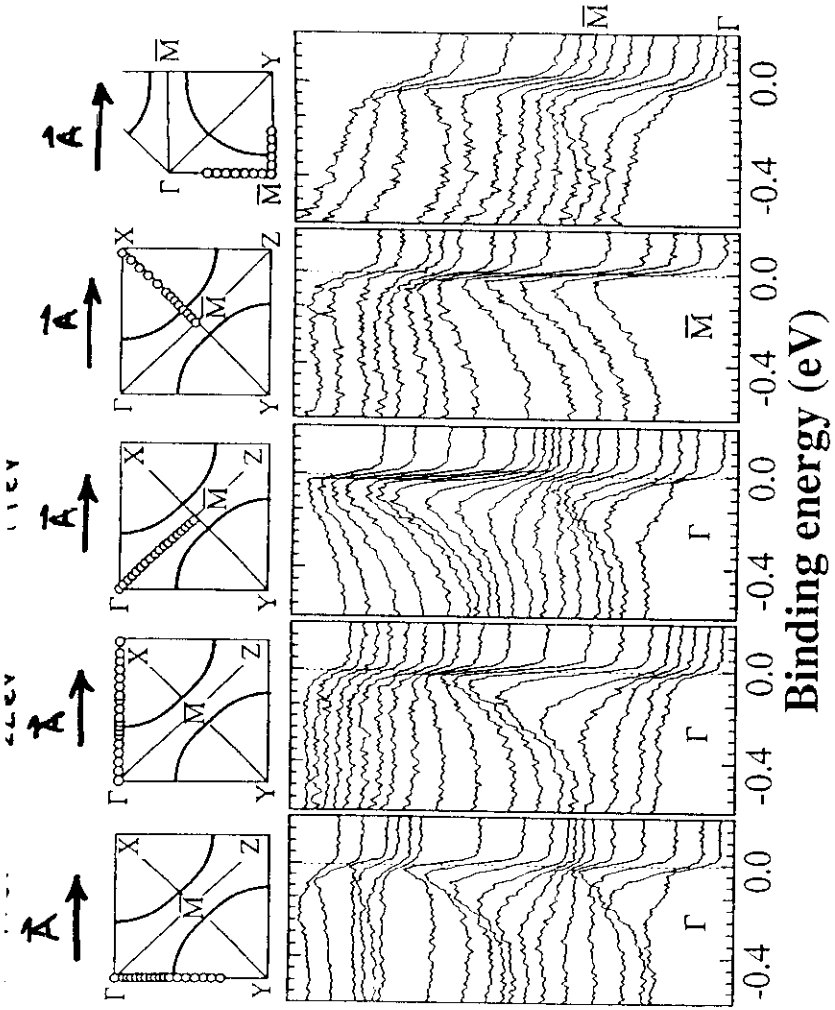
  line width Σ'' decreases sharply as T is lowered

  $\Rightarrow$ Σ'' determined by e-e interactions
- intensity increase due to $\Sigma'' \downarrow$ and sum rule

  not a "BCS pile up"
- dip feature
- T changes by 100 K
  spectral shifts down to 100 meV $\sim 10^3$ K

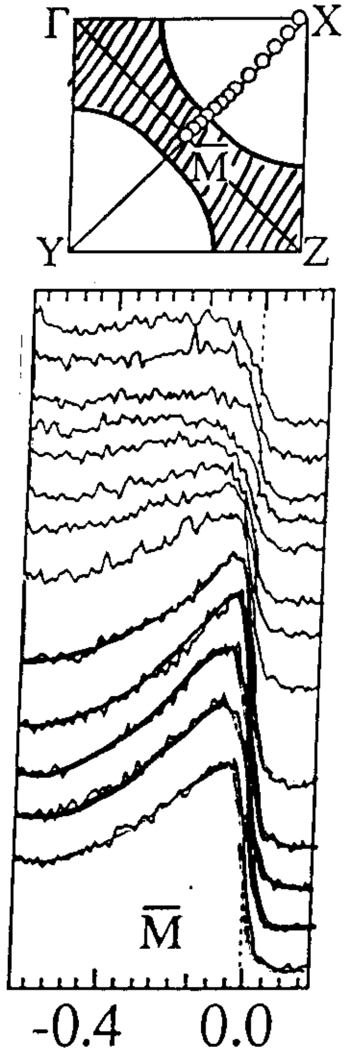
II. Electronic Excitations in Bi 2212

mostly normal state



Ding et al, PRL (1996)

Bi2212 (T_c = 87K)
T = 95K



NO QUASIPARTICLE PEAKS IN THE NORMAL STATE!

ARPES as an experimental probe of the momentum distribution $n(\vec{k})$

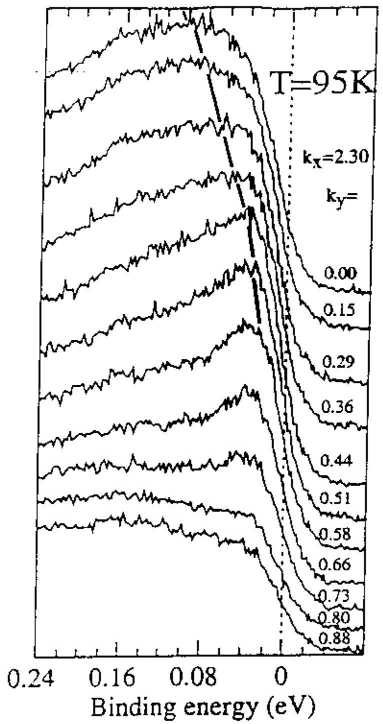
$$\int_{-\infty}^{\infty} d\omega \; I(\vec{k},\omega) = I_0(\vec{k}) \int_{-\infty}^{\infty} d\omega \, f(\omega) A(\vec{k},\omega)$$

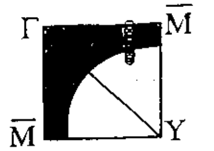
$$= I_0(\vec{k}) \, n(\vec{k})$$

$I_0(\vec{k})$: can be obtained from electronic structure calculations – for now, assume constant or slowly varying

other probes of $n(\vec{k})$:

- Compton scattering (all bands)
- e^+ annihilation (only chains)





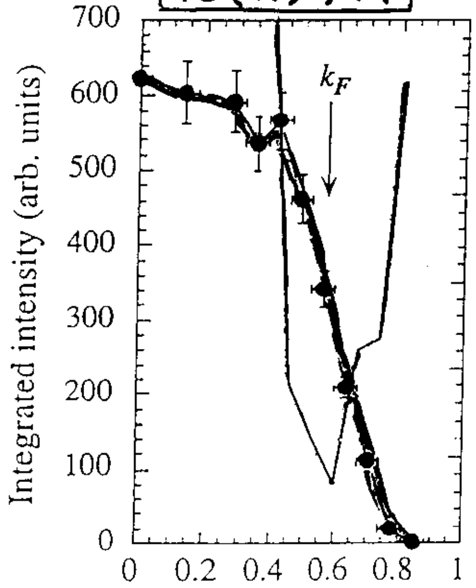
Ding et al PRL (1996)

Campuzano et al PRB (1996)

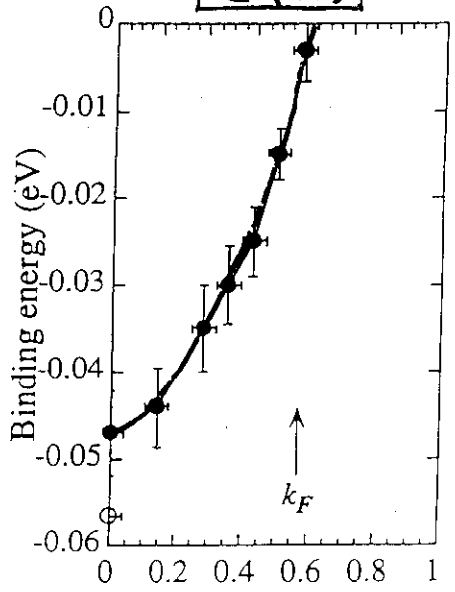
Bi2212 ARPES measurements of:

- "BAND STRUCTURE" $\epsilon(\vec{k})$
- MOMENTUM DISTRIBUTION $n(\vec{k})$
- FERMI SURFACE

"$n(\vec{k})$"; $\vec{k}_F$

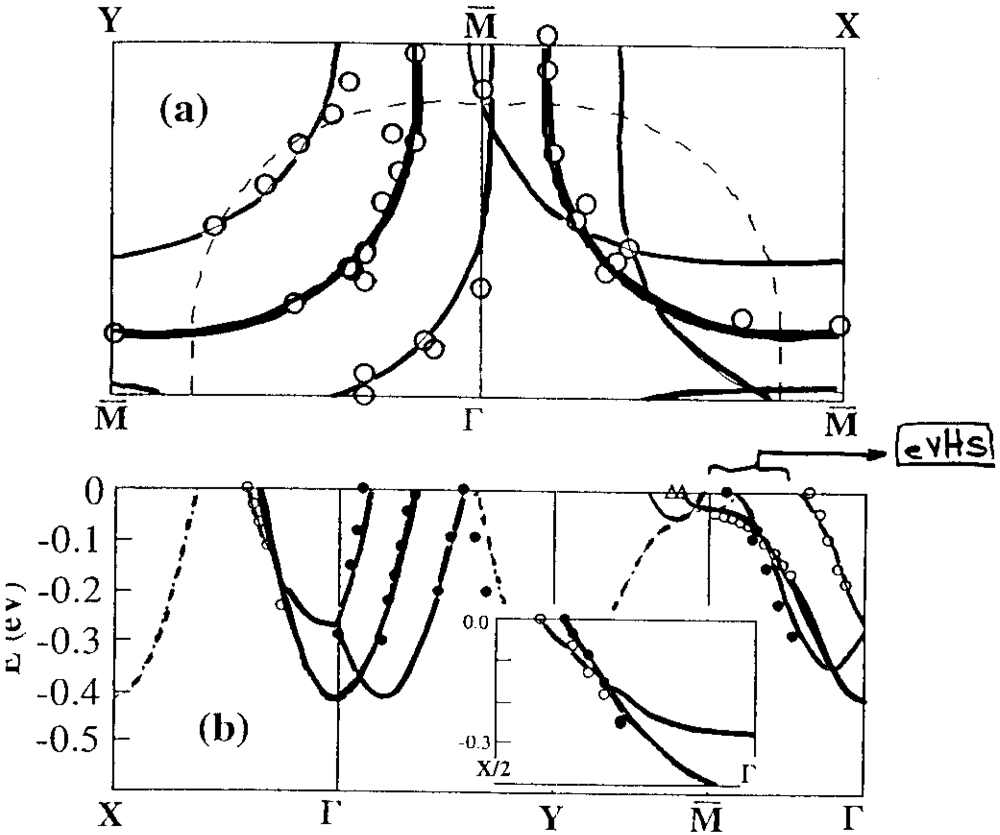


$\epsilon(\vec{k})$



Dispersion & Fermi Surface

Bi 2212 (normal state)



● = odd ; O = even ; Δ = mixed

Main band

± Q umklapps $\vec{Q} = (0.21\pi, 0.21\pi)$

SL along ΓY

"shadow bands"

all spectral features fall into one of three categories :

(1) main CuO band

FS area ≡ 0.17 holes / Cu

(2) $\pm \vec{Q}$ umklapp bands

$\vec{Q} = (0.21\pi, 0.21\pi)$ along ΓY

SL distortion in Bi-O layer

(3) some evidence for "shadow bands"

(π,π) "fold back" of magnetic or structural origin ?

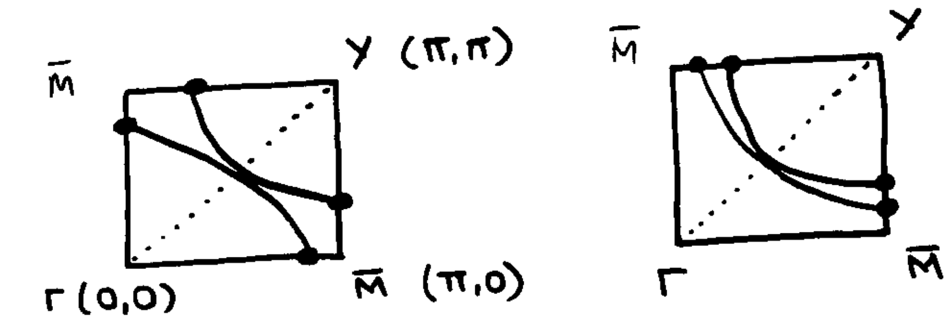
Detailed polarization analysis :

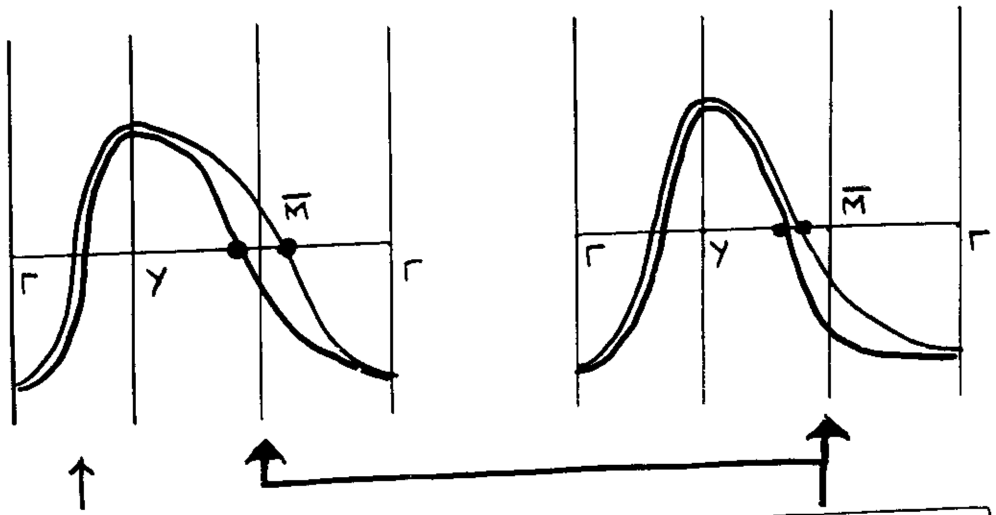
* previously puzzling, apparent breakdown of selection rules in X quadrant now understood as SL effect

* only one FS (≡ two degenerate FSs).

No FS "enclosing" Γ point

Bilayer Splitting ?





degenerate along ΓX, ΓY

maximum splitting at $\bar{M}$ point !

$t_\perp(\vec{k}) \sim [\cos k_x - \cos k_y]^2$

[OK Anderson et al
PW Anderson et al]

Split F.S. depends sensitively on
* doping level & * BiO pockets

look for bilayer splitting at $\bar{M}$ point (below ε_F)

$T > T_c$: very broad line shape

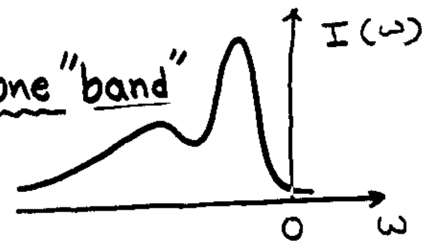
$\Sigma'' \sim \epsilon_k$

cannot hope to resolve bilayer splitting

$T < T_c$: obtain dip feature !

hypothesis A : one "band"

single spectral function



$$I \propto |\langle \psi_f | \vec{p}\cdot\vec{A} | \psi_i \rangle|^2 \, A(\vec{k},\omega) \, f(\omega)$$

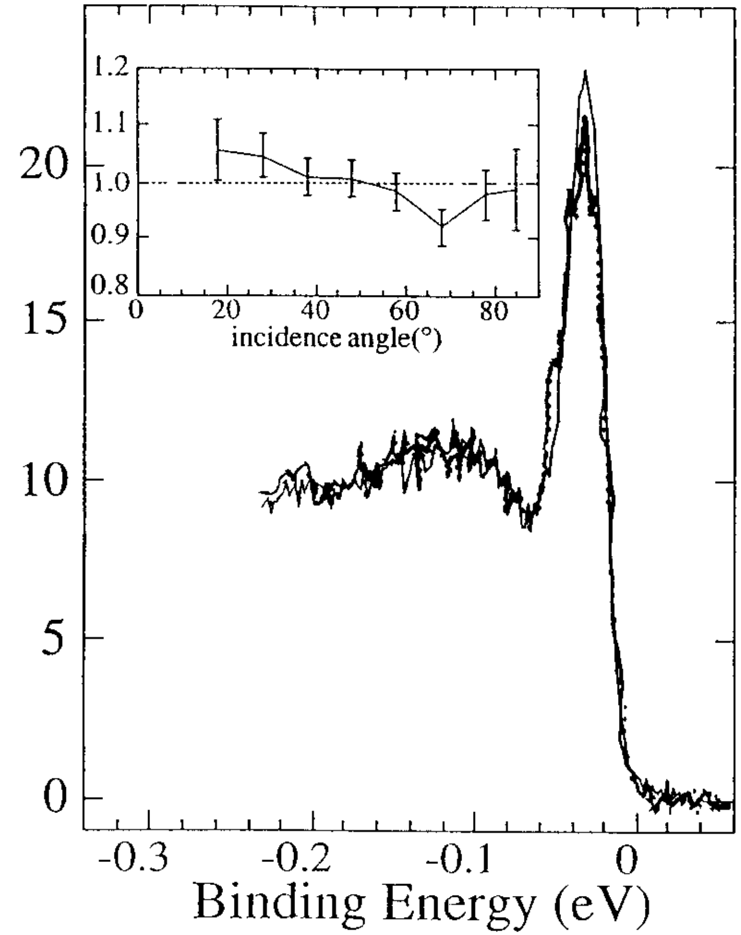
hypothesis B : two "bands"

two independent matrix elements

$$I \propto [M_1^2 A_1(k,\omega) + M_2^2 A_2(k,\omega)] \, f(\omega)$$

Bi 2212 ($T_c = 87$ K) $T = 13$ K

Ding et al PRL (1996)



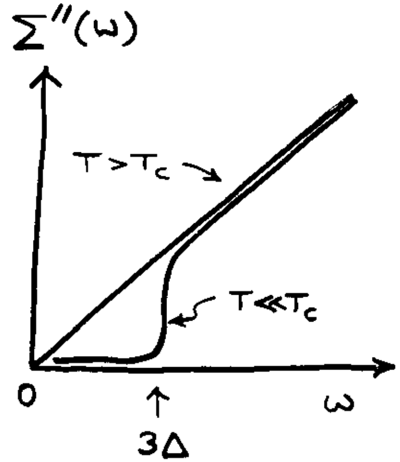
—— 18° } angle of incidence
—— 85° } of photon beam
w.r.t. normal to surface

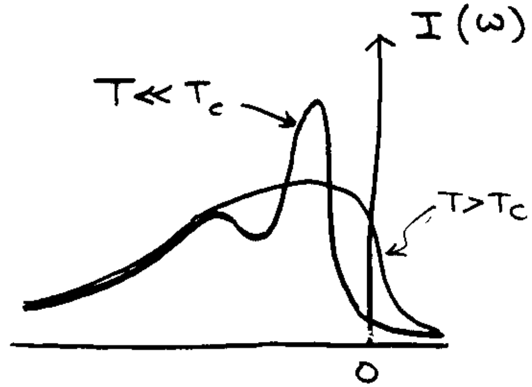
entire EDC, including dip feature, governed by single matrix element

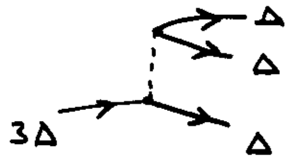
i.e. one spectral function

<u>many-body interpretation of dip</u>

Varma + Littlewood '92
Coffey + Coffey '93







<u>Dip</u>:
- ARPES
- Tunneling
- angle integrated PES

✓ Zasadzinski (1993): Dip in tunneling G(V) scales with gap feature for a number of cuprates

No evidence for bilayer split bands in Bi 2212

even below T_c where a sharp quasiparticle peak is seen!

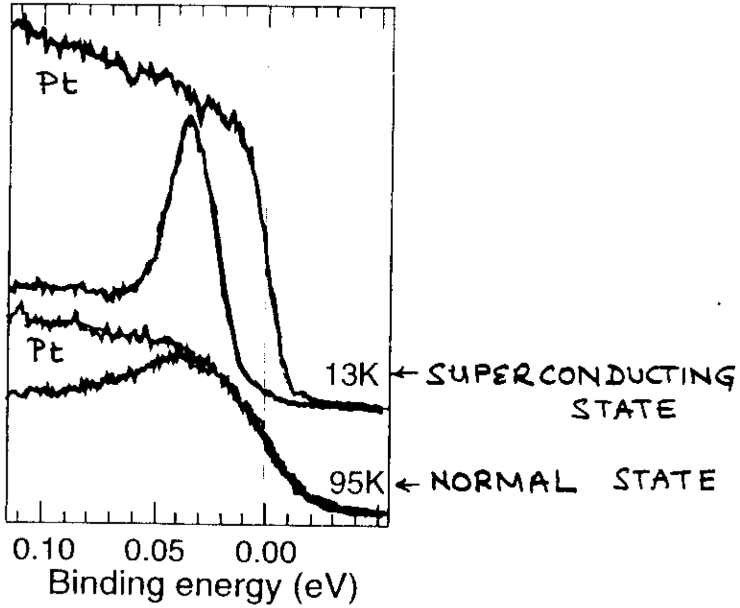
remarks:

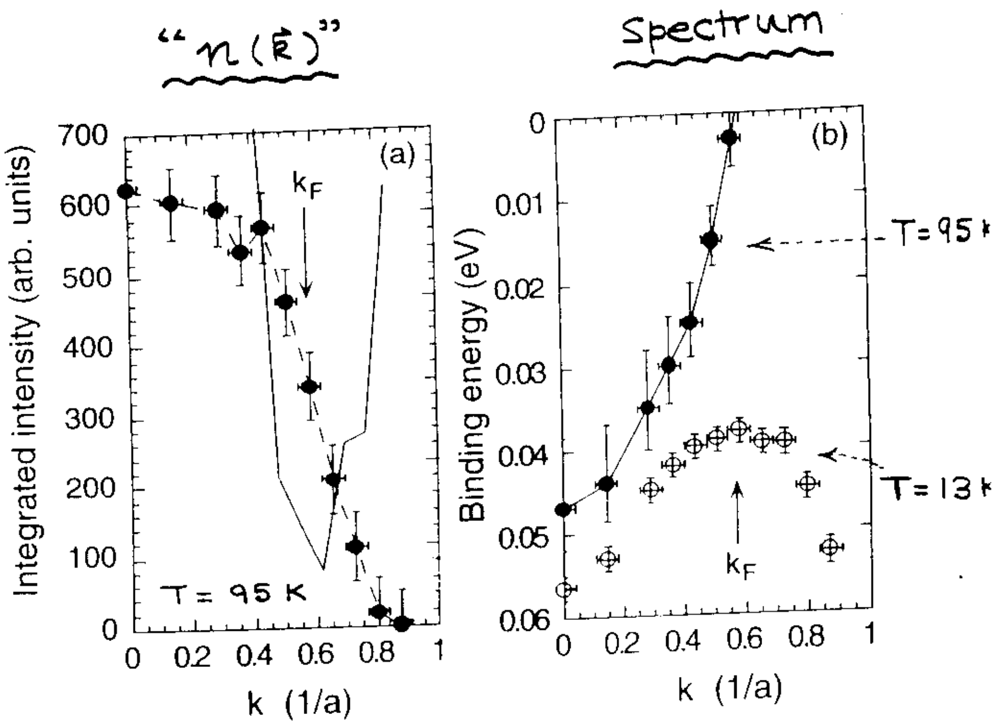
- P.W. Anderson's prediction
- cf. YBCO

  some evidence for two Cu-O bands

* incoherent c-axis transport probes the much weaker coupling between one bilayer and another bilayer

III. Gap Anisotropy in Bi 2212





J. Campuzano et al, PRB (1996)

- particle-hole mixing
- $\epsilon_{\vec{k}} \longrightarrow \sqrt{\epsilon_{\vec{k}}^2 + |\Delta(\vec{k})|^2}$

$\Rightarrow$ SC GAP !

"FERMI SURFACE": locus in $\vec{k}$-space

- rapid variation of $n(\vec{k})$
- gapless excitations $(T > T_c)$

$\longleftrightarrow$ locus of min. gap $(T < T_c)$

early data: Ding et al. 1995

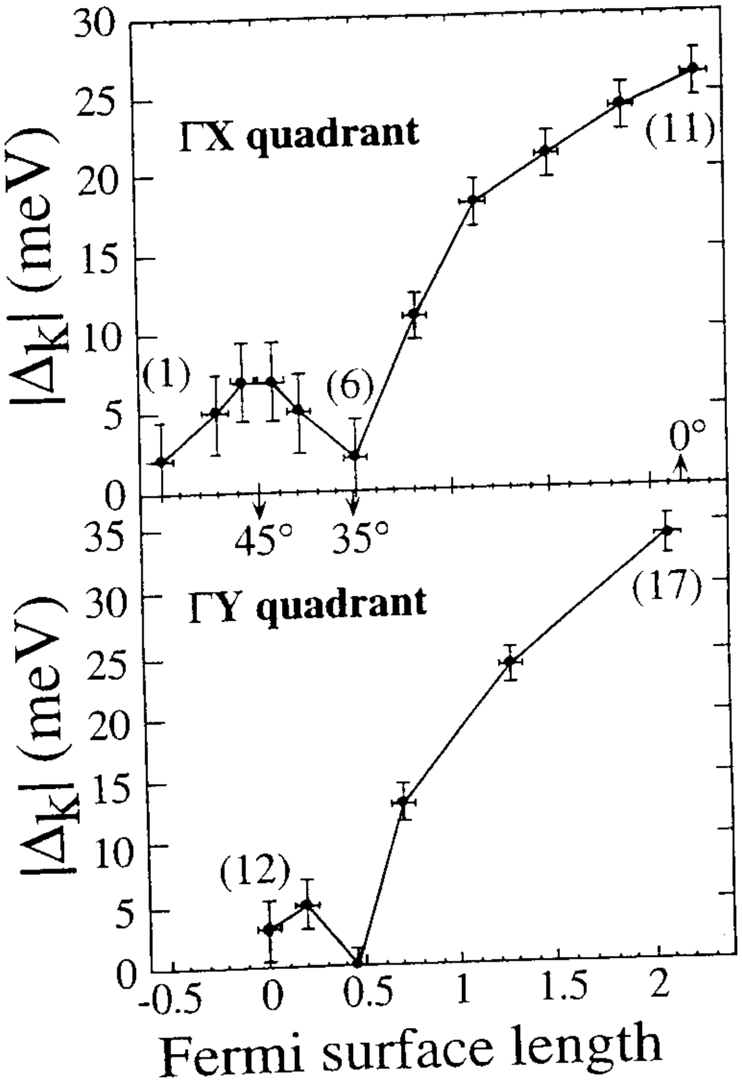
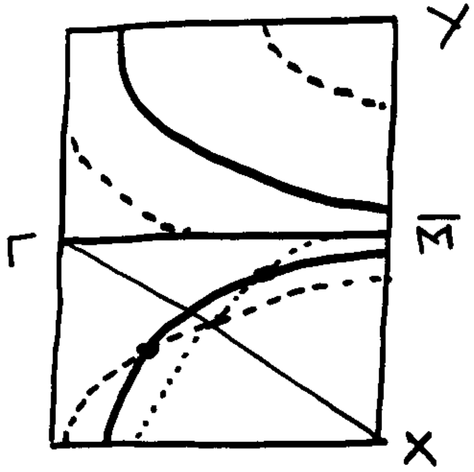


Fig. 4

ΓX //

ΓY 45°



Nodes coincide with main FS and superlattice FS crossing points!

$Cu \longrightarrow O$

main band : Cu $d_{x^2-y^2}$ orbital

⇒ odd w.r.t. ΓX

hump along ΓX seen in ΓX ∥ polarizn

⇒ initial state even in ΓX

∴ hump is not on main CuO band

it is on the even SL band

$\psi(\vec{k}+\vec{Q}) - \psi(\vec{k}-\vec{Q})$

$\vec{k}$ along ΓX

$\vec{Q}$ = SL vector

$\mathcal{R}$: reflection in ΓX

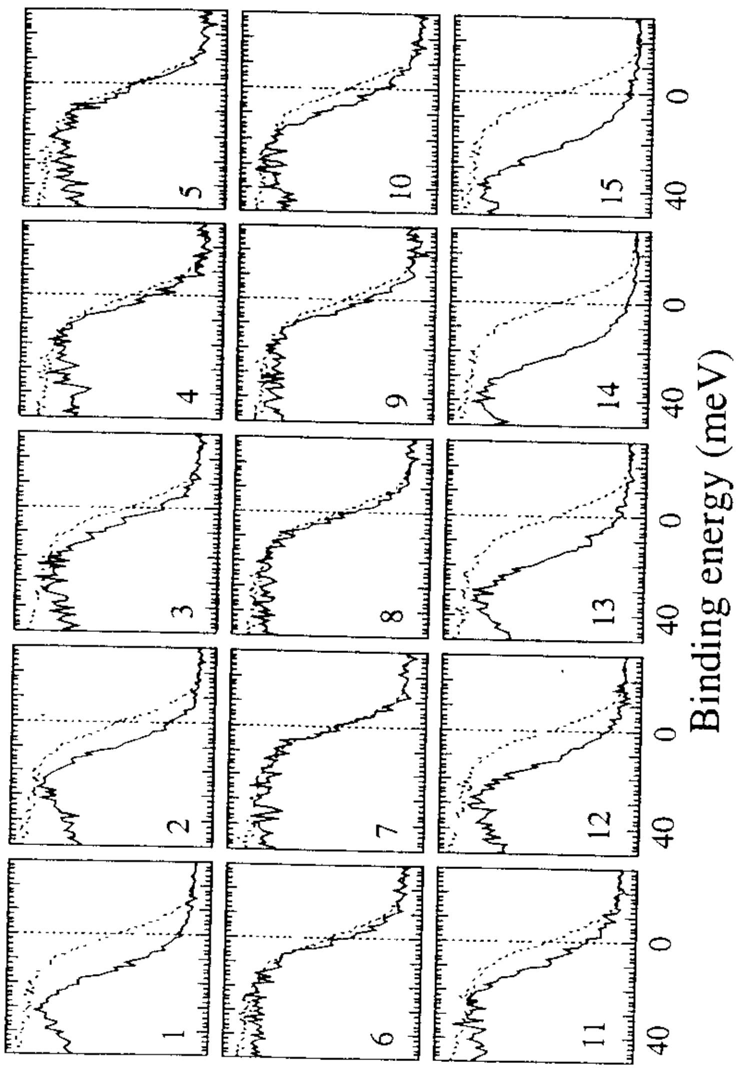
$\mathcal{R}\,\psi(\vec{k}+\vec{Q}) = -\psi(\vec{k}-\vec{Q})$

⇒ Y quadrant gap is intrinsic gap

Bi 2212 $T_c = 87\,K$ T = 13 K

Y quadrant

ΓY ⊥



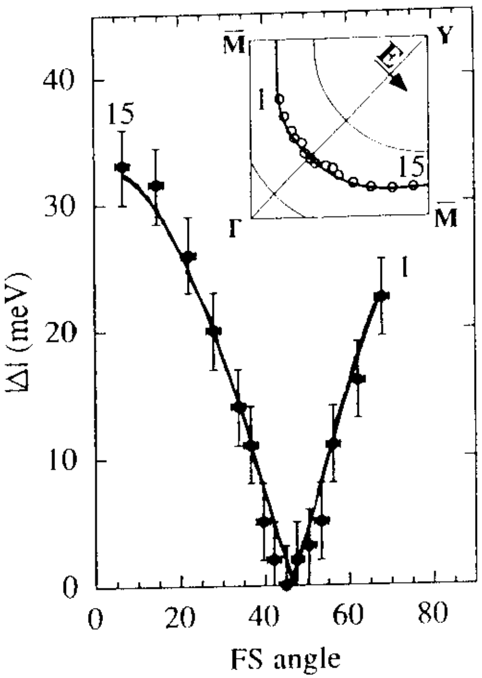
Bi 2212 $T_c = 87\,K$ $T = 13\,K$

Y- quad

ΓY ⊥ ; no SL problems!

consistent with:

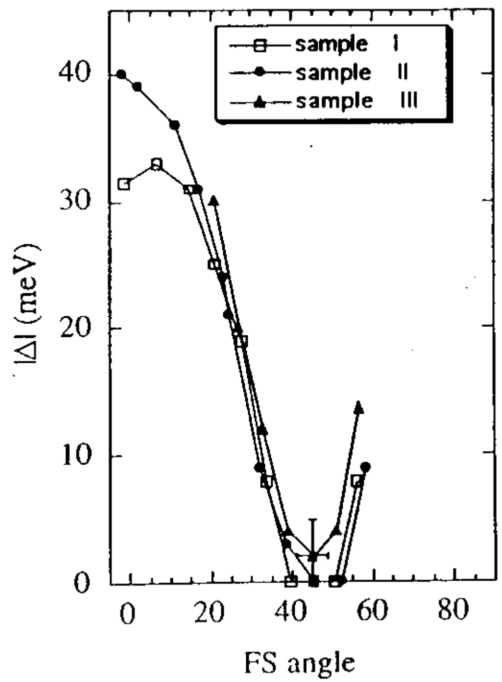
$$|\Delta(\vec{k})| = \Delta_0 \, |\cos k_x - \cos k_y|$$



Ding et al, (1996)

Bi 2212 $T_c \simeq 90$ K

sample-to-sample variations in SC gap.



IV. Underdoped

$Bi_2 Sr_2 Ca Cu_2 O_{8+\delta}$:

Pseudo gaps above T_c

ref: Ding et al., Nature (1996)

Is the normal state of a short coherence length SC necessarily a Fermi liquid?

No ! • local pairing correlations develop at $T^* > T_c$
• phase coherence at T_c

C. Sa de Melo, M. Randeria, J.R. Engelbrecht
PRL 71, 3202 (1993)

pseudo gap in $A(\vec{k},\omega)$
$T_c < T < T^*$

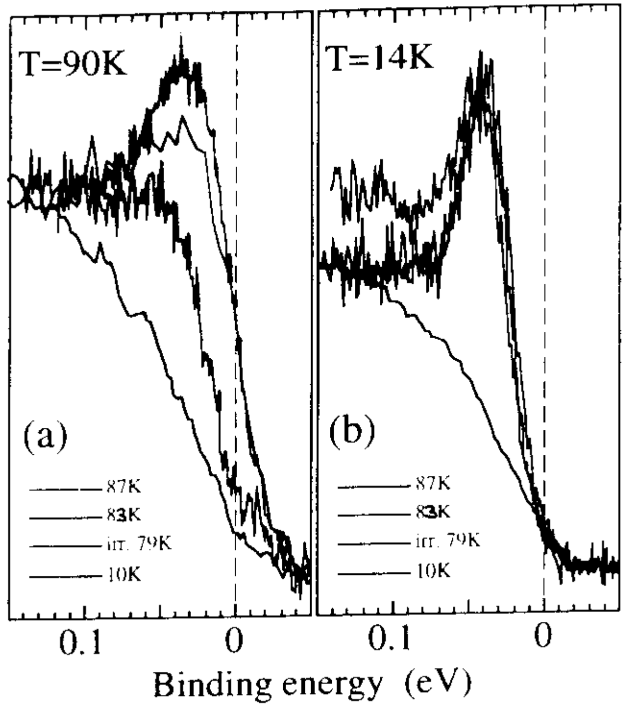
$\Rightarrow$ spin gap in magn. corrlns.

* $N(0)$ is T-dep
* $\chi(T) \sim N(0)$ with $\frac{d\chi}{dT} > 0$
* $1/T_1T \sim \chi(T)$
* $\frac{dn}{d\mu}$ not T-dep
* deviations from Fermi liq. theory in a highly degenerate Fermi system .... $n(\vec{k})$

Randeria, N. Trivedi, A. Moreo & R.T. Scalettar
PRL 69, 2001 (92)

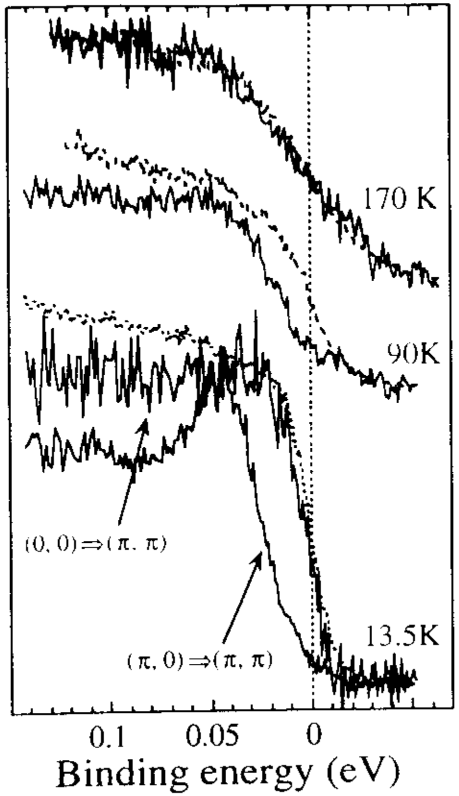
Trivedi & M. Randeria
PRL 75, 312 (1995)

Ding et al., Nature (1996)



• carrier concentration v/s. disorder
• underdoping $\Rightarrow$ very broad normal state spectra
• quasi-particle peak recovered below T_c !

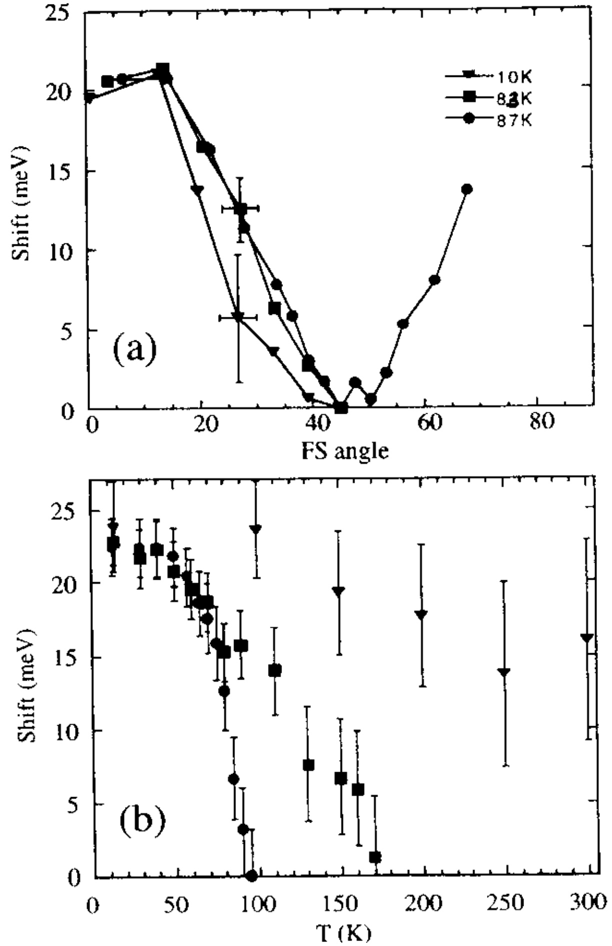
$T_c < T < T^*$: normal state pseudo-gap



T_c = 83 K, lightly underdoped Bi2212

- gap persists along $(\pi,0) \to (\pi,\pi)$ in normal state $T < T^* \simeq 170$ K
- F.S. with gapless excitations for $T > T^*$

- same $\vec{k}$-dependence as SC gap $T < T_c$



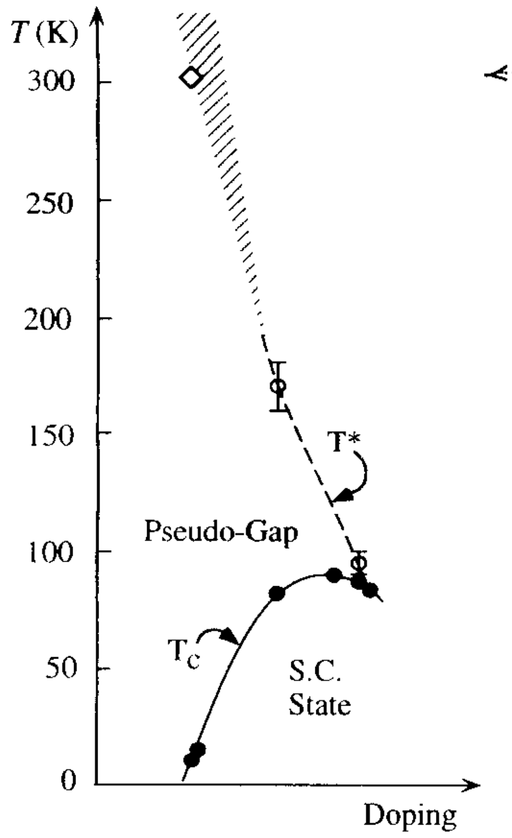
▼ T_c = 10

■ T_c = 83

● T_c = 87

- smooth evolution of gap through T_c.
- magnitude indep. of T_c (underdoping)

Phase Diagram for $Bi_2 Sr_2 Ca Cu_2 O_{8+x}$



$T^* > 300$ K for $T_c = 10$ K sample

T_c : SC transition temp

T^* : pseudo-gap vanishes and F.S. is recovered

Summary :

- $f(\omega)\, A(\vec{k}, \omega)$ interpretation of ARPES
  - * sum rules
- experimental probe of $n(\vec{k})$
- electronic excitations :
  - * dispersion
  - * Fermi surface
  - * anomalous line shape $T > T_c$
  - * below T_c : gap
    - T-dep. of line width
    - dip feature
  - * absence of bilayer splitting !
- selection rules + superlattice
- SC gap : $|\cos k_x - \cos k_y|$
- underdoped samples
  - * pseudo-gap for $T_c \leq T \leq T^*$
  - * smooth evolution through T_c
  - * same $\vec{k}$-dep. as SC gap
  - * large F.S. recovered at T^*