Constituents of the “kink” in high-Tc cuprates

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Outline

• Introduction to ARPES

• Self-consistent analysis of ARPES spectra

• Nodal direction of cuprates
Introduction to ARPES

What do we measure?
Samples should be

1. Easily cleavable – perfect surface
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2. 2D – to neglect $k_z$ dispersion
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2. 2D – to neglect $k_z$ dispersion
3. Free of superstructure
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3. Free of superstructure

4. High $T_c$
Samples should be

1. Easily cleavable – perfect surface

2. 2D – to neglect $k_z$ dispersion

3. Free of superstructure

4. High $T_c$

$\rightarrow$ Bi(Pb)-2212
Samples should be

1. Easily cleavable – perfect surface

2. 2D – to neglect $k_z$ dispersion

3. Free of superstructure

4. High $T_c$

\[ \text{Bi}(\text{Pb})-2212 \]

but bilayer splitting – we need different $hv$
Photoemission Spectrum
Angle-Resolved Photoemission (ARPES)
Angle Resolved Analyser

Detector

Sample

Energy vs. Momentum

Energy vs. Angle
ARPES with Synchrotron Light

Scienta hemispherical analyzer

Entrance slit

Photoelectrons

Toroidal mirror

Exit slit

Scan

Plane mirror

Spherical mirror

4-jaw aperture

Undulator

Sample

Detector

$\theta_x$

$E_k$

$\chi$

$\gamma$

Damasceelli RMP 2003
Basics: electron dispersion
Basics: electron dispersion

MDC dispersion
Photocurrent

\[ I(k, \omega) = G_k \{ M(k) [A(k, \omega) f(\omega)] \otimes R_{\omega, k} + B(\omega) \} \]

geometrical prefactor

momentum and energy resolution

matrix elements

Fermi cutoff

extrinsic background
$I(k,w)$ - Energy Distribution Map

$I(k,w)$ - Momentum Distribution Curve

$I(k_x,k_y,w)$ - Momentum Distribution Map

Borisenko PRB 2001
Precise Cryo-Manipulator

0.1° precision

15 K < T < 400 K

UHV
Fermi-surface map
Momentum-energy space

Binding energy (eV)

Momentum (Å⁻¹)

min max

Borisenko PRB 2001
Bare band structure

What is underneath?
Fermi surface evolution with doping

\[ S_{FS} = (1 - x)/2 \]

“Large Fermi surface”
Band structure: TBF

$$\varepsilon(k_x, k_y) = \Delta \varepsilon - 2t(\cos k_x + \cos k_y) + 4t' \cos k_x \cos k_y - 2t''(\cos 2k_x + \cos 2k_y)$$

$$\Delta \varepsilon \approx 0.4 \text{ eV}$$
$$t \approx 0.4 \text{ eV}$$
$$t' \approx 0.1 \text{ eV}$$
$$t'' \approx 0.05 \text{ eV}$$
Bare band structure

| 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                   |

Kordyuk *PRB* 2003
Good agreement with LDA
(no signature of Mott insulator)

vHs is essential for HTSC
Quasiparticle spectral weight

What is relevant in ARPES spectra?
Nodal direction (GX)

No gap, simple bare dispersion.
Extrinsic background
Extrinsic background depends on excitation energy

Kordyuk *PRL* 2002

Borisenko *PhyC* 2004

Kaminski *PRB* 2004
One more complication: **nodal splitting**

![Image of nodal splitting](image)

**b**

OD73
50 eV

**c**

Kordyuk PRB 2004
Nodal splitting

\[ \Delta k = 0.012 \text{ 1/Å} \]

\[ \Delta \varepsilon = 50 \text{ meV (bare!)} \]
IF
one use
superstructure-free high quality samples
with negligible $k_z$ dispersion (Bi(Pb)-2212)
and
rid of the background
and bilayer splitting effect,

one may get an access to the
quasiparticle spectral function.
Quasiparticle spectral function

![Graph showing the quasiparticle spectral function with energy and momentum axes.]
Quasiparticle spectral function

Abrahams *PNAS* 2000

Kordyuk *PRL* 2002

Haslinger *EPL* 2002
Self-energy approach

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

\[ \Sigma'(\omega) = \omega - \varepsilon(k_m) \]

\[ \Sigma''(\omega) = -\nu_F W(\omega) \]
Self-energy approach: fitting procedure

\[ \Sigma'(\omega) = \frac{v_F}{2} (k_m^2(\omega) - k_F^2) + \omega, \]

\[ \Sigma''(\omega) = -v_F W(\omega) \sqrt{k_m^2(\omega) - W^2(\omega)}. \]

\[ \Sigma'(\omega) = K K \Sigma''(\omega) \]

Three parameters

bare band parameter: \( v_F \) or \( \omega_0 \)

tail parameters: \( \omega_c \) and \( n \)
Kramers-Kronig transform

$$\Sigma'(\omega) = \mathcal{K}\mathcal{K} \Sigma''(\omega)$$

\[
\Sigma''(\omega) = - \begin{cases} 
\alpha \omega^2 + C & \text{for } |\omega| < \omega_c, \\
0 & \text{for } |\omega| > \omega_c,
\end{cases}
\]

\[
\lambda = \frac{2}{\pi} \left( \alpha \omega_c - \frac{C}{\omega_c} \right) \approx \frac{2}{\pi} \alpha \omega_c
\]

\[
\lambda = 4\alpha \omega_c / \pi
\]
Kramers-Kronig transform

\[ \Sigma'(\omega) = KK \Sigma''(\omega) \]

\[ \lambda = - \left( \frac{d \Sigma'}{d \omega} \right)_{\omega=0} \]

\[ \lambda = \frac{-2}{\pi} \int_{0}^{\infty} \frac{\Sigma''(\omega) - \Sigma''(0)}{\omega^2} \, d\omega \]
Kramers-Kronig transform

\[ \Sigma'(\omega) = \text{KK} \Sigma''(\omega) \]

\[
\Sigma''(\omega) = \begin{cases} 
\Sigma''_{\text{width}}(|\omega|) & \text{for } |\omega| < \omega_m, \\
\Sigma''_{\text{mod}}(\omega) & \text{for } |\omega| > \omega_m,
\end{cases}
\]

\[ \Sigma''_{\text{mod}}(\omega) = -\frac{\alpha \omega^2 + C}{1 + \left|\frac{\omega}{\omega_c}\right|^n} \]

Kordyuk PRB 2005
Kramers-Kronig transform

\[ \Sigma'(\omega) = KK \Sigma''(\omega) \]

Kordyuk PRB 2005
Real Self-Energy

\[ \nu_F = 3.82 \pm 0.17 \text{ eVÅ} \]

\[ \lambda = 0.87 \pm 0.12 \]
Real Self-Energy

Self-consistency: LDA + self-energy

Well defined quasi-particles

Kink phenomenology

Kordyuk PRB 2005
"Kinks"

Kaminski *PRL* 2001

Bogdanov *PRL* 2000

Johnson *PRL* 2001

Lanzara *Nature* 2001
Phenomenology of the kink

\[ \Sigma' (\text{eV}) \]

- UD77
- OD75

\[ \omega (\text{eV}) \]

Kordyuk *PRB* 2005
Quasiparticle scattering rate

What is the main scatterer?
Scattering rate kink

Kordyuk PRL 2004
Scattering rate:

**T-dependence**

![Graph showing T-dependence](image)

**Doping dependence**

![Graph showing Doping dependence](image)
Scattering rate:
Some conclusions

There are two channels:
1\textsuperscript{st} electron-electron scattering and
2\textsuperscript{nd} electron-boson scattering
Scattering rate kink

Bi-2212 UD85

MDC FWHM (Å⁻¹)

Energy (eV)

25 K
40 K
220 K
25 K – 220 K
40 K – 220 K

Bi(La)-2201 OP32

Energy (eV)

25 K
60 K
25 K – 60 K

Kordyuk PRL 2004
Nodal electrons couple to ...

Doping dependence: $\text{UD}^\uparrow$
$\text{OD}^\downarrow$

Temperature dependence:
$< T_c$ for OD
$< T^*$ for UD

Parity: odd boson
Conclusions

“Careful and systematic analysis” of ARPES data implies KK consistency.

“Kink” needs to be quantified!

Meanwhile, under “kink” we imply the kinked doping and temperature dependent part of the self-energy. Besides the huge Auger-like scattering this is the main interaction channel seen by ARPES.

Kink appears below $T^*$ line on the $T-x$ phase diagram.

Irrelevant “kink” can have many reasons: e.g., superstructure, bilayer splitting, superconducting gap or, for overdoped samples, a sharp maximum of the $\text{Re}\Sigma(\omega)$ due to vHs approaching Fermi level.
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