High-Temperature Superconductors: A View from K-Space

Mark S. Golden
Van der Waals-Zeeman Institute
University of Amsterdam

© Mark S. Golden

Condensed Matter Physics Group, University of Amsterdam
Yingtai Huang

Spectroscopy Group, IFW Dresden
Sergey Borisenko, Alexander Kordyuk, Andreas Koitzach, Sibylle Legner, Christian Dür, Martin Knapier, Thomas Pichler, Roland Höbel, Dieter Müller, Jörg Fink, Claus Schneider, Frank Matthes, Robert Frömter
IFF, IFW Dresden

Crystals
Helmut Berger
B. Liang, A. Maliouk, C. T. Lin, Bernhard Keimer
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 Graziosi

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

Money
FOM, EU, BMBF, DFG, SMWK
High-Temperature Superconductors: A View from K-Space

Outline

- ARPES as k-space microscopy
  - results from the Bi$_2$Sr$_2$CaCu$_2$O$_{8+x}$ 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 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

spectroscopy

☆ offers a direct probe of the electronic states
☆ is now a 'standard' test of any aspiring theories
High-Temperature Superconductors: A View from K-Space

Spectroscopies with electrons

PES XPS IPES XAS AES EELS

N-1 N-1 N+1 N, can be ≈ N+1 N-2 N

Angle resolved photoemission spectroscopy

ARPES
High-Temperature Superconductors: A View from K-Space

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'

\[ \left| \frac{k}{k_h} \right| = \frac{\sqrt{2mE_{\text{kin}}}}{E_{\text{kin}}(eV)} \sin \theta = 0.512 \sqrt{E_{\text{kin}}(eV)} \sin \theta \]
High-Temperature Superconductors: A View from K-Space

**k-space microscopy**

- $\theta, \Phi$ precision < 0.1°
- $-90^\circ < \Phi < +160^\circ$
- $-90^\circ < \theta < +160^\circ$

- $4k_B T$ at 5 K
- $\Delta E_{\text{tot}} = 2 \text{ meV}$
- $\Delta \theta = 0.1^\circ$

- 5 < $T_{\text{sample}}$ < 300 K

- low bandwidth, high intensity
- variable energy
- variable polarisation

The nodal direction (0,0)-(\(\pi,\pi\)) as an illustration

- $\Gamma$ = node
- $A$ = antinode

Dr. Mark Golden, Amsterdam (KITP Correlated Electrons 10/09/02)
High-Temperature Superconductors: A View from K-Space

**ARPES with an angle multiplexing analyser**

Energy Distribution Curves

\[ I(\mathbf{k},E) \]

Momentum Distribution Curves

....this all lands on the detector in 5 mins.!

**What physical quantities are measured in photoemission?**

\[ I \propto \sum_{f,i} \left| \langle f | \mathbf{p} \cdot \mathbf{A} | i \rangle \right|^2 A(\mathbf{k},E)f(E) \]

**Spectral function:**

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

**BUT**

the matrix element is always present:

\[ \rightarrow \text{dependence on photon energy, polarisation...} \]
Representing ARPES data in 2D

E_{D\text{C}} - I(k_x,k_y,\omega)

Energy

E_{D\text{M}} - I(k_x,k_y,\omega)

MDC - I(k_x,k_y,\omega)

EDM - I(k_x,k_y,\omega)

Momentum

Divide raw signal

I(E_F)

I(E_F) / I_{int}

I(E_F) / I(250\text{meV})

Borisenko et al., PRB64, 094513 (2001)
High-Temperature Superconductors: A View from K-Space

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

Outline
- ARPES as k-space microscopy
- results from the Bi$_2$Sr$_2$CaCu$_2$O$_8$ 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 underdoped regime
Determination of the
Fermi surface topology

'The Experimental' Fermi surfaces of HTSC

HTSC Fermi surface:
- hole-like?
- electron-like?
- perfect nesting?
- stripey?

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

0.8(\pi,0)
High-Temperature Superconductors: A View from K-Space

**Why Bi$_2$Sr$_2$CaCu$_2$O$_8$?**

- Bi-O planes
- CuO$_2$ planes
- Cleave here!

**LEED**

- Pristine Bi2212

**Suppressed by Pb-doping**

*Primary photoelectron*

*Diffraction replicas*

*Excellent cleavage surface*
Pristine Bi-2212 Fermi surface map

main FS
shadow FS
diffraction replicas
high intensity ribbons

Pb-doped Bi2212:

$\text{Bi}_{2-x}\text{Pb}_x\text{Sr}_2\text{CaCu}_2\text{O}_8$
The Fermi surface of Pb-doped Bi-2212

T = 300 K (OD72K)
High-Temperature Superconductors: A View from K-Space

The Fermi surface of Pb-doped Bi-2212

- main FS
- shadow FS

Constant energy surfaces: $\omega$ dependence (OD69K)

- symmetric ‘breathing’;
- FS closes around $\Gamma$ only very late

300K, $h\nu = 21$ 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)$_2$Sr$_2$CaCu$_2$O$_8$

2CuO$_2$ planes: close together

→ antibonding and bonding states

due to c-axis bilayer coupling

 maximal near $(\pi,0)$

 zero along $(0,0)$-$(\pi,\pi)$

Could the antibonding band give an electron-like FS?
High-Temperature Superconductors: A View from K-Space

c-axis bi-layer splitting

Normal state FS map:
BLS 'invisible'

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

Binding energy (eV)

Momentum (Å⁻¹)

BB AB

OD69K

hv = 21.2 eV
T = 30 K

OD69K

hv = 38 eV
T = 30 K

Kordyuk, Borisenko et al., 2002

© Mark S. Golden

Tight binding fit to the OD69K data

TABLE 1: Tight-binding parameters of the CuO conducting band of Bi-2212.

<table>
<thead>
<tr>
<th>Sample</th>
<th>t (eV)</th>
<th>t' (eV)</th>
<th>t'' (eV)</th>
<th>t₃ (eV)</th>
<th>Δε (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>OD 69 K</td>
<td>0.40</td>
<td>0.090</td>
<td>0.045</td>
<td>0.082</td>
<td>0.43</td>
</tr>
<tr>
<td>UD 77 K</td>
<td>0.39</td>
<td>0.078</td>
<td>0.039</td>
<td>0.082</td>
<td>0.39</td>
</tr>
</tbody>
</table>

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

© Mark S. Golden

\[ t_{uvb} = \Delta \varepsilon - 2t (\cos k_x + \cos k_y) + 4t' \cos k_x \cos k_y - 2t'' (\cos 2k_x + \cos 2k_y) \]
\[ \pm t_3 (\cos k_x - \cos k_y)^2 / 4. \]
High-Temperature Superconductors: A View from K-Space

Outline

- ARPES as k-space microscopy
- results from the Bi$_2$Sr$_2$CaCu$_2$O$_8$ 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 underdoped regime

Dr. Mark Golden, Amsterdam (KITP Correlated Electrons 10/09/02)
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

\[ |k| = 1.09 \text{ Å}^{-1} \]

[by the way:
clear BLS in UD!]

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

Azimuthal MDC's

• BB vs. AB can be 'tuned' via \( \nu \):

20' sapprox =

38: BB > AB

50: AB > BB

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

© Mark S. Golden

Dr. Mark Golden, Amsterdam (KITP Correlated Electrons 10/09/02)
High-Temperature Superconductors: A View from K-Space

**How to determine the gap**

- **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

**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
High-Temperature Superconductors: A View from K-Space

**k-dependence of AB leading edge gap**

- If $50\text{meV}$ at $E_F$
- Map of LEG' s
- Plot LEG' s vs. FS angle $\phi$

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

**AB leading edge gap vs. FS angle**

- $\Delta(\phi) = \Delta_{\text{max}} |\cos(2\phi)|$

UD 77K

Borisenko et al., IFW Dresden, cond-mat 0208418, PRB(RC), in press
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: $$\Delta(\phi) = \Delta_{\text{max}} |\cos(2\phi)|$$
- higher gap harmonics: $$\Delta(\phi) = \Delta_1 |\cos(2\phi)| + \Delta_2 |\cos(6\phi)|$$
  here = 27% $$\cos(6\phi)$$
- other pairing symmetries?
  $$d_{x^2-y^2} + is; d_{x^2-y^2} + id_{xy}$$

Outline

- ARPES as k-space microscopy
- results from the Bi$_2$Sr$_2$CaCu$_2$O$_8$ 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 underdoped regime
The $(\pi,0)$ peak-dip-hump in over doped Bi2212 superconducting state.

The spectral function at $(\pi,0)$ 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

- $(\pi,\pi)$ 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 $(\pi,\pi)$-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 \((\pi,\pi)\) mode seen in INS results in peaked \(\text{Im}\Sigma\)
eats away spectral weight at \(\Delta_c + \Omega\)

\(\uparrow\) no BLS \(\downarrow\)

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

- well developed picture for \((\pi,\pi)\)-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 \((\pi,\pi)\)-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 \((\pi,0)\) ` only in sc state:
  
  \[ T < T_c \quad (T_c \text{ ca. 90K}) \text{ in Bi-2212 based materials} \]

- 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 \(h\nu 19-22\) eV

- Dip position vs. doping: fits with \((\pi,\pi)\) mode from neutrons

- Peak is non-dispersive along \((0,0)-(\pi,0)-(2\pi,0)\)

All published PDHs are recorded with \(19<h\nu<22.5\) eV

- Dessau et al., PRL1991
- Hwu et al., PRL1991
- Loeser et al., PRB1997
- Ding et al., PRL2001
- Feng et al., Science2000
- Ding et al., PRL1996
- Fedorov et al., PRL1999
High-Temperature Superconductors: A View from K-Space

The 'old peak-dip-hump edifice

- PDH seen near \((\pi,0)\) only in sc state:
  
  \[ T < T_c \quad (T_c \text{ ca. } 90\text{K}) \text{ in Bi-2212 based materials} \]

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

- PDH lineshape didn’t alter on modifying \(A(z)\) (via incidence angle)
  
  \[ \text{all spectra published to date are with } h\nu \text{ 19-22 eV} \]

- Dip position vs. doping: fits with \((\pi,\pi)\) mode from neutrons

- Peak is non-dispersive along \((0,0)-(\pi,0)-(2\pi,0)\)

- the \((\pi,0)\) point of modulated Bi2212 is dangerous!
  
  \[ \rightarrow \text{use modulation-free PbBi-2212} \]

To Pb or not to Pb?

\[ E = E_F \]

\[ 300\text{K} \]

\[ h\nu = \]

\[ 21 \text{ eV} \]

\[ \text{Bi2212} \]

\[ \text{Pb-Bi2212} \]

Kordyuk, Borisenko et al., 2001, IFW Dresden

Dr. Mark Golden, Amsterdam (KITP Correlated Electrons 10/09/02)
High-Temperature Superconductors: A View from K-Space

The experiment

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

let's pick out some characteristic data...

18 eV

25 eV

32 eV

39 eV

46 eV

53 eV

60 eV

65 eV

hv dependence - OD69K

Kordyuk et al., PRL89, 077003 (2002)
High-Temperature Superconductors: A View from K-Space

Cafeteria (self-service) lineshape - OD69K

looks familiar . . .

hump only

500 meV BE

Kordyuk et al., PRL89, 077003 (2002)

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

- lineshape depends strongly on \( h_\nu \)
  - it depends strongly on matrix elements

- self-energy can’t depend on \( h_\nu \)
  - reject the 'single spectral function' scenario for
    the 'classic' PDH

[also the 'SPR' linked to \( n_s \) or \( Z \) would be \( h_\nu \) dependent]

Possible alternative:

Two features: PEAK and HUMP which react differently to
altering \( h_\nu \)
**Can we simulate the spectra?**

- **OD**
- **Good!**
- **Toy model:**
  - spectral function 1
  - spectral function 2
  - background
- **Broad hv range**
- **Poor**

**Fitting function**

\[
I(\omega, T, hv) \propto \left[ (M_a(hv)A(\omega, \varepsilon_a, T) + M_b(hv) \right. \\
\left. \times A(\omega, \varepsilon_b, T)) f(\omega, T) \right] \otimes R_\omega + B(\omega, T)
\]

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

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

\[
\alpha = 1.1 \pm 0.1, \quad \beta = 2
\]
High-Temperature Superconductors: A View from K-Space

**Fit vs. experiment: 'matrix elements'**

- **OD**
- **bonding**
- **antibonding**
- 2 component fit

Kordyuk et al., PRL89, 077003 (2002)

**Toy model vs. one-step ARPES calculations**

- **bonding = 'hump'**
- **antibonding = 'peak'**

Lindroos et al., PRB65, 054514 (2002)

Kordyuk et al., PRL89, 077003 (2002)
Consequences....

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

**BUT:**
- \((\pi, \pi)\) mode interpretation not tenable for OD

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

Feedback effects near \((\pi, 0)\) in **underdoped** Bi2212

normal & superconducting state
High-Temperature Superconductors: A View from K-Space

hv dependence in UD 77K at (\(\pi, 0\))

- again, lineshape depends on hv

- is it the same as in overdoped?

NO! subtle, yet crucial differences

i) no spectrum without a dip or plateau
ii) details of hv dependence differ

⇒ toy model

Three component ‘toy model’ fits

Idea:

- select hv that shows only AB band....

third component clearly follows AB band
**Targeting \( h\nu \)**

Bonding band has local minima at \( h\nu \) 29 and 50 eV

...these \( h\nu \) show ‘pure’ AB spectrum

**\((\pi,0)\) antibonding band EDC’s**

<table>
<thead>
<tr>
<th>( h\nu )</th>
<th>( \nu )</th>
<th>( T )</th>
</tr>
</thead>
<tbody>
<tr>
<td>29 eV</td>
<td>UD77K</td>
<td>30 K</td>
</tr>
<tr>
<td>50 eV</td>
<td>UD77K</td>
<td>30 K</td>
</tr>
</tbody>
</table>

UD: dip or plateau

OD: smooth

Antibonding band has an ‘intrinsic’ peak dip-hump at \((\pi,0)\)

Peak ↔ dip separation = 38-40 meV

Dr. Mark Golden, Amsterdam (KITP Correlated Electrons 10/09/02)
High-Temperature Superconductors: A View from K-Space

Energy distribution maps: cut through \((\pi, 0)\) for \(T < T_c\)

- **AB & BB**
- **BB strong**
- **AB only**

'B wipe out' of spectral weight in UD

UD: AB and BB bands indistinguishable below \(T_c\)
Hi gh-Temperature Superconductors: A View from K-Space

\textbf{'Wipe out' disappears above }T_c\textbf{ }

\textbf{UD 'wipe out' gone above }T_c\textbf{ }

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

© Mark S. Golden

Dr. Mark Golden, Amsterdam (KITP Correlated Electrons 10/09/02)
High-Temperature Superconductors: A View from K-Space

T-dependence of ($\pi, 0$) PDH

- UD
- OD

many body PDH gone above $T_c$

band structure PDH remains above $T_c$

Fingerprints of the mode......

- Lives at ca. 38-40 meV energy
- Strongest effects closer to ($\pi, 0$)
- Only significant effects for $T < T_c$
- Coupling in UD much stronger than OD
- Odd symmetry w.r.t. bilayer (interband scattering)

$\rightarrow$ data: Feng/Chuang, theory: Eschrig&Norman

Dr. Mark Golden, Amsterdam (KITP Correlated Electrons 10/09/02)
**Rehabilitation of the bi-layer splitting**

- multilayer splitting becomes an advantage:

  OD  
  optD  
  UD  

  materials’ dependence of band structure + doping dependence of $\varepsilon_{AB}$ and $\varepsilon_{BB}$ + odd (interband) character of feedback =

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

---

**Correlation between $T_c^{\max}$ and $r$ parameter**

$r \sim t'/t$ obonding band of multilayer HTSC

$T_c^{\max}$

Pavarini et al., PRL 87 047003 (2001)
High-Temperature Superconductors: A View from K-Space

Outline

- ARPES as k-space microscopy
- results from the Bi$_2$Sr$_2$CaCu$_2$O$_y$ 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 underdoped regime
- next workshop...
High-Temperature Superconductors: A View from K-Space

Condensed Matter Physics Group, University of Amsterdam
Yingtai Huang

Spectroscopy Group, IFW Dresden
Sergey Borisenko, Alexander Kordyuk
Andreas Koitzsch, Sibylle Legner, Christian Dürr
Martin Knupfer, Thomas Pichler, Timur Kim
Roland Hübel, Dieter Müller
Jörg Fink, Claus Schneider, Frank Matthes, Robert Frömter IFF, IFW Dresden

Crystals
Helmut Berger
B. Liang, A. Maliouk, C. T. Lin, Bernhard Keimer
Guang Yang, Stuart Abell

Experimental collaboration
Fred Schiller, Serguei Molodtsov, Clemens Laubschat
Rolf Foliath
Michael Sing, Ralph Claessen
Stefano Turchini, Stefano Zennaro
Cesare Graziol

Crystal characterisation
K. Nenkov, D. Eckert

Money
FOM, EU, BMBF, DFG, SMWK

Dr. Mark Golden, Amsterdam (KITP Correlated Electrons 10/09/02) 39