ARPES studies of cuprates

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Goals of lecture

• Understand why gaps are important and various ways that gap is extracted in ARPES experiments

• Superconducting gap
  • How does one know it is a superconducting gap?
  • Momentum dependence of d-wave superconducting gap

• Pseudogap: enhance understanding of what it is exactly

• Electron-doped cuprates
What kind of gaps are there in condensed matter?

- Band gaps
- CDW gaps
- SDW gaps
- Superconducting gaps
- Hybridization gaps
- Pseudogaps

Why is it important to measure gaps?

Information about robustness and symmetry of a given phase.
Bogoliubov quasiparticles

\[
\begin{pmatrix}
\epsilon_k - \epsilon_F \\
\Delta^*
\end{pmatrix}
\begin{pmatrix}
\Delta \\
-(\epsilon_k - \epsilon_F)
\end{pmatrix}
\begin{pmatrix}
 u_k \\
v_k
\end{pmatrix}
= E_k
\begin{pmatrix}
 u_k \\
v_k
\end{pmatrix}
\]

Solutions to the matrix equation are simple.

At \( k_F \): \( |u_k|^2 = |v_k|^2 \).

Superposition of hole and electron states, with probabilities \( |u_k|^2 \) and \( |v_k|^2 \).
Observing Bogoliubov quasiparticles in ARPES

\[ E_k = -\sqrt{\varepsilon_k^2 + \Delta_k^2} \]

\[ T_c = 108K \]

Matsui et al. PRL 90 (2003)
Observing Bogoliubov quasiparticles in ARPES

$E_k = -\sqrt{\varepsilon_k^2 + \Delta_k^2}$

Energy distribution curves (EDCs)

- **Intensity** as a function of binding energy at fixed momentum
- Usual way of studying gaps

$T_c = 108$K

Assessing a gap, step 1: remove Fermi-Dirac cutoff

How?

- One way: divide spectrum by Fermi-Dirac function, convolved with instrument energy resolution
- Necessary if gap edge is sufficiently close to $E_F$

Matsui et al. PRL 90 (2003)
Assessing a gap, step 2: quantify gap

In this paper, $\Delta(k)$ along the cut was quantified by fitting to two lorentzians:

- Peak position $\rightarrow \Delta$
- Peak intensity $\rightarrow |u_k|^2, |v_k|^2$

Matsui et al. PRL 90 (2003)
Comparison to BCS theory

What correspondences between theory and experiment are there?

Matsui et al. PRL 90 (2003)
Mini-conclusions

- In superconducting state of cuprates quasiparticles appear to follow the same phenomenology as in BCS superconductors.
- Superconducting gap can be quantified by:
  - Dividing out Fermi-Dirac function
  - Finding $k_F$
  - Measuring energy position of quasiparticle peak

Superconducting gap is defined at $k_F$, so most papers only show EDCs at $k_F$. 
Cuprates have $d_{x^2-y^2}$ pairing symmetry

- Cuprate superconducting gap is anisotropic in momentum space
- ARPES is a momentum-resolved spectroscopic tool
Detour/disclaimer: fermi surface

Discussion of superconducting gap and pseudogap assumes a locus in momentum space, similar to a Fermi surface, even if Fermi liquid theory may not be applicable.
Detour/disclaimer: fermi surface

Brillouin zone and Fermi surface

Discussion of superconducting gap and pseudogap assumes a locus in momentum space, similar to a Fermi surface, even if Fermi liquid theory may not be applicable.
Cuprates have $d_{x^2-y^2}$ pairing symmetry

What is the evidence for a $d_{x^2-y^2}$ gap?

- Going across $T_c$: Leading-edge shift at momentum where antinode should be, none where node should be
- Spectral weight redistribution at antinode

Shen et al. PRL 70 (1993)
Momentum dependence of superconducting gap

\[ \Delta(k_x, k_y) = \frac{\Delta_0}{2} [\cos k_x - \cos k_y] \]

\[ |\Delta(k_x, k_y)| = \frac{\Delta_0}{2} |\cos k_x - \cos k_y| \]

\[ \Delta(\theta) = \Delta_0 \cos 2\theta \]
Momentum dependence of superconducting gap

- Gap at each momentum determined from leading edge midpoint (distance between inflection point or ½ height and $E_F$)
- $E_F$ determined from polycrystalline metal

H. Ding et al, PRB 54 (1996)
Momentum dependence of superconducting gap

Remove Fermi-Dirac cutoff by symmetrizing

1. Flip EDC about EF:
   \[ A(k_F, \omega)f(\omega) \rightarrow A(k_F, -\omega)f(-\omega) \]

2. Add flipped EDC to original EDC:
   \[ A_{sym}(k_F, \omega) = A(k_F, \omega)f(\omega) + A(k_F, -\omega)f(-\omega) \]

3. This removes FD cutoff if there is particle-hole symmetry
   \( A(k, \omega) = A(k, -\omega) \), which is true at \( k_F \) for a SC

4. Visualization tool: single peak=no gap, double peak=gap

Extract superconducting gap at each Fermi surface point by fitting to a phenomenological model (Norman et al, Phys. Rev. B 57, R11093 (1998))

Meng et al, PRB 79, 024514 (2009)
Momentum dependence of superconducting gap

2 ways to parametrize where you are on the Fermi surface:

1. Fermi surface angle ($\Phi$)
   Advantage: intuitive to know where you are on Fermi surface

2. Expression for $d_{x^2-y^2}$ gap to leading order
   \[ \frac{1}{2} |\cos k_x a - \cos k_y a| \]
   Advantage: easy to see if gap function has higher order terms

Meng et al, PRB 79, 024514 (2009)
Summary, part 1

How do we know if there is a gap in the spectrum?
- Leading edge shifts away from Fermi level
- Quasiparticle peak (after accounting for Fermi-Dirac cutoff) is not at $\omega = 0$ at $k = k_F$

How do we account for/remove Fermi-Dirac cutoff?
- Divide by Fermi function
- Compare measured spectrum to polycrystalline metal
- Symmetrize

How to we quantify the magnitude of the gap?
- Quasiparticle peak position
- Leading edge midpoint
- Fitting to a model
Summary, part 1

How do we know a gap has superconducting origin?
- Onsets at $T_c$
- Bogoliubov quasiparticle dispersion and spectral weight

What evidence for $d_{x^2-y^2}$ pairing does ARPES provide?
- Opening of a gap at antinodal momentum but not nodal momentum below $T_c$
- Momentum dependence of gap magnitude consistent with $d_{x^2-y^2}$ pairing
  - $\Delta(\theta) \propto \cos(2\theta)$
  - $\Delta(k) \propto \frac{1}{2} |\cos k_x - \cos k_y|$
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The pseudogap in **hole-doped** cuprates

- Is the ‘normal’ state accessed above $T_c$ or in sufficiently high magnetic field
- Onsets at $T^*$, which decreases with increasing doping
- Apparent in almost every experiment which couples to low-energy electrons

Discovery of ARPES signatures of pseudogap


Gap at antinodal momentum remains above $T_c$!

More modern ARPES data in pseudogap state to better visualize what is happening

Tc=92K

- Antinode: change in lineshape across Tc, but gap unchanged
- Node: Fermi arc above Tc
- Gap quantified by fitting symmetrized spectra to phenomenological model

More modern ARPES data in pseudogap state to better visualize what is happening

Depletion of spectral weight at $E_F \, T<T^*$

- Symmetrized EDCs at $k_F$ at antinode
- Normalize at high energy
- Subtract highest temperature trace

Kondo et al. Nat. Phys. 7 (2011)
Summary of ARPES signatures of pseudogap

- Antinode
  - Gap persists above $T_c$ until $T^*$
  - Change in lineshape
  - Starting from high $T$: depletion of spectral weight below $T^*$

- Node
  - Extended region of gapless excitations (Fermi arc)
Competing explanations for pseudogap

Pseudogap is phase-disordered superconductor


Pseudogap is distinct ordered phase


Complication: evidence for both superconducting fluctuations and symmetry breaking (unrelated to SC) at $T^*$
Evidence for ‘preformed pairs’

- Magnitude of gap unchanged across Tc

In this scenario, Fermi arc is attributed to d-wave gap which has been thermally broadened.

(note: the images on this slide are from a paper arguing for the opposite scenario, but they are used here for their data quality)
Evidence for ‘two-gaps’

- Distinct phenomenology in different regions of Fermi surface

In this scenario, Fermi arc is attributed to portion of Fermi surface where superconductivity once dominated and superconducting gap closed at $T_c$.

Non-monotonic momentum dependence of SC spectral weight suggests another order coexists with SC below $T_c$.

In this scenario, Fermi arc is attributed to portion of Fermi surface where superconductivity once dominated and superconducting gap closed at $T_c$.

Summary, part 2

• Signatures of pseudogap in ARPES
  • Gap above Tc in antinodal region of Fermi surface
  • In pseudogap state, DOS at $E_F$ does not go all the way to zero
  • Extended gapless region where node of SC gap used to be (Fermi arc)

• Competing explanations for pseudogap
  • Pre-formed pairs without phase coherence
  • A non-superconducting order which causes a gap
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Key message: antiferromagnetism and hot spots

FS reconstruction due to doubling of unit cell from AF order

Short-range correlations: “hot spots”

Normal state gap in electron-doped cuprates

- Normal-state gap in electron-doped cuprates is maximum at hotspot, not at antinodes
- Phenomenology well explained by short-range AF fluctuations

Superconducting gap in electron-doped cuprates

Matsui et al. PRL 94 (2005)

Consistent with d-wave, but gap is maximum at hot stop not at brilliouin zone boundary

How was gap assessed in this experiment?
Other misc. foci of ARPES studies of cuprates

Dispersion anomalies

Zhang et al. PRL 100, 107002 (2008)

Purpose: possibly related to pairing glue

Size and shape of Fermi surface

Hashimoto et al. PRB 77, 094516 (2008)

Purpose:
• What is the doping, really?
• What Fermi surface instabilities are likely?
Conclusions

• ARPES has contributed to studies of superconducting gap and pseudogap because both states involve a spectral gap at $E_F$ and are anisotropic in momentum space

• Gaps are studied via energy distribution curves (EDCs) which look at intensity vs energy at a fixed momentum

• Many ways to quantify gaps (leading edge shift, quasiparticle peak position, fitting to a model) and in the pseudogap regime, spectral weight depletion is an important metric too