Cuprate high-$T_c$ superconductivity: Insights from a model system

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Outline

- Introduction
  - HTSC and the cuprates
  - Spectroscopic methods applied to the high-$T_c$ problem
- Model system $\text{HgBa}_2\text{CuO}_{4+\delta}$
- Topics:
  1. The neutron resonant mode
  2. Pseudogap magnetism
  3. Energy $2\Delta_{sc}$ and above
- Summary
$T_c$ over the years

courtesy of Rudi Hackl
Cuprates: crystal and electronic structure

Fisher et al., in *Handbook of high-temperature superconductivity*, Springer (2007)

Cuprates: crystal and electronic structure

three-band model

t_{dp} \ll U, t_{dp} \ll \Delta_{dp}

\mathit{t}_p, \mathit{t}_p' \text{ negligible}

t-J model

\begin{align*}
\text{(c)} & \quad \begin{array}{c}
\varepsilon_p \\
B \quad \text{NB} \\
\varepsilon_p' \\
\varepsilon_F \\
AB
\end{array} \\
\text{(d)} & \quad \begin{array}{c}
\varepsilon_p \\
B \quad \text{NB} \\
\varepsilon_p' \\
\varepsilon_F \\
LHB \quad \text{UHB}
\end{array} \\
\text{(e)} & \quad \begin{array}{c}
LHB \\
B \quad \text{NB} \\
UHB
\end{array} \\
\text{(f)} & \quad \begin{array}{c}
LHB \\
T \quad \text{ZRS} \\
UHB
\end{array}
\end{align*}
$d$-wave pairing near a spin-density-wave instability

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(Received 23 June 1986)

We investigate the three-dimensional Hubbard model and show that paramagnon exchange near a spin-density-wave instability gives rise to a strong singlet $d$-wave pairing interaction. For a cubic band the singlet ($d_{x^2-y^2}$ and $d_{3z^2-r^2}$) channels are enhanced while the singlet ($d_{xy}, d_{xz}, d_{yz}$) and triplet $p$-wave channels are suppressed. A unique feature of this pairing mechanism is its sensitivity to band structure and band filling.

Unconventional SC near AF instability

Some important questions

- Q: What’s the pairing symmetry?
- Q: What causes the pseudogap above $T_c$?
- Q: Is there a competing order other than AFM?
- Q: Which bosonic modes are important?
- Q: What’s the minimal microscopic model?
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ARPES


STM/STS

Optical conductivity


Cooper et al., *PRB* 47, 8233 (1993)

van Heumen *et al., PRB* 79, 184512 (2009)
Raman scattering

Hg1201


Sugai et al., PRB 68, 184504 (2003)
Neutron scattering

Haug et al., PRL 103, 017001 (2009)

YBCO

La$_2$CuO$_4$

Headings et al., PRL 105, 247001 (2010)
(Resonant) X-ray scattering


Some important questions

Q: What’s the pairing symmetry?
   A: $d$-wave.

Q: What causes the pseudogap above $T_c$?
   A: There is evidence for both pre-formed pairs and competing order.

Q: Is there a competing order other than AFM?
   A: CDW, SDW, intra-unit-cell order are all possible.

Q: Which bosonic modes are important?
   A: Both magnetic excitations and phonons are prominent.
      
      (Which one is the “pairing glue” is a separate question!)

Q: What’s the minimal microscopic model?
   A: Single-band models are accepted as there is no strong violation.
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$T_c$ over the years


courtesy of Rudi Hackl
Model system HgBa$_2$CuO$_{4+\delta}$

- Single layer, tetragonal
- Single Cu site, flat Cu-O sheet
- Doping disorder confined to far away from the Cu-O sheets
- Highest $T_c$ (max. 97 K) among single-layer compounds

$Y$Ba$_2$Cu$_3$O$_{6+\delta}$

$T_{c,\text{max}} = 92$ K

HgBa$_2$CuO$_{4+\delta}$ (Hg1201)

$T_{c,\text{max}} = 97$ K
Challenges from the synthesis

- Mercury is toxic 😞
- Synthesis requires high pressure
- Purity against crystal size

Principles of synthesis:
Pure and big single crystals

Barišić, YL, et al., PRB 78, 054518 (2008)

Work since 2008

Neutron scattering

Optical conductivity

ARPES

STM/STS

XPS

Pressure

REXS/RIXS

Ultrasound

NMR

μSR

Magneto-transport

Kerr effect

Microwave

SHG

IXS

Raman scattering
Neutron scattering

Properties of neutron
charge 0, spin 1/2
magnetic moment (P), energy (E)
and momentum (k)
scattering due to nuclear and electromagnetic interaction

Thermal neutron
$E = 10–100$ meV, $k = 2–7$ Å⁻¹
match typical energy and momentum in solid state physics

\[ I(Q, \omega) \propto \mathcal{F}_{r,t} \int \, d\mathbf{r}' \langle b(\mathbf{r}' - \mathbf{r}, 0) b(\mathbf{r}', t) \rangle \]

\[ \mathbf{k}_i - \mathbf{k}_f \equiv \mathbf{Q} \]
\[ E_i - E_f \equiv \hbar \omega \to \omega \]
Raman scattering
Optical ellipsometry

\[ \sigma_1 \sim \omega \varepsilon_2 \]

\[ \varepsilon(\omega) = (n + i\kappa)^2 = 1 + \frac{e^2 N}{\varepsilon_0 m V} \frac{1}{(\omega_0^2 - 2i\beta\omega - \omega^2)} \]
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The neutron resonant mode


YBCO$_{6.6}$

Inosov et al., Nat. Phys. 6, 178 (2010)

Ba(FeCo)$_2$As$_2$

Fong et al., Nature 398, 588 (1999)

Bi2212

He et al., Science 295, 1045 (2002)

TI2202

Stock et al., PRL 100, 087001 (2008)
Resonant mode in Hg1201

Yu, YL et al., PRB 81, 064518 (2010)
Resonant mode in Hg1201

Yu, YL et al., PRB 81, 064518 (2010)
Resonant mode in Hg1201

- We confirmed the universal presence of the resonant mode
- Sign-changing $\Delta_{sc}$ connected by $q_{\text{res}}$: as expected from $d$-wave

Coherence factor:

$$\frac{1}{2} \left( 1 - \frac{\Delta(k)\Delta(k + q^*)}{\mathcal{E}(k)\mathcal{E}(k + q^*)} \right)$$

Conventional wisdom: $E_r \propto T_c$
Superconducting gap: $\Delta_{sc}$

Fauque et al., *PRB* 76, 214512 (2007)


Pushp et al., *Science* 324, 1689 (2009)
Universal $E_r$-$\Delta_{SC}$ scaling

- $\Delta$ is not proportional to $T_c$ in underdoped systems
- One should consider both resonant modes in bilayer systems

Yu, YL et al., Nature Physics 5, 873 (2009)
Implication

- Unexpected from a simple RPA excitonic picture

\[ \chi(q, \omega) = \frac{\chi_0(q, \omega)}{1 + J(q) \chi_0(q, \omega)} \]

- Implies a much deeper connection between magnetic fluctuations (entire spectrum) and superconductivity

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“Orbital current” order

Varma, *PRB* 73, 155113 (2006)

Bourges & Sidis, *C.R. Physique* 12, 461 (2011)
Spin-polarized neutron scattering

Properties of neutron

charge 0, spin 1/2
magnetic moment (P), energy (E)
and momentum (k)

scattering due to nuclear and
electromagnetic interaction

Spin-flip scattering all comes from electromagnetic interaction
Intra-unit-cell order: initial evidence

Fauqué et al., *PRL* 96, 197001 (2006)

Bourges & Sidis, *C.R. Physique* 12, 461 (2011)
Intra-unit-cell order: confirmed in Hg1201

(1 0 1) Bragg peak

YL et al., PRB 84, 224508 (2012)
Intra-unit-cell order: evidence from STM/STS

Lawler et al., *Nature* **466**, 347 (2010)
New excitations in the pseudogap state

AF-type fluctuations near $(1/2,1/2)$, including the resonance

New excitations

Related publications:
YL et al., Nature 468, 283 (2010)
YL et al., Nat. Phys. 8, 404 (2012)

Spin waves in La$_2$CuO$_4$
Coldea et al., PRL 86, 5377 (2001)
Samples

“OP95”

“UD65”
Unusual aspect of the resonance data
Verification of magnetic origin

Measured in spin-flip geometry
Almost disperseless excitation

Sample: OP95
A second excitation branch
Verification of magnetic origin

\[ 2 \times |I_{S} - I_{Q}| = \text{arb. units} \]

- **OP95**
- **UD65**

\[ \text{Energy (meV)} \]

\[ \sim 125 \text{ hours} \]

(whole beam time)

\[ \sim 6 \text{ hours} \]
$T$ dependence

**c**

- **OP95**
  - $(0, 0, 4.6)$ 53 meV
  - $(0.2, 0.2, 5.2)$ 53 meV
  - $(1.08, 1.08, 0)$ 32 meV

**d**

- **UD65**
  - $(0.2, 0.2, 6.0)$ 54 meV
  - $(0.5, 0.5, 4.4)$ 39 meV
Q dependence

OP95

4K - 230K

Intensity (arb. units)

Energy (meV)

Differ by 90° sample rotation
Connection to signal maxima at (1/2,1/2)
New excitation summary

- Two almost disperseless modes
- Verified to be magnetic
- Set in below $\sim 7^*$
- One energy decreases with doping
- Mysterious $Q$ dependence of intensity
- Connection to AF fluctuations

YL et al., Nature 468, 283 (2010)
YL et al., Nat. Phys. 8, 404 (2012)
Electron-boson coupling

van Heumen et al., PRB 79, 184512 (2009)
Electron-boson coupling

Lee et al., Nature 442, 546 (2006)
Electron-boson coupling

Inverted from high-resolution ARPES data taken by Xingjiang Zhou’s group

Yun et al., PRB 84, 104521 (2011)
What are these excitations?

1. Excitations from “orbital currents”?
   - 😊 Two modes, same $T^*$ as seen by neutron diffraction
   - 😞 Q-dependence, relation to AF fluctuations
   

2. Admixture between AF fluctuations and phonons?
   - 😊 Multiple modes, Q-dependence, coincidence with AF fluctuation maxima
   - 😞 Lack of systematic theory

3. Local modes?
   - 😊 Weak dispersion, Q-dependence
   - 😞 Coincidence with AF fluctuation maxima, large spectral weight

See, *e.g.*, Martin *et al.*, *PRB* 70, 224514 (2004)
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Phonon-mediated superconductivity

Lattice vibration

Magnetic fluctuation mediated superconductivity

Desire to form pairs

Magnetism

A feedback effect due to pairing can be expected on the magnetic fluctuations
More “juice” at higher energy

LSCO $x=0.16$

LSCO $x=0.22$

Le Tacon et al., *Nat. Phys.* 7, 725 (2011)

**Hg1201**, data taken last week at SLS with Le Tacon, Tabis, Braicovich

How about correlation between high-energy magnetic excitations and SC as we change temperature and doping?
Raman scattering


Sugai et al., PRB 68, 184504 (2003)
Samples

Freshly prepared sample surface (50x)

Our $p$- and $T$-range

Temperature (K)

Hole concentration

$T_c$
Hg1201, UD77
($T_c = 77$ K)

**a**

$\chi''(\omega, T)$ (arb. units)

**b**

$\chi''(\omega, T) - \chi''(\omega, 330 \text{ K})$ (a.u.)

- **Pair-breaking peak**
- **two-magnon peak**
- **gap**

Raman shift $\omega$ (cm$^{-1}$)
Both!

High-energy feedback effect

- Enhancement of two-magnon peak when the gap opens
- Pre-formed pairs observed around the same temperature

High-energy feedback effect similar to the resonant mode!

Reasons for the “two-magnon” name:
- Selection rule is correct ($B_{1g}$)
- Energy agrees with reported values
- “Leading edge” insensitive to doping

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- Q: Is there a competing order other than AFM?
  A: CDW, SDW, intra-unit-cell order are all possible.

- Q: Which bosonic modes are important?
  A: Magnetic excitations, phonons, AND perhaps modes with *mixed degrees of freedom*.

- Q: What’s the minimal microscopic model?
  A: Single-band models may be insufficient.
Collaborators

**Neutron Scattering**
- Guichuan Yu (U. Minnesota)
  - Martin Greven (U. Minnesota)
  - Paul Steffens (ILL, Grenoble)
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  - Nikola Egentenmeyer (PSI, Villigen)
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  - Victor Balédent (LLB, Saclay)
  - Yvan Sidis (LLB, Saclay)
  - Philippe Bourges (LLB, Saclay)

**Raman Scattering**
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**Theory**
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**Samples and Characterization**
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Thank you!