Polaronic Effects in the Lightly Doped Cuprates

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ARPES Studies of the Cuprates

Physics of “Lightly Doped” Mott Insulators?

“High-Temperature Superconductivity is the physics of strong correlations”

Temperature (K)

Hole Doping (x)

Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$
Bi$_2$Sr$_2$CuO$_{6+\delta}$
YBa$_2$Cu$_3$O$_{7-\delta}$
Phase Diagram of $\text{Ca}_{2-x}\text{Na}_x\text{CuO}_2\text{Cl}_2$

- $T_{c,\text{max}} = 28$ K @ $x = 0.18$
- $x = 0 : T_N = 247$ K
- $x = 0.05 : \text{No SC or Néel order}$
- $x = 0.10 : T_c \sim 13$ K
- $x = 0.12 : T_c = 22$ K

Hole Doping ($x$)

AFI

SC

Grown under high pressures ($\sim 4$ GPa)

Tetragonal $\text{K}_2\text{NiF}_4$ Structure

Undistorted square CuO$_2$ planes

Y. Kohsaka et al., JACS (2002)
Many-Body Interactions in Cuprates

Studying interactions of many holes with spin, lattice, charge degrees of freedom an intractable theoretical problem...

Can we simplify the problem (both experimentally and theoretically?)
A Single Hole in the Mott Insulator

ARPES on Mott insulator: Reflects dynamics of a single hole!

A logical starting point for understanding relevant interactions
Band Structure Predictions: Non-Interacting

Kinetic Energy Only
Mott Insulator: Magnetic Interactions

KE & Magnetism

\[ \mathcal{H} = -t \sum_{\langle ij \rangle, \sigma} (c_{i \sigma}^\dagger c_{j \sigma} + \text{h.c.}) + J \sum_{\langle ij \rangle, \sigma} (\mathbf{S}_i \cdot \mathbf{S}_j - \frac{n_i n_j}{4}) \]
A Single Hole in the Mott Insulator

-0.5
0
-1

Energy (eV)

(0.7\pi, 0.7\pi)

(0.14\pi, 0.14\pi)

(\pi/2, \pi/2)

(0, 0)

(\pi, 0)

(\pi, \pi)

(0, 0)

Wavevector (r.l.u.)

Energy (eV)

LDA

\textit{t-J} model

Experiment
Comparison with Fermi Liquid

**Ca$_2$CuO$_2$Cl$_2$**

1. Peak Width ~ 300 meV  
2. Gaussian Lineshape  
3. Separation of $\mu$ from peak

**Sr$_2$RuO$_4$**

1. Peak Width ~ 10 meV  
2. Lorentzian (FL) Lineshape  
3. Peak approaches $\mu$
Electron-Boson Interactions in Cuprates

“Ubiquitous”

Campuzano, Dessau, Fink, Johnson, Lanzara, Norman, Z.-X. Shen, Takahashi
The Franck-Condon Effect

\[ \mathcal{H} = \epsilon_0 c^\dagger c + \sum_q \omega_q a_q^\dagger a_q + \sqrt{g \omega_0^2} \sum_q c^\dagger c(a_q + a_{-q}^\dagger) \]

Equivalent to Franck-Condon broadening

D.W. Turner, 1970
Comparison with Fermi Liquid

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![Graph for Ca$_2$CuO$_2$Cl$_2$](image1)

$g \sim 10$

![Graph for Sr$_2$RuO$_4$](image2)

$g << 1$
Theoretical Treatments of Polaron Physics

A. Mishchenko & N. Nagaosa

O. Rosch & O. Gunnarsson

**Centroid (first moment) of spectral weight tracks**

*“frozen lattice” dispersion!*


Doping Evolution of the Cuprates

Emergence of the Sharp Nodal Quasiparticles

Resolving the Long-Standing Controversy over the Doping Evolution of the Chemical Potential

Shift into LHB / UHB

Midgap States

Z.-X. Shen et al., PRB 44, 12098
P.G. Steeneken et al., PRL 90, 247005
N.P. Armitage et al., PRL 88, 257001
Y. Kohsaka et al., JPSJ 72, 1018

J.W. Allen et al., PRL 64, 595
R.O. Anderson et al., PRL 70, 3163
A. Ino et al., PRL 79, 2101
N. Harima et al., PRB 64, 220507
Chemical Potential Shift: $O 2p_\pi$ & $O 2p_z$
Evolution of Low Energy States
Evolution of Low Energy States

Franck-Condon Broadening in Photoemission

**Cuprates**
- A.S. Alexandrov
- O. Rosch (2005)

**Ionic Insulators**

**I-D Peierls**
- L. Perfetti (2001)

**Manganites**
- D.S. Dessau (1998)
- V. Perebeinos (2000)
- Y.D. Chuang (2000)

**Vanadates**
- K. Okazaki (2001)

**Magnetite**
- D. Schrupp (2004)

“The activation-type temperature dependence of hole-mobilities in transition-metal oxides ... provided the initial stimulus for the present work.”
Strong Interactions in the Cuprates

KE & Magnetism & Lattice

A.S. Mishchenko & N. Nagaosa (PRL ‘04);
O. Rosch & O. Gunnarsson (PRL ‘04, EPJ B ‘05)
Determining the Origin of Broadening

LHB states tied to spin, charge, and lattice degrees of freedoms.

O \(2p_\pi\) and Ca \(3p\) states have no overlap with LHB or Cu \(3d\) orbitals. Therefore, represents primarily lattice contribution.

Use these states as a simple benchmark!
Franck-Condon Broadening: Core Levels

Core Hole lifetimes in Alkali Halides (KCl, KI, KF)

- Lineshape and temperature dependence in ionic insulators very different from simple metals
- Gaussian lineshapes suggested lattice (Franck-Condon) broadening dominant
- Significant temperature broadening (unexpected from electron-hole decay)

P.H. Citrin et al., PRL (1974)
also G.K. Wertheim & Y. Baer
Comparison of Lineshape

- Both LHB & O\textit{2p}_\pi states exhibit Gaussian lineshapes
- Franck-Condon Broadening exists for uncorrelated non-LHB state (O\textit{2p}_\pi)

K.M. Shen \textit{et al.}, submitted
J.J.M. Pothuizen \textit{et al.}, PRL (1997)
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**Kyoto University (Samples)**: Masaki Azuma and Mikio Takano

**University of Oregon (Samples)**: Lance Miller

Conclusions

• Spectral features of insulating cuprates (and many TMOs!) can be understood in a polaronic / Franck-Condon model

• Quasiparticles grow from near zero intensity when doped away from insulator, and this QP band controls $\mu$

• FCB present in other uncorrelated electronic states, suggesting a strong lattice contribution

K.M. Shen et al., submitted (2005)