Cuprate Superconductors: Towards materials specific calculations

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Acknowledgements

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Thomas Maier, Thomas Schulthess / ORNL

Ole K. Andersen, Tanusri Dasgupta, Ove Jepsen / MPI Stuttgart

Funding:

DOE / CMSN

Computer time:

Cray X1 / ORNL

Figures:

superconductors.org

DOE

APS
Outline

1. Superconductivity Background
2. Model theories (?)
3. Materials specific simulation (?)
4. Next Steps and Summary
Superconductivity


H. K. Onnes
1913 Nobel Prize (He)
Conventional Superconductors

- Pairing due to phonon-mediated pairing potential
- Fermi-liquid Normal State
- Moderately Correlated Systems
- s-wave
The Isotope Effect (the smoking gun)

BCS

\[ T_c = \omega_D e^{-1/N(0)} V \]

Migdal-Eliashberg

local approximation

\[ \Sigma(k,\omega) \approx \Sigma(\omega) \]
Pairing is due to potential energy recovery

System recovers substantial potential energy by forming pairs. However, paired electrons must occupy states outside the Fermi sea, i.e. states with an increased kinetic energy.
New superconductors (’86)

Pressure 168K

DOE figure
Cuprates: Unusual Superconductors

- No BCS-like phonon/isotope “smoking gun”
- Mechanism?
- Non-Fermi liquid underdoped normal state (pseudogap)
- Doped Mott insulator
- d-wave
- Kinetically Driven Pairing

Alex Müller and Georg Bednorz
1987 Nobel Prize
Complex phase diagram

Unlike BCS, must dope to ~15% holes for highest $T_c$
Kinetic Energy Reduction
(opposite of BCS)


$A_{1+D} = - \text{kinetic energy}$

Kramers-Kronig

Kinetic Energy reduction is roughly 1 meV > condensation energy!
Meanwhile...

(Back in the real world)
Industrial manufacture of HTSC wires, power machinery (motors, generators) exploiting high current densities achievable
Outstanding questions
(19 years later)

• What is the principal mechanism?
  • Electrons? Phonons? Both? Other?
• Does material A, B, or C have higher Tc?
• Influence of pressure, magnetic fields?
• Other materials with same mechanism?
  c.f. new BCS-like MgB2 in 2001, 39K
• ...many others
Outline

1. Superconductivity Background
2. Model theories
   a. Hubbard model
   b. DCA simulations
3. Materials specific simulation
4. Next Steps and Summary
Focus on Cu-O layers

Quasi 2D system
SC is in plane
Half-filled when undoped
Antiferromagnet
The Hubbard Model of the Cuprates

CuO$_2$ Planes

Hubbard Model with $8t = W \approx U$
Anderson 87, Zhang-Rice 88

Note: A few model parameters ($t,U$) fit to experiment
The Energy Scales in the Hubbard Model

The Bandwidth \( W = 8t \)

\[ \cdots \quad \text{N(E)} \quad \cdots \]

The local Coulomb repulsion \( U \)

\[ \begin{align*}
\text{Energy} & \\
0 & \quad 2\varepsilon + U \\
\varepsilon & \\
\text{Moment Formation} & \\
\end{align*} \]

\[ \begin{align*}
E_1 &= -\frac{t^2}{U} \\
E_2 &= 0 \\
J &= 2(E_1 - E_2) \\
\text{Antiferromagnetic exchange} &
\end{align*} \]

Note: A few model parameters \((t,U)\) fit to experiment
Pairing Mechanism: Holes in AF background

One hole motion breaks AF bonds

A bound second hole restores the AF bonds


Pseudogap due to SRO or pre-formed pairs, Pairing due to kinetic energy gain
Outline

1. Superconductivity Background

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Effective Medium

Periodic Lattice

Dynamical Cluster Approximation

Solve self-consistently

Difficult to solve accurately directly
## Cluster Approximations

**Dynamical Cluster Approximation: Expansion around the DMF/CPA Solutions**

<table>
<thead>
<tr>
<th>$N_c$</th>
<th>1</th>
<th>4</th>
<th>8</th>
<th>16</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\text{effective medium}$</td>
<td>$\text{cluster}$</td>
<td>$\text{DMFA}$</td>
<td>$\text{effective medium}$</td>
<td>$\text{cluster}$</td>
</tr>
</tbody>
</table>

\[
\sum_{\text{lattice}} \approx \sum_{\text{cluster}}
\]

DCA papers http://www.physics.uc.edu/~jarrell
We Solve The Cluster Problem with Quantum Monte Carlo (QMC)

Expensive! 1-1000+ cpu hours per temperature and doping
Many temperatures and dopings per phase diagram
Small cluster results
Phase Diagram $N_c=4$

$U=W=2.0$ $N_c=4$

- Pseudogap
- d-wave superconductivity
- AF
- Fermi Liquid Like

$T$, $\delta$ axes
Energies for $T < T_c$

Kinetic energy reduction entering SC phase
Small cluster DCA Hubbard calculations display key features of cuprate phase diagram
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1. Superconductivity Background
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3. Materials specific simulation
4. Next Steps and Summary
Outstanding questions
(19 years later)

• What is the principal mechanism?
  • Electrons? Phonons? Both? Other?

  Mostly electronic

• Does material A, B, or C have higher Tc?

• Influence of pressure, magnetic fields?

• Other materials with same mechanism?
  • c.f. new BCS-like MgB2 in 2001, 39K
Focus on Cu-O layers

Need to include entire structure, additional orbitals
First-principles calculations

Use zero-temperature LDA density functional calculations for structure and bonding

Although these band-structure methods “fail”, structure and bonding are close to experiment: hope/look for trends.
Method

1. DFT LDA ground state

Obtain parameters

2. Multi-band Hubbard Hamiltonian

3. Phase Diagram
Can this work?
LDA+DMFT

Similar method recovers structural phase transition in Pu

Kotliar Nature 410 793 (2001)
Trends from DFT
PRL 87 047003 (2001)
DFT Orbitals

Well-localized Cu d orbital obtained: small materials differences.

O px, py: strong hybridization.

La$_2$CuO$_4$  
HgBa$_2$CuO$_4$
DFT Orbitals
Some far from atomic picture
Hopping meV

HgBa2CuO4
Tl2Ba2CuO6
TlBaLaCuO5
La2CuO4
Ca2CuO2Cl2

Increasing Tc
DFT Results

• ~6 terms appear significant, in this basis

  Parametric studies are possible

• Parameters are close to empirical parameters used in model calculations

• Some trends apparent e.g. txyI (=tpp) increases with increasing Tc. Similar to single band observations, but inconclusive.
LDA+DCA results
Few % variation in U; similar in all materials

Any Tc dependence must reside in orbitals or additional interactions (e.g. phonons)
HgBa₂CuO₄
“near-neighbor” parameters

Tc

Inverse d pairing susceptibility vs. T (arb. units)
Near-neighbor parameters

Full HgBa$_2$CuO$_4$ Parameters
No SC transition
Band structure v. important
Hopping meV

Increasing Tc

“Kills” SC Transition

HgBa2CuO4
Tl2Ba2CuO6
TlBaLaCuO5
La2CuO4
Ca2CuO2Cl2
Parametric Results

2nd NN Cu-O hybridization strongly governs Tc

Toy model: +ve sign, Tc increased ~60% from reference
Outline

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Next Steps

Investigating influence of DFT ground state

    More accurate calculations underway

If we fail, we will have shown “something extra” is needed to describe HTSC in real materials.

If we succeed, we expect to obtain “materials trends” in real HTSC materials.
Oxygen Superstructures Throughout the Phase Diagram of (Y, Ca)Ba$_2$Cu$_3$O$_{6+x}$

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(Received 12 November 2003; published 7 October 2004)

The doping dependence of short-range lattice superstructures in (Y, Ca)Ba$_2$Cu$_3$O$_{6+x}$ has been studied with high-energy x-ray scattering. We observe diffuse features with a well defined periodicity which depend on the oxygen concentration but not on the charge carrier concentration. In addition, we find that diffuse scattering is absent in underdoped YBa$_2$Cu$_4$O$_8$, which does not sustain oxygen defects. Our combined data highlight that the diffuse scattering arises from short-range oxygen ordering and associated lattice distortions. Signatures of stripe ordering or fluctuations are not seen and therefore must be much weaker.

DOI: 10.1103/PhysRevLett.93.157007

PACS numbers: 74.72.Bk, 61.10.Eq, 74.25.-q
Four-Unit-Cell Superstructure in the Optimally Doped YBa$_2$Cu$_3$O$_{6.92}$ Superconductor

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(Received 23 December 2003; published 7 October 2004)

Diffuse x-ray scattering measurements reveal that the optimally doped YBa$_2$Cu$_3$O$_{6.92}$ superconductor is intrinsically modulated due to the formation of a kinetically limited 4-unit-cell superlattice, $q_0 = (\frac{1}{4}, 0, 0)$, along the shorter Cu-Cu bonds. The superlattice consists of large anisotropic displacements of Cu, Ba, and O atoms, respectively, which are correlated over $\sim$3–6 unit cells in the $ab$ plane, and appears to be consistent with the presence of an O-ordered “ortho-IV” phase. Long-range strains emanating from these modulated regions generate an inhomogeneous lattice which may play a fundamentally important role in the electronic properties of yttrium-barium-copper-oxides.
Summary

Small cluster DCA Hubbard calculations display key features of cuprate phase diagram.

LDA+DCA calculations are feasible. We are testing fundamental assumptions of many cuprate theories.

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