Closing in on an Explanation for High-Temperature Superconductivity

Thomas A. Maier
Oak Ridge National Laboratory

T.C. Schulthess
M. Jarrell, A. Macridin
D. Scalapino
D. Poilblanc

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Superconductivity - Zero resistance state

**Discovery:**
- Zero resistance state
  H. Kamerlingh Onnes (1911)

**Meissner-Ochsenfeld effect:**
- Superconductors repel magnetic fields
  Meissner & Ochsenfeld (1933)

**Explanation:**
- Bardeen-Cooper-Schrieffer theory (1957)
- BCS theory generally accepted in early 1970s
BCS Theory - Fermions, Bosons and Cooper pairs

- **Fermions** (Electrons)
- **Bosons**
- **Phonons** (lattice vibrations) glue fermions into Cooper pairs (boson-like)

Energy gap prevents scattering that leads to resistivity

Energy gap: $\Delta E$
Cuprate high-temperature superconductors

**Discovery:**
- Bednorz & Müller (1986)

**Properties:**
- Insulators or bad metals
  (conv. superconductors are good metals)

**Critical temperatures:**
- \( T_c \sim 40\text{K} - 150\text{K} \)
  (well above liquid nitrogen boiling point)

**20 years of intense research:**
- No consensus on a general theory
- No predictive power for \( T_c \) in known materials
- No predictive power for design of new materials
Applications of superconductors

**Large volume, stable magnetic fields**
- MRI and NMR machines
- Mass spectrometers
- Particle accelerators
- Maglev trains

**Josephson effect**
- Josephson junctions (SQUIDS)
- Digital circuits

**High power capacity at lower voltage**
- Cables (3-5x more power capacity than conv. AC cables, 10x more than DC cables)
- Motors and generators

Source: www.amsc.com
Outline

- Brief introduction into superconductivity
- Background: 2D Hubbard model and the DCA/QMC method
- Breakthroughs and future work
From cuprate materials to the Hubbard model

Cuprate structure

CuO-planes

2D Hubbard Model

Basic properties:
- Moment formation
- Antiferromagnetic exchange

\[ \mathcal{H} = -t \sum_{\langle ij \rangle, \sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \]

Energy

\[ J = \frac{4t^2}{U} \]
**The challenge: A quantum multi-scale problem**

<table>
<thead>
<tr>
<th>Atomic scale</th>
<th>Nano-scale</th>
<th>Macro-scale</th>
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</thead>
<tbody>
<tr>
<td>- Strong local correlations</td>
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<td></td>
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<tr>
<td>- Moment formation</td>
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<tr>
<td>~ nm</td>
<td>- Antiferromagnetic correlations</td>
<td></td>
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<tr>
<td></td>
<td>- Cooper pairs</td>
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<td></td>
<td>- Inhomogeneities</td>
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<td></td>
<td>~ μm</td>
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</tr>
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<td></td>
<td>- Macroscopic quantum effects</td>
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**Theory:**

- Atomistic description
  - Complexity $\sim 4^N$
- Thermodynamics Continuum description
  - $N \sim 10^{23}$
The solution: Quantum cluster methods

Atomic scale
- Strong local correlations
- Moment formation

Nano-scale
- Antiferromagnetic correlations
- Cooper pairs
- Inhomogeneities

Macro-scale
- Macroscopic quantum effects

Explicitly treat correlations within a localized cluster

Coherently embed cluster into effective medium

Quantum cluster theories review:
Maier, Jarrell, Pruschke & Hettler, Rev. Mod. Phys. ‘05
**Sketch of the DCA/QMC method**

Quantum cluster theories review:
Maier, Jarrell, Pruschke & Hettler, Rev. Mod. Phys. '05

Essential assumption:
Correlations are short-ranged

Bulk lattice

Size $N_c$ clusters

Integrate out remaining degrees of freedom

Reciprocal space

$\Sigma(k, z) \approx \Sigma(K, z)$

Embedded cluster with periodic boundary conditions

DCA
**DCA cluster mapping & cluster solver**

Computationally expensive part

\[ G_0(R, \tau) \]

\[ G_0(K, z) = [ \tilde{G}^{-1}(K, z) + \Sigma(K, z) ]^{-1} \]

\[ \tilde{G}(K, z) = \frac{N_c}{N} \sum_{\tilde{k}} [ z - \epsilon_{K+\tilde{k}} - \Sigma(K, z) ]^{-1} \]

\[ \Sigma(K, z) = G_0^{-1}(K, z) - G_c^{-1}(K, z) \]
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Superconductivity in Hubbard model on Cray X1(E)

Pairing mechanism in Hubbard model on Cray XT3/4

Role of inhomogeneities on Cray XT5
Evidence for superconductivity in 2D Hubbard model

2005 on Cray X1(E):
- Superconducting transition in 2D Hubbard model in largest accessible clusters
- Superconducting susceptibility diverges at finite temperature $T \sim 0.025t$ (~100K)

$$P_d = \int_0^\beta d\tau \langle \Delta_d(\tau)\Delta_{d}^\dagger(0) \rangle$$

Understanding the pairing mechanism

2006 - 2008 on Cray XT3/XT4:
- Study of mechanism responsible for pairing in the Hubbard model
- Analyze the particle-particle vertex in the normal state
- Electron spin is responsible for pairing interaction

Why pairing in a model with purely repulsive interactions?

Doping a Mott insulator:
Physics dominated by Coulomb energy, kinetic energy is frustrated

Brinkman & Rice, PRB (1970)
Why pairing in a model with purely repulsive interactions?

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Hole localization due to increase in exchange energy!
Relieve kinetic frustration through pairing

Paired hole restores antiferromagnetic background

(Hirsch, PRL ’87; Bonca et al., PRB ‘89; Dagotto et al., PRB ‘90)
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Spin fluctuation model

**Spin fluctuation mechanism:**

Pairing arises from exchange of spin fluctuations

\[ \Gamma_{pp}(k, \omega; k', \omega') \approx \frac{3}{2} \bar{U}^2 \chi(k - k', \omega - \omega') \]

- Calculate \( T_c \) in spin-fluctuation model and compare with actual \( T_c \)


<table>
<thead>
<tr>
<th>(&lt;n&gt;)</th>
<th>0.95</th>
<th>0.90</th>
<th>0.85</th>
</tr>
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<tbody>
<tr>
<td>( T_{c0} )</td>
<td>0.080</td>
<td>0.074</td>
<td>0.067</td>
</tr>
<tr>
<td>( T_{c0}^{(1)} )</td>
<td>0.100 (25%)</td>
<td>0.087 (18%)</td>
<td>0.074 (10%)</td>
</tr>
<tr>
<td>( T_{c0}^{(2)} )</td>
<td>0.108 (35%)</td>
<td>0.084 (14%)</td>
<td>0.064 (4%)</td>
</tr>
<tr>
<td>( T_{c0}^{(3)} )</td>
<td>0.105 (31%)</td>
<td>0.081 (9%)</td>
<td>0.058 (13%)</td>
</tr>
</tbody>
</table>

Miyake et al., PRB 34, 6554 (1986)
Scalapino et al., PRB 34, 8190 (1986)
Review: Monthoux et al., Nature ‘07
Theories based on the coupling between spin fluctuations and fermionic quasiparticles are among the leading contenders to explain the origin of high-temperature superconductivity, but estimates of the strength of this interaction differ widely. Here, we analyse the charge- and spin-excitation spectra determined by angle-resolved photoemission and inelastic neutron scattering, respectively, on the same crystals of the high-temperature superconductor $\text{YBa}_2\text{Cu}_3\text{O}_6$. We show that a self-consistent description of both spectra can be obtained by adjusting a single parameter, the spin-fermion coupling constant. In particular, we find a quantitative link between two spectral features that have been established as universal for the cuprates, namely high-energy spin excitations and ‘kinks’ in the fermionic band dispersions along the nodal direction. The superconducting transition temperature computed with this coupling constant exceeds 150 K, demonstrating that spin fluctuations have sufficient strength to mediate high-temperature superconductivity.

"The superconducting transition temperature computed with [the spin fluctuation model] exceeds 150 K, demonstrating that spin fluctuations have sufficient strength to mediate high-temperature superconductivity"
Spin fluctuations vs. RVB: Mouse vs. Elephant

P.W. Anderson, Science 316, 1705 (2007): “We have a mammoth (U) and an elephant (J) in our refrigerator - do we care much if there is also a mouse?”

Resonating Valence Bond mechanism:

\[ V_{RVB} = -J(\cos k_x - \cos k_y)(\cos k'_x - \cos k'_y) \]

\[ V_d \approx \frac{3}{2} \bar{U}^2 \chi(k - k', w - w') \]

\[ -\bar{J}(\cos k_x - \cos k_y)(\cos k'_x - \cos k'_y) \]

Thomas A. Maier - Fall Creek Falls 2009
Are we done?

Many open questions!!

For example:

- What is the reason for the factor 5 difference in transition temperature between different cuprates?
- What is the role of the nano-scale electronic structure inhomogeneities?
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Role of inhomogeneities on Cray XT5

2005

2006-2008

2009 -

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Disorder & inhomogeneities

Hubbard model with diagonal disorder:

\[ \mathcal{H} = -t \sum_{\langle ij \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + \sum_i U_i n_{i\uparrow} n_{i\downarrow} + \sum_{i, \sigma} V_i n_{i\sigma} \]

- \( U_i \in \{U + \Delta U, U - \Delta U\} \)
- \( V_i \in \{V, 0\} \)
- \( N_c = 16 \rightarrow N_d = 2^{16} \) disorder configurations

Disorder-average cluster Green’s function:

\[ G_c(X_i - X_j, z) = \frac{1}{N_c} \sum_{\nu=1}^{N_d} G_c^{\nu}(X_i, X_j, z) \]

Required communication

Peta- or exascale problem!
Cray XT5 portion of Jaguar @ NCCS

Peak: 1.382 TF/s
Quad-Core AMD
Freq.: 2.3 GHz
150,176 cores
Memory: 300 TB
For more details, go to www.nccs.gov
QMC parallelism: Multiple random walkers

- Updates: dgemm
- Measurements: zgemm
- Thermalization
- Sample
- QMC time

Required communication

Amdahl’s law
**DCA++ code: Concurrency**

- QMC cluster solver
- Disorder configurations
- DCA cluster mapping
- MPI AllReduce

- ~10^3 random walkers
- ~10^2 - 10^4 disorder configurations

- OpenMP/CUDA
Multi-core/GPU/Cell: threaded programming

Multi-core: OpenMP or pthreads

NVIDIA G80: CUDA, cuBLAS

IBM Cell

Work on GPUs motivated mixed single-precision/double-precision model
Mixed single-precision/double-precision model

- Run in single-precision
  - QMC cluster solver
  - DCA cluster mapping

- Keep in double-precision

• No loss of precision
• But significant speedup
  - Up to 1.9x faster on CPU
• Speedup on GPU
  - NVIDIA 8800GTS vs. 2.0GHz Opteron
  - Up to 19x for offloading HF-updates onto GPU

Results are identical within error bars!

Sustained performance of DCA++ on Cray XT5

Weak scaling with number of disorder configurations, each running on 128 Markov chains on 128 cores (16 nodes)

- Mixed precision
- Double precision

Time to solution (sec.)

Number of disorder configurations

Sustained performance (TFlop/s)

Number of Cores

Speedup = 1.9
**Preliminary results**

**Hubbard model with random disorder:**
- Inhomogeneities can enhance the pairing interaction but generally suppress the superconducting transition temperatures.

![Graph showing temperature ($T_c$) versus doping ($x$) for a 4-site cluster with $U=8t$. The graph compares homogeneous and disordered cases.](image)

- The graph shows that $T_c$ increases with doping $x$ for both homogeneous and disordered cases, with the disordered case having a slightly lower $T_c$ for a given $x$.
Future work

Understand the interplay between inhomogeneities and superconductivity:
- Are inhomogeneities good or bad for superconductivity?
- What about stripes?
- Is there an optimum inhomogeneity for which $T_c$ is maximum?
- Can $T_c$ be enhanced in composite systems or artificial multi-layers?

Understand the large difference in transition temperature between different cuprate materials:
- Perform material specific simulations
Summary

New algorithms and computer hardware allow to gain insight into the high-$T_c$ pairing mechanism

- Superconductivity in 2D Hubbard model with realistic parameters
- Fundamental understanding of the pairing mechanism responsible for superconductivity
- Phenomenological model for critical temperature based on spin fluctuations allows experimental validation

Understanding the role of inhomogeneities is needed for a comprehensive theory of high-$T_c$

- Unique opportunity for high-end computing (peta- or exascale problem)
- Random disorder related to dopant atoms
- Spin and charge stripes
- Optimal inhomogeneity
- DCA++ provides a unique computational tool to study these questions