ADVANCING OUR UNDERSTANDING OF HIGH-TEMPERATURE SUPERCONDUCTORS THROUGH EXTREME SCALE COMPUTING

Thomas A. Maier
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Next Generation Multi-Scale Quantum Simulation Software for Strongly Correlated Materials

- Order of magnitude increase in number of electrons that can be simulated using Quantum Monte Carlo (QMC) codes.

- New QMC solver for dynamic mean field theory that scales linearly in inverse temperature rather than cubic.

- Highly parallel solver for multi-scale parquet quantum modeling of correlated materials

- INCITE 2010 award: 17M hours on ORNL Cray XT

See posters by Ed D’Azevedo & Z. Bai!
Next Generation Multi-Scale Quantum Simulation Software for Strongly Correlated Materials


"Dimensional trend in CePt2In7, Ce-115 compounds, and CeIn3", M. Matsumoto, M.J. Han, J. Otsuki, S.Y. Savrasov, arXiv:1004.5457 (2010)


"First Principle Simulations of Heavy Fermion Cerium Compounds Based on the Kondo Lattice", M. Matsumoto, M.J. Han, J. Otsuki, S. Y. Savrasov, Phys. Rev Lett. 103, 096403 (2009).

"Doping Driven (π, 0) Nesting and Magnetic Properties in Iron Chalcogenide Superconductors", M.J. Han, S.Y. Savrasov, Phys. Rev. Lett. 103, 067001 (2009);


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ACKNOWLEDGEMENTS

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Mike Summers             ORNL

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Computational resources:
NCCS @ ORNL
**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 - FERMIIONS, BOSONS AND COOPER PAIRS

Fermions
(Electrons)

Bosons

Phonons (lattice vibrations) glue fermions into Cooper pairs (boson-like)

\[ \Delta E \]

Energy gap prevents scattering that leads to resistivity
CUPRATES HIGH-TEMPERATURE SUPERCONDUCTORS

Discovery:
- Bednorz & Müller (1986)

Properties:
- Insulators or bad metals (conv. superconductors are good metals)
- Many complex phenomena

Critical temperatures:
- $T_c \sim 40K - 150K$ (well above liquid nitrogen boiling point)

25 years of intense research:
- No consensus on a general theory
- No predictive power for $T_c$ in known materials
- No guidance for design of new materials
OUTLINE

– Brief introduction into superconductivity

– Background: 2D Hubbard model & dynamic cluster quantum Monte Carlo approximation (DCA-QMC)

– Gaining insight into superconductivity through computing
FROM CUPRATED MATERIALS TO THE HUBBARD MODEL

Cuprate structure

CuO-planes

2D Hubbard Model

Basic properties:
- Moment formation

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

- Antiferromagnetic exchange

Energy

\[ U \]

\[ J = 4t^2/U \]
A QUANTUM MULTISCALE PROBLEM

Atomic scale
- Strong local correlations
- Moment formation

Nano-scale
- Antiferromagnetic correlations
- Cooper pairs
- Inhomogeneities

Macro-scale
- Macroscopic quantum effects

Theory:
- Atomistic description
  - Complexity $\sim 4^N$
- Thermodynamics Continuum description
  - $N \sim 10^{23}$
Coherently embed cluster into effective medium

Explicitly treat correlations within a localized cluster

Nano-scale
- Antiferromagnetic correlations
- Cooper pairs
- Inhomogeneities

Macro-scale
- Macroscopic quantum effects

Atomic scale
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- Antiferromagnetic correlations
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Explicitly treat correlations within a localized cluster

Coherently embed cluster into effective medium

CLUSTER DYNAMIC MEAN FIELD METHODS

DMFT:
Metzner & Vollhardt, PRL '89;
Müller-Hartmann, Z. Phys. '89; Georges et al., RMP '96

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

QMC to sample exponentially large number of electronic configurations in effective cluster problem

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

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

2005 2006-2008 2009 -
SUPERCONDUCTIVITY IN 2D HUBBARD MODEL

2005 on Cray X1(E):

- Superconducting transition in largest accessible clusters
  \[ T_c \sim 0.025t \text{ for } U = 4t, <n> = 0.9 \]
  Maier, Jarrell, Schulthess, Kent & White, PRL '05

4-site cluster: Antiferromagnetism, pseudogap & superconductivity
Jarrell, Maier et al., EPL '01
(Simulations on IBM Power4 “Cheetah”)
Superconductivity in Hubbard model on Cray X1(E)

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Role of inhomogeneities on Cray XT5
PAIRING MECHANISM

- 2006 - 2008 on Cray XT3/4:
  - Study of mechanism responsible for superconductivity in the Hubbard model
  - Analyze the particle-particle irreducible vertex function

\[
\Gamma_{pp} = \Lambda_{irr} + \Gamma_{ph} + \Gamma_{ph}
\]

- Electron spin is responsible for pairing

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

Brinkman & Rice, PRB (1970)
Doping a Mott insulator: Physics dominated by Coulomb energy, kinetic energy is frustrated

(Brinkman & Rice, PRB ’70)
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(Brinkman & Rice, PRB ’70)
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 ’70)

SPIN-MEDIATED PAIRING

Hole localization due to increase in exchange energy!
Paired hole restores antiferromagnetic background

(Hirsch, PRL ’87; Bonca et al., PRB ‘89; Dagotto et al., PRB ‘90)
Paired hole restores antiferromagnetic background

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Further characterization of pairing interaction

- Dynamics associated with spin-fluctuation spectrum
  \[ \Gamma^{pp}(\omega, \omega') \sim \chi_s(\omega - \omega') \]

- Spin-fluctuation representation reproduces \( T_c \) within 30%
  \[ \Gamma^{pp}(k, k') \approx \frac{3}{2} \bar{U}^2 \chi_s(k - k') \]

- Relative importance of spin-fluctuation and instantaneous resonating valence bond mechanism

Maier et al., PRB 75, 134519 (2007), PRB 76, 144516 (2007)
Maier, Poilblanc & Scalapino, PRL ‘08
Superconductivity in Hubbard model on Cray X1(E)

Pairing mechanism in Hubbard model on Cray XT3/4

Role of inhomogeneities on Cray XT5

- 2005
- 2006-2008
- 2009 -
 ROLE OF INHOMOGENEITY?

- **Nanoscale electronic inhomogeneity**
  - Stripes  
    (Tranquada et al. ’95, Mook et al., ’00)
  - Checkerboard charge modulations  
    (Hanaguri, Davis et al., ’04)
  - Random SC gap modulations  
    (Lang, Davis et al., ’02, Gomes, Yazdani et al., ’07)
Hubbard model with diagonal disorder:

\[ H^{(\nu)} = -t \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + \sum_i U^{(\nu)} n_{i\uparrow} n_{i\downarrow} + \sum_{i,\sigma} V^{(\nu)}_{i} n_{i\sigma} \]

\[ \forall \nu, \quad P(\{V_i\}) = \prod_{i=1}^{N_c} P_i(V_i) \quad P_i(V_i) = \begin{cases} x & \text{if } V_i = V \\ (1-x) & \text{if } V_i = 0 \end{cases} \]

\[ N_c = 16 \rightarrow N_d = 2^{16} \]

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

\[ V_i \in \{V, 0\} \]

\[ \text{Disorder-average cluster Green's function} \]

\[ \text{Peta- or exascale problem!} \]
DCA++ CODE: EFFICIENCY

- DCA cluster mapping
- QMC cluster solver
- Disorder configurations
- Random walkers

MPI AllReduce

~10^2 - 10^4 disorder configurations

~10^3 random walkers

pthreads/CUDA

DCA cluster mapping
RANDOM DISORDER SUPPRESSES SC

Leading d-wave eigenvalue; $U=4t$, $N_c=16A$

$$\lambda_d \text{ leading eigenvalue of } \Gamma^{pp} P_d^0$$

$$P_d = \frac{P_d^0}{1 - \Gamma^{pp} P_d^0}$$

- Random disorder reduces $T_c$, but only by about 20%
Good hole mobility


Strong pairing region

- Experimental evidence for optimization of SC in striped state
  
  
  Li et al., PRL 99, 067001 (2007)
Imposed potential and charge modulation

Stripes can significantly enhance superconductivity

Maier et al., PRL 104, 247001 (2010)
Advances in algorithms and computers have increased our ability to answer more and more complex questions.

- Evidence for superconductivity in coarse-grained Hubbard model of cuprate high-temperature superconductors
- Mechanism for pairing that leads to superconductivity
- Effect of nanoscale electronic inhomogeneities

Future?

- Predictive materials-specific simulations of correlated electron systems

Computer power:
- ~ 5 TFlops
- ~ 100 TFlops
- ~ 1 PFlops
- ~ MultiPFlop ...
- ExaFlop
Why is there a factor 5 difference in the transition temperature between different cuprates?

- Multi-orbital Hubbard models
- Energy-dependent Coulomb interactions
- Parameters systematically determined from DFT