High-temperature superconductors

Armitage, Fournier, Greene, RMP (2009)

• Competing order
  – Current loops: Varma, PRB 81, 064515 (2010)
  – Stripes or nematic: Kivelson et al. RMP 75 1201(2003); J.C.Davis
  – d-density wave: Chakravarty, Nayak, Phys. Rev. B 63, 094503 (2001); Affleck et al. flux phase
  – SDW: Sachdev PRB 80, 155129 (2009) ...
Fermi surface plots

Hubbard repulsion $U$ has to…

be not too large

increase for smaller doping

Hankevych, Kyung, A.-M.S.T., PRL, sept. 2004

B. Kyung et al., PRB 68, 174502 (2003)
Resistivity (TPSC)

D. Bergeron, V. Hankevych, B. Kyung, and A.-M.S.T.

Dominic Bergeron
Im $\Sigma$ for e-doped QCP (TPSC)

D. Bergeron, D. Chowdury, M. Punk, S. Sachdev, A.-M.S.T.
High-temperature superconductors

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What is under the dome?

Mott Physics away from $n = 1$

• Or Mott Physics?
Hubbard model

1931-1980

\[ H = - \sum_{<ij>\sigma} t_{i,j} \left( \hat{c}_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger \hat{c}_{i\sigma} \right) + U \sum_i n_{i\uparrow} n_{i\downarrow} \]

Effective model, Heisenberg: \( J = 4t^2 / U \)
Method
Mott transition and Dynamical Mean-Field Theory. The beginnings in $d = \infty$

- Compute scattering rate (self-energy) of impurity problem.
- Use that self-energy ($\omega$ dependent) for lattice.
- Project lattice on single-site and adjust bath so that single-site DOS obtained both ways be equal.

W. Metzner and D. Vollhardt, PRL (1989)
A. Georges and G. Kotliar, PRB (1992)
M. Jarrell PRB (1992)

DMFT, ($d = 3$)
2d Hubbard: Quantum cluster method

Hettler …Jarrell…Krishnamurty PRB 58 (1998)
Kotliar et al. PRL 87 (2001)

REVIEWS
Maier, Jarrell et al., RMP. (2005)
Kotliar et al. RMP (2006)
AMST et al. LTP (2006)
• Missing:
  – Long wavelength fluctuations

• Included:
  – Short-range dynamical and spatial correlations

• Long range order:
  – Allow symmetry breaking in the bath (mean-field)
Outline

- Method
- $T=0$ phase diagram with competing order
- Finite $T$ phase diagram
  - Normal state (no LRO, what is below the dome)
    - First order transition
    - Widom line and pseudogap
  - Superconductivity
$T = 0$ phase diagram: cuprates

Phase diagram

Exact diagonalization as impurity solver ($T=0$).
CDMFT global phase diagram

AND Capone, Kotliar PRL (2006)

Armitage, Fournier, Greene, RMP (2009)
Consistent with following experiments

H. Mukuda, Y. Yamaguchi, S. Shimizu, … A. Iyo JPSJ 77, 124706 (2008)
Magnetic phase diagram of YBCO

\[ T = 0 \] phase diagram

The glue
Im $\Sigma_{an}$ and electron-phonon in Pb

Maier, Poilblanc, Scalapino, PRL (2008)
The glue


Wakimoto … Birgeneau
PRL (2004)
The glue and neutrons

**FIG. 3** (color online). Q-integrated dynamic structure factor $S(\omega)$ which is derived from the wide-$H$ integrated profiles for LBCO 1/8 (squares), LSCO $x = 0.25$ (diamonds; filled for $E_i = 140$ meV, open for $E_i = 80$ meV), and $x = 0.30$ (filled circles) plotted over $S(\omega)$ for LBCO 1/8 (open circles) from [2]. The solid lines following data of LSCO $x = 0.25$ and 0.30 are guides to the eyes.

Finite temperature

The Mott transition
$n = 1$, unfrustrated cubic lattice

$J = \frac{4t^2}{U}$
Local moment and Mott transition

$n = 1$, unfrustrated square lattice
Doping-induced Mott transition \((t' = 0)\)

Not just adding new piece:
Lesson from DMFT, first order transition + critical point governs phase diagram

G. Sordi, K. Haule, A.-M.S.T
PRL, \textbf{104}, 226402 (2010)
and
C-DMFT

Continuous-time Quantum Monte Carlo calculations to sum all diagrams generated from expansion in powers of hybridization.


Mean-field is not a trivial problem! Many impurity solvers.

Here: continuous time QMC

P. Werner, PRL 2006
P. Werner, PRB 2007
K. Haule, PRB 2007
Doping driven Mott transition

Gull, Werner, Millis, (2009)
Link to Mott transition up to optimal doping

Doping dependence of critical point as a function of $U$

H. Park, K. Haule, and G. Kotliar

PRL 101, 186403 (2008)
Characterisation of the phases ($U=6.2t$)

$U > U_{MIT}$:
1. Mott insulator (MI)
2. Underdoped phase (UD):
   $\delta < \delta_c$
3. Overdoped phase (OD):
   $\delta > \delta_c$
4. Coexistence/forbidden region

Here "optimal doping" $\delta_c =$ doping at which the 1st order transition occurs

How does the UD phase differ from the OD phase?

Smaller $D$ and $S$
Density of states
Density of states

Khosaka et al. Science 315, 1380 (2007);
Density of states
Density of states
Spin susceptibility
Spin susceptibility

Underdoped Hg1223

Julien et al. PRL 76, 4238 (1996)
Plaquette eigenstates
Pseudogap $T^*$ along the Widom line
The Widom line

arXiv:1110.1392
What is the Widom line?

- it is the continuation of the coexistence line in the supercritical region
- line where the maxima of different response functions touch each other asymptotically as $T \to T_p$
- liquid-gas transition in water: max in isobaric heat capacity $C_p$, isothermal compressibility, isobaric heat expansion, etc
- DYNAMIC crossover arises from crossing the Widom line!

McMillan and Stanley, Nat Phys 2010

Phase diagram
Summary: normal state

- Mott physics extends way beyond half-filling
- Pseudogap is a phase
- Pseudogap $T^*$ is a Widom line
- High compressibility (stripes?)
Finite $T$ phase diagram

Superconductivity
arXiv:1201.1283v1
Unified phase diagram
Cuprates (doping driven transition)
Cuprates (doping driven transition)

Meaning of $T_c^d$

- Local pair formation

$T_{\text{pair}}$


ARPES Bi2212
$T_2$

Magnetoresistance, LSCO
Fluctuating vortices

Giant proximity effect

$T_c = 32 \, K$

$T_c < 5K$

Morenzoni et al.,
Nature Comms. 2 (2011)
Actual $T_c$ in underdoped

- **Quantum and classical phase fluctuations**

- **Magnitude fluctuations**

- **Competing order**

- **Disorder**
Gaussian amplitude fluctuations in Eu-LSCO

Chang, Doiron-Leyraud et al.
Phase fluctuations and disorder?

Monolayer LSCO, field doped


Figure 2 | Superconductor–insulator transition driven by electric field.
a. Temperature dependence of normalized resistance $r = R_C(x; T) / R_Q$ of an initially heavily underdoped and insulating film (see Supplementary Fig. 12 for linear scale). The device (Supplementary section B) employs a coplanar Au gate and DEME-TFSI ionic liquid. The carrier density, fixed for each curve, is tuned by varying the gate voltage from 0 V to −4.5 V in 0.25 V steps; an insulating film becomes superconducting via a QPT. The inset highlights a separatrix independent of temperature below 10 K. The open circles are the actual raw data points; the black dashed line is $R_C(x; T) = R_Q = 6.45 \text{ k}\Omega$. b. The inverse representation of the same data, that is, the $r_T(x)$ dependence at fixed temperatures below 20 K. Each vertical array of (about 100) data points corresponds to one fixed carrier density, that is, to one $r_c(T)$ curve in Fig. 2a.

The colours refer to the temperature, and the continuous lines are interpolated for selected temperatures (4.5, 6.0, 8.0, 10.0, 12.0, 15.0 and 20.0 K). The crossing point defines the critical carrier concentration $x_c = 0.06 \pm 0.01$, and the critical resistance $R_c = 6.45 \pm 0.10 \text{ k}\Omega$. c. Scaling of the same data with respect to a single variable $u = |x - x_c| T^{-1/\nu}$, with $\nu = 1.5$. This figure is derived by folding panel b at $x_c$ and scaling the abscissa of each $r_T((x - x_c))$ curve by $T^{-2/\nu}$. For $4.3 \text{ K} < T < 10 \text{ K}$, the discrete groups of points of Fig. 2b collapse accurately onto a two-valued function, with one branch corresponding to $x$ larger and the other to $x$ smaller than $x_c$. The critical exponents are identical on both sides of the superconductor–insulator transition. The raw data points cover the interpolation lines almost completely, except close to the origin.
Effect of disorder

Superconductivity in underdoped vs BCS
First-order transition leaves its mark
Summary: superconductivity

- Below the dome finite $T$ critical point (not QCP) controls normal state
- First-order transition destroyed but traces in the dynamics
- $T^*$ different from $T_c^d$
- Actual $T_c$ in underdoped
  - Competing order
  - Long wavelength fluctuations (see O.P.)
  - Disorder
Projects
BIG QUESTIONS:

• What is the pairing mechanism in pnictides and cuprates?
• Is the same fundamental scenario common to all unconventional superconductors?
• What limits the critical temperature $T_c$?
• What is the pseudogap phase of cuprates?
• Collaboration with Rutgers:
  – Normal state finite $T$ phase diagram of 2d Hubbard model and competition between superconductivity and antiferromagnetism at finite $t'$ with CDMFT for more realistic comparisons with experiment.
  – Competition between antiferromagnetism and pseudogap phase to clearly differentiate the two phenomena at strong coupling.
High temperature superconductivity

• Collaboration with Rutgers continued-1:
  – Improved algorithms
    • Skip list for CT-HYB
  – Compute vertex corrections to obtain
    • The highly non-BCS zero temperature superfluid density
      – High Tc
      – Organics (McKenzie)
    • Resistivity, to verify whether it is linear in temperature.
Collaboration with Rutgers continued-2
- Include realistic band structure effects to understand the difference in $T_c$ between different compounds: single layer vs multilayer and electron vs hole doped compounds.
High temperature superconductivity

• To understand the mechanism of strongly correlated superconductivity study
  – Effect of near-neighbor repulsion
  – Effect of retardation in three-band model

• Improve the methodology to include long wavelength fluctuations in CDMFT
  – Make the vertex self-consistent to satisfy Pauli principle and achieve consistency between lattice and impurity for double occupancy (à la TPSC).
  – Achieve self-consistency between one- and two-particle quantities
High temperature superconductivity

• Benchmark CDMFT + DCA against large system calculations by
  – Comparing with results obtained on the Hubbard ladder and also on the square lattice at half-filling where there is no sign problem.
Heterostructures

BIG QUESTION

• Can we create new states of matter at interfaces, or design materials that exhibit desired states such as higher-temperature superconductivity?
Heterostructures

• Compute with CDMFT and from first-principles (DFT) the charge distribution and ordered-states in the high-Tc $p$-$n$ junction (hole-doped on electron-doped high Tc) to look for interface superconductivity arising between two non-superconducting compounds. Project in collaboration with the experimental group of P. Fournier.
BIG QUESTIONS:
• Is there a quantum spin liquid in nature?
• What new phenomena exist in frustrated magnetic materials?
• Can the sign problem be solved for frustrated quantum spin systems?
Theoretical phase diagram BEDT

\[ X = \text{Cu}_2(\text{CN})_3 \ (t' \sim t) \]


Spin Liquids

• Obtain the finite temperature phase diagram of the κ-BEDT layered organic superconductors with CDMFT and CTQMC to find how antiferromagnetism leaves room for spin liquid as we move towards the isotropic triangular lattice.

• In the spin-liquid phase, check whether there is a linear specific heat and Pauli susceptibility despite insulating behavior.
Sponsors:
Mammouth
Merci
Thank you