Repelled, yet attracted: the case of strongly correlated superconductivity

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McGill, 26 February, 2015
How to make a metal

Courtesy, S. Julian
Superconductivity
Attraction mechanism in the metallic state
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Attraction mechanism in the metallic state

\[ p \rightarrow p' \rightarrow -p \rightarrow -p' \]
#1 Cooper pair, #2 Phase coherence

\[ E_P = \sum_{p,p'} U_{p-p'} \psi_{p, p'}^\dagger \psi_{p', p'} \]

\[ E_P = \sum_{p,p'} U_{p-p'} \left( \langle \psi_{p, p'} \rangle \psi_{p', p'}^\dagger + \psi_{p, p'}^\dagger \langle \psi_{p', p'} \rangle \right) \]

\[ |\text{BCS}(\theta)\rangle = \ldots + e^{iN\theta}|N\rangle + e^{i(N+2)\theta}|N + 2\rangle + \ldots. \]
Half-filled band is metallic?
Half-filled band: Not always a metal

NiO, Boer and Verway

Peierls, 1937

Mott, 1949
\[ H = - \sum_{<ij> \sigma} t_{i,j} \left( c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma} \right) + U \sum_i n_{i\uparrow} n_{i\downarrow} \]

Effective model, Heisenberg: \( J = 4t^2 / U \)
Superconductivity and attraction?
Cuprates
High-temperature superconductors

Armitage, Fournier, Greene, RMP (2009)
Hubbard on anisotropic triangular lattice


\[ H = \sum_{ij\sigma} (t_{ij} - \delta_{ij} \mu) c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \]

\[ n=1, \text{ varying } t'/t \]

Kagawa et al.
Nature Physics 5, 880 (2009)

\[ t \approx 50 \text{ meV} \]
\[ \Rightarrow U \approx 400 \text{ meV} \]
\[ t'/t \sim 0.6 - 1.1 \]
Phase diagram for organics

Phase diagram \((X=\text{Cu}[\text{N(CN)}_2]\text{Cl})\)


F. Kagawa, K. Miyagawa, + K. Kanoda

B_g for C_{2h} and B_{2g} for D_{2h}

Powell, McKenzie cond-mat/0607078
Perspective

\[ \frac{U}{t} \]

\[ t \]

\[ t' \]

\[ \delta \]
Outline

• Method
• $T=0$ phase diagram
  – The « glue »
• Finite $T$ phase diagram
  – Normal state
    • First order transition
    • Widom line and pseudogap
  – Superconductivity
Method

“The effect of concept-driven revolution is to explain old things in new ways. The effect of tool-driven revolution is to discover new things that have to be explained.”

Freeman Dyson *Imagined Worlds*
Mott transition and Dynamical Mean-Field Theory.
The beginnings in $d = \text{infinity}$

- 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)
DMFT as a stationary point

\[ \delta \Omega_t [\Sigma(t')] = 0 \]

\[ \Omega = \Omega_t [\Sigma] \]

\[ \Sigma = \Sigma (t) \]

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

• Included:
  – Short-range dynamical and spatial correlations

• Missing:
  – Long wavelength p-h and p-p fluctuations
C-DMFT

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

Why important

\[ Z = \int D[\psi^{\dagger}, \psi] e^{-\mathcal{S}_{c} - \int_{0}^{\beta} d\tau \int_{0}^{\beta} d\tau' \sum_{k} \psi^{\dagger}_{K}(\tau) \Delta(\tau, \tau') \psi_{K}(\tau')} \]

Effective local impurity problem

\[ \Delta(i\omega_n) = i\omega_n + \mu - \Sigma_c(i\omega_n) \]

\[ - \left[ \sum_{k} \frac{1}{i\omega_n + \mu - t_c(\tilde{k}) - \Sigma_c(i\omega_n)} \right]^{-1} \]
$T = 0$ phase diagram $n = 1$

Phase diagram
Exact diagonalization as impurity solver ($T=0$).
Theoretical phase diagram BEDT

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


$T = 0$ phase diagram: cuprates

Phase diagram

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

\begin{align*}
U/t &= 8 \\
t'/t &= -0.3 \\
t''/t &= 0.2 \\
\beta &= 50 \\
\omega_c &= 1.5
\end{align*}


Armitage, Fournier, Greene, RMP (2009)

AND Capone, Kotliar PRL (2006)
A bit of physics: superconductivity and repulsion
\[ \Delta_p = - \frac{1}{2V} \sum_{p'} U(p - p') \frac{\Delta p'}{E_{p'}} \left( 1 - 2n(E_{p'}) \right) \]

Exchange of spin waves?
Kohn-Luttinger
\[ T_c \text{ with pressure} \]

D. J. Scalapino, E. Loh, Jr., and J. E. Hirsch
P.R. B 34, 8190-8192 (1986).
Béal–Monod, Bourbonnais, Emery
P.R. B. 34, 7716 (1986).
Kohn, Luttinger, P.R.L. 15, 524 (1965).
AFM Quantum critical point
A cartoon strong correlation picture


\[
J \sum_{\langle i,j \rangle} S_i \cdot S_j = J \sum_{\langle i,j \rangle} \left( \frac{1}{2} \hat{c}_i^\dagger \vec{\sigma} c_i \right) \cdot \left( \frac{1}{2} \hat{c}_j^\dagger \vec{\sigma} c_j \right)
\]

\[
d = \langle \hat{d} \rangle = \frac{1}{N} \sum_{\vec{k}} \left( \cos k_x - \cos k_y \right) \langle c_{\vec{k},\uparrow}^\dagger c_{-\vec{k},\downarrow} \rangle
\]

\[
H_{MF} = \sum_{\vec{k},\sigma} \varepsilon(\vec{k}) c_{\vec{k},\sigma}^\dagger c_{\vec{k},\sigma} - 4Jm \hat{m} - Jd(\hat{d} + \hat{d}^\dagger) + F_0
\]

Pitaevskii Brückner:
Pair state orthogonal to repulsive core of Coulomb interaction

Kotliar and Liu, P.R. B 38, 5142 (1988)
Miyake, Schmitt–Rink, and Varma
P.R. B 34, 6554-6556 (1986)
The glue
Raising the question

Is There Glue in Cuprate Superconductors?
Philip W. Anderson
Many theories about electron pairing in cuprate superconductors may be on the wrong track.

Retardation

\[ V_{el-ph}^{eff}(\vec{q}, \omega) = \frac{e^2}{4\pi\varepsilon_0(q^2 + k^2_{TF})} \left[ 1 + \frac{\omega^2_{ph}(\vec{q})}{\omega^2 - \omega^2_{ph}(\vec{q})} \right] \]

“We have a mammoth and an elephant in our refrigerator—do we care much if there is also a mouse?”
Im $\Sigma_{an}$ and electron-phonon in Pb

Maier, Poilblanc, Scalapino, PRL (2008)
The superconducting order parameter scales like $J$.
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.

Wakimoto … Birgeneau PRL (2007);
PRL (2004)
Resilience to near-neighbor repulsion $V$

$$\hat{H}_{\text{Hubbard}} = - \sum_{\langle i,j \rangle_{1,2,3}\sigma} \left( t_{ij\sigma} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + c.c. \right) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} + V \sum_{\langle i,j \rangle} \hat{n}_i \hat{n}_j - \mu \sum_i \hat{n}_{i\sigma}$$

$YBa_2Cu_3O_7$:

$t = 1 \quad t' = -0.3 \quad t'' = 0.2$

We expect superconductivity to disappear when:

- In weakly correlated case $U/W < 1$
  $$V > \frac{U^2}{W}$$

- In mean-field strongly correlated case
  $$V > J$$
  $$V = 400 \text{ meV} \quad J = 130 \text{ meV}$$

In cuprates:

$$U_c = V_c / \left[ 1 + N(0) V_c \ln \left( E_F / \omega_c \right) \right]$$

Resilience to near-neighbor repulsion

David Sénéchal

Alexandre Day

Vincent Bouliane

Sénéchal, Day, Bouliane, AMST PRB 87, 075123 (2013)
$V$ also increases $J$
Binding aspects of V

\[ J = \frac{4t^2}{U - V} \]

J increases with V explaining better pairing at low frequency

But V also induces more repulsion at high frequency, explaining the negative impact at high frequency on binding
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Finite $T$ phase diagram

Normal state of the cuprates
Weak vs Strong correlations

$n = 1$, unfrustrated $d = 3$ cubic lattice

$J = 4t^2 / U$

Heisenberg

Mott

Slater
Local moment and Mott transition

$n = 1, d = 2$ square lattice

Understanding finite temperature phase from a mean-field theory down to $T = 0$

Critical point visible in $V_2O_3$, BEDT organics
Finite $T$ phase diagram

Normal state of the cuprates
Not just adding new piece:
Lesson from DMFT, first order transition + critical point governs phase diagram

Doping-induced Mott transition \((t' = 0)\)

G. Sordi, K. Haule, A.-M.S.T
PRL, 104, 226402 (2010)
and
First order transition at finite doping

$n(\mu)$ for several temperatures: $T/t = 1/10, 1/25, 1/50$
The critical point

U=6.2t
Normal state phase diagram

G. Sordi, K. Haule, A.-M.S.T
PRL, 104, 226402 (2010)

μ = 0, H. Park, K. Haule, and G. Kotliar,
Link to Mott transition up to optimal doping

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

Smaller $D$ and $S$
Characterisation of the phases (\(U=6.2t\))

\[ U > U_{\text{MIT}}: \]
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?
Finite $T$ phase diagram

Pseudogap in the normal state and the Widom line
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 $T \to T_c$
- 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

The Widom line
Rapid change also in dynamical quantities
Density of states
Density of states

Khosaka et al. *Science* **315**, 1380 (2007);
Spin susceptibility
Spin susceptibility

Underdoped Hg1223
Julien et al. PRL 76, 4238 (1996)
Plaquette eigenstates
Pseudogap $T^*$ along the Widom line
What is the minimal model?

H. Alloul arXiv:1302.3473

Fig 1 Spin contribution $K_\delta$ to the $^{89}$Y NMR Knight shift [11] for YBCO$_{6.6}$ permit to define the PG onset $T^*$. Here $K_\delta$ is reduced by a factor two at $T\sim T^*/2$. The sharp drop of the SC fluctuation conductivity (SCF) is illustrated (left scale) [23]. We report as well the range over which a Kerr signal is detected [28], and that for which a CDW is evidenced in high fields from NMR quadrupole effects [33] and ultrasound velocity data [30]. (See text.)
Two crossover lines

P. Sémon, G. Sordi, A.-M.S.T., Phys. Rev. B 89, 165113/1-6 (2014)
C-axis resistivity

Summary: normal state

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

Superconductivity

P. Sémon, G. Sordi, A.-M.S.T., Phys. Rev. B 89, 165113/1-6 (2014)
P. Sémon, G. Sordi, A.-M.S.T., Phys. Rev. B 89, 165113/1-6 (2014)
Larger clusters

- In 2x2 $T_c$ vanishes extremely close to half-filling. In larger cluster, earlier.
- Local pairs in underdoped (2x2)

8 site DCA, $U=6t$

Gull Parcollet Millis,
PRL 110, 216405 (2013)
Meaning of $T_c^d$

- Local pair formation


Bandwidth control and doping control of the Mott transition in organics
Theoretical phase diagram BEDT

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


Sénécha, Sahebsara, Phys. Rev. Lett. 97, 257004
A doped BEDT organic

Doped BEDT

Widom line in organics

Charles-David Hébert, Patrick Sémon, AMT
\[ t' = 0.4t \]
t' = 0.4t overview
Generic case
Summary: organics

- Agreement with experiment
  - SC: larger $T_c$ and broader $P$ range if doped
  - Larger frustration: Decrease $T_N$ and $T_c$
  - Normal state metal to pseudogap crossover

- Predictions
  - First order transition at low $T$ in normal state (or remnants in SC state)

- Physics
  - SC dome without a AFM-QCP. Follows first-order.
  - SC from short range $J$.
  - $T_c$ decreases at Widom line
Main collaborators

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