Insulators, metals, pseudogaps and cuprate superconductivity

A.-M. Tremblay

Rutherford, June 20th, 2013
How to make a metal

Courtesy, S. Julian
Superconductivity
Attraction mechanism in the metallic state
Attraction mechanism in the metallic state
Attraction mechanism in the metallic state
Attraction mechanism in the metallic state
Attraction mechanism in the metallic state
#1 Cooper pair, #2 Phase coherence

\[ E_P = \sum_{p,p'} U_{p-p'} \psi_{p\uparrow,-p\downarrow}^* \psi_{p'\uparrow,-p'\downarrow} \]

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

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

NiO, Boer and Verway

Peierls, 1937

Mott, 1949
« Conventional » Mott transition

Figure: McWhan, PRB 1970; Limelette, Science 2003
Quantum Criticality in 3 Families of Superconductors

AFM and superconductivity

L. Taillefer, Annual Reviews of CMP 2010
Weakly or strongly correlated?

L. Taillefer, Annual Reviews of CMP 2010

CePd$_2$Si$_2$  CeIn$_3$
Model

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

$H = - \sum_{<ij>\sigma} t_{i,j} \left( c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma} \right) + U \sum_i n_i^\uparrow n_i^\downarrow$

Effective model, Heisenberg: $J = 4t^2 / U$
Strong vs weak coupling
Local moment and Mott transition

\( n = 1, \) unfrustrated \( d = 3 \) cubic lattice

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

Diagram showing the transition between Slater, AFM, and Heisenberg phases with the Mott transition indicated by a dashed line.
Local moment and Mott transition

$n = 1, d = 2$ square lattice

Critical point visible in $V_2O_3$, $BEDT$ organics

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

What is under the dome?
Mott Physics away from $n = 1$

• Or Mott Physics?
Stripes and reconstructed Fermi surface

Competing CDW order

- Parker, C. V. et al. Fluctuating stripes at the onset of the pseudogap in the high-Tc superconductor B2Sr2CaCu2O8Cx. Nature 468, 677680 (2010).
Three broad classes of mechanisms for pseudogap

- Rounded first order transition
- \( d = 2 \) precursor to a lower temperature broken symmetry phase
- Mott physics

- 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) ...

- Or Mott Physics?
e-doped cuprates: precursors

NCCO


Vilk, A.-M.S.T (1997)
Kyung, Hankevych, A.-M.S.T., PRL, 2004

\[ z = 1 \]
Hot spots from AFM quasi-static scattering

$d = 2$

Armitage et al. PRL 2001
Back to hole-doped
What is the minimal model?

H. Alloul arXiv:1302.3473

Fig 1 Spin contribution $K_s$ to the $^{89}$Y NMR Knight shift [11] for YBCO$_{5.6}$ permit to define the PG onset $T^*$. Here $K_s$ is reduced by a factor two at $T^*$. 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.)
Pseudogap from Mott physics


Competing order is a consequence of the pseudogap, not its cause:
Hole-doped cuprates as Mott insulators
Mott-Ioffe-Regel limit

\[ \sigma = \frac{ne^2\tau}{m} \]

\[ k_F\ell = \frac{2\pi}{\lambda_F} \ell \sim 2\pi \]

\[ \sigma_{MIR} = \frac{e^2}{\hbar d} \]
Hole-doped cuprates and MIR limit

LSCO 17%, YBCO optimal

Gurvitch & Fiory
PRL 59, 1337
(1987)

MIR limit
Mean-free path
~ Fermi wavelength

Dominic Bergeron et al. TPSC
PRB 84, 085128 (2011)

Optical and dc conductivity of the two-dimensional Hubbard model in the pseudogap regime and across the antiferromagnetic quantum critical point including vertex corrections
Spectral weight transfer

Meinders et al. PRB 48, 3916 (1993)
Experiment: X-Ray absorption

Chen et al. PRL 66, 104 (1991)


Number of low energy states above $\omega = 0$ scales as $2x +$
Not as $1+x$ as in Fermi liquid

Meinders et al. PRB 48, 3916 (1993)
Charge-transfer insulator

Meinders et al. PRB 48, 3916 (1993)
Hall coefficient

Ando et al. PRL 92, 197001 (2004)
Outline

• Method
• $T=0$ phase diagram
• Finite $T$ phase diagram
  – Normal state (no LRO, what is below the dome)
    • First order transition
    • Widom line and pseudogap
  – Superconductivity
Method
**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)
Another way to look at this (Potthoff)

\[ \Omega_t[G] = \Phi[G] - Tr[(G_{0t}^{-1} - G^{-1})G] + Tr \ln(-G) \]

\[ \frac{\delta \Phi[G]}{\delta G} = \Sigma \]

\[ \Omega_t[\Sigma] = \Phi[G] - Tr[\Sigma G] - Tr \ln(-G_{0t}^{-1} + \Sigma) \]

Still stationary (chain rule)

\[ \Omega_t[\Sigma] = F[\Sigma] - Tr \ln(-G_{0t}^{-1} + \Sigma) \]

With \( F[\Sigma] \) Legendre transform of Luttinger-Ward funct.

\[
\Omega_t[\Sigma] = F[\Sigma] + \text{Tr} \ln(-(G_0^{-1} - \Sigma)^{-1})
\]

is stationary with respect to \( \Sigma \) and equal to grand potential there.

\[
\Omega_t[\Sigma] = \Omega_{t'}[\Sigma] - \text{Tr} \ln(-(G_0'^{-1} - \Sigma)^{-1}) + \text{Tr} \ln(-(G_0^{-1} - \Sigma)^{-1}).
\]

Vary with respect to parameters of the cluster (including Weiss fields)

**Variation of the self-energy, through parameters in** \( H_0(t') \)

• 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
Finite $T$ phase diagram

Normal state of the cuprates
Doping-induced Mott transition ($t'=0$)

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

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


Doping driven Mott transition, $t' = 0$

<table>
<thead>
<tr>
<th>Method</th>
<th>$t'$</th>
<th>Orbital selective</th>
<th>U</th>
<th>Critical point</th>
<th>Ref.</th>
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<tbody>
<tr>
<td>D+C+H 8</td>
<td></td>
<td></td>
<td>7</td>
<td></td>
<td>Werner et al. cond-mat (2009)</td>
</tr>
<tr>
<td>D+C+H 4</td>
<td>-0.3</td>
<td></td>
<td>10,6</td>
<td></td>
<td>Gull et al. EPL (2008)</td>
</tr>
<tr>
<td>D+C+H 8</td>
<td></td>
<td></td>
<td>7</td>
<td></td>
<td>Liebsch, Merino… (2008)</td>
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<td></td>
<td></td>
<td>Ferrero et al. PRB (2009)</td>
</tr>
</tbody>
</table>

K. Haule, G. Kotliar, PRB (2007)

Vildhyadhiraja, PRL (2009)
Doping driven Mott transition

\[ T = 0.25 \, t \]

Gull, Parcollet, Millis
arXiv:1207.2490v1

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

Doping dependence of critical point as a function of \( U \)

- Correlated metal
- PG

\( U_{\text{MIT}} \)

\( T_{\text{cr}} \)

\( \mu_{c2} \)

\( \mu_{c1} \)
First order transition at finite doping

\[ n(\mu) \text{ for several temperatures:} \]
\[ T/t = 1/10, 1/25, 1/50 \]
Link to Mott transition up to optimal doping

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

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)
What is the minimal model?

H. Alloul arXiv:1302.3473

Fig 1 Spin contribution $K_s$ to the $^{89}$Y NMR Knight shift [11] for YBCO$_{5.6}$ permit to define the PG onset $T^*$. Here $K_s$ 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.)
C-axis resistivity

Plaquette eigenstates
Pseudogap $T^*$ along the Widom line
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 $T \to T_p$.
- 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!

Pseudogap $T^*$ along the Widom line

Widom line: defined from maxima of charge compressibility
\[ \kappa = \frac{1}{n^2} \left( \frac{dn}{d\mu} \right)_T \]
divergence of $\kappa$ at the (classical) critical point!
Phase diagram
What is the minimal model?

H. Alloul arXiv:1302.3473

Fig 1 Spin contribution $K_s$ to the $^{89}$Y NMR Knight shift [11] for YBCO$_{5.6}$ permit to define the PG onset $T^*$. Here $K_s$ 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.)
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

Sordi et al. PRL 108, 216401 (2012)
\[ \Delta_p = -\frac{1}{2V} \sum_{p'} U(p - p') \frac{\Delta_{p'}}{E_{p'}} \left( 1 - 2n \left( E_{p'} \right) \right) \]

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

Béal–Monod, Bourbonnais, Emery
P.R. B. 34, 7716 (1986).
D. J. Scalapino, E. Loh, Jr., and J. E. Hirsch
P.R. B 34, 8190-8192 (1986).
Kohn, Luttinger, P.R.L. 15, 524 (1965).

A cartoon strong coupling picture


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

\[ d = \langle \hat{d} \rangle = \frac{1}{N} \sum_{\mathbf{k}} (\cos k_x - \cos k_y) \langle \mathbf{c}_\mathbf{k}^\dagger \mathbf{c}_{\mathbf{k}^\prime} \rangle \]

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

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

Miyake, Schmitt–Rink, and Varma
P.R. B 34, 6554-6556 (1986)
Unified phase diagram
Cuprates (doping driven transition)
Cuprates (doping driven transition)

Pseudogap vs pair

$T_{\text{pair}}$

ARPES
Bi2212

Meaning of $T_c^d$: Local pair formation


However, our measurements demonstrate that the nodal gap does not change with reduced doping. The pairing strength does not get weaker or stronger as the Mott insulator is approached; rather, it saturates.
Fluctuating region

Infrared response

Dubroka et al. 106, 047006 (2011)
Magnetoresistance, LSCO
Fluctuating vortices

Giant proximity effect

\[ T_c = 32\, K \]
\[ T_c < 5K \]

Morenzoni et al.,
Nature Comms. 2 (2011)

Figure 6 | Depth profile of the local field at different temperatures. The
Actual $T_c$ in underdoped

- **Quantum and classical phase fluctuations**

- **Magnitude fluctuations**

- **Competing order**

- **Disorder**
Larger clusters

- Is there a minimal size cluster where $T_c$ vanishes before half-filling?
- Learn something from small clusters as well
- Local pairs in underdoped
Larger cluster 8 site DCA

FIG. 8. Superfluid stiffness $\rho_s$ determined in the superconducting state at $T = t/60$ from Eq. 15, as a function of doping.

Gull, Millis, arxiv.org:304.6406
Gaussian amplitude fluctuations in Eu-LSCO

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

Monolayer LSCO, field doped

Effect of disorder

Summary

- 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
Main collaborators

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Dominic Bergeron
Sarma Kancharla
Marcello Civelli
Gabriel Kotliar
Massimo Capone
Merci

Thank you