Strongly correlated superconductivity: cuprates and organics

A.-M. Tremblay

Advances in strongly correlated electronic systems
Minneapolis - 13 June 2016
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
\[ E_P = \sum_{p,p'} U_{p-p'} \psi_{p \uparrow, -p \downarrow} \psi_{p' \uparrow, -p' \downarrow} \]

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

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

NiO, Boer and Verway

Peierls, 1937

Mott, 1949
« Conventional » Mott transition

Figure: McWhan, PRB 1970; Limelette, Science 2003
Two pillars of Condensed Matter Physics

• Band theory
  – DFT
  – Fermi liquid Theory
    • Metals
    • Semiconductors: transistor

• BCS theory of superconductivity
  – Broken symmetry
  – Emergent phenomenon
    • Also in particle physics, astrophysics…
« Phase » and emergent properties

- Emergent properties
  - e.g. Fermi surface
    - Shiny
    - Quantum oscillations (in B field)
- Many microscopic models will do the same
  - Electrons in box or atoms in solid, Fermi surface
  - Concept of Fermi liquid
  - Often hard to « derive » from first principles (fractionalization - gauge theories)
Atomic structure
Breakdown

For references, September 2013 Julich summer school
Strongly Correlated Superconductivity
http://www.cond-mat.de/events/correl13/manuscripts/tremblay.pdf
2. The 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

1931-1980

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

Attn: Charge transfer insulator
\[
U = 0
\]

\[
H = -\sum_{<ij>\sigma} t_{i,j} \left( c_{i\sigma}^{\dagger} c_{j\sigma} + c_{j\sigma}^{\dagger} c_{i\sigma} \right)
\]

\[
c_{i\sigma} = \frac{1}{\sqrt{N}} \sum_{k} e^{i\mathbf{k} \cdot \mathbf{r}_i} C_{k\sigma}
\]

\[
H = \sum_{k,\sigma} \varepsilon_k C_{k\sigma}^{\dagger} C_{k\sigma}
\]

\[
|\Psi\rangle = \prod_{k,\sigma} c_{k\sigma}^{\dagger} |0\rangle
\]
\( t_{ij} = 0 \)

\[
H = - \sum_{i,j} \alpha t_{ij} c_i^\dagger c_j + \sum_i n_i \uparrow n_i \downarrow
\]

\[
|\Psi\rangle = \prod_i c_{i\uparrow}^\dagger \prod_j c_{j\downarrow}^\dagger |0\rangle
\]

\( U \sum_i n_{i\uparrow} n_{i\downarrow} \)
Interesting in the general case

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

Mott transition

Effective model, Heisenberg: \( J = 4 t^2 / U \)
Spectral weight transfer

Meinders et al. PRB 48, 3916 (1993)
Outline

1. Introduction
2. The model
3. Weakly and strongly correlated antiferromagnets
   1. Qualitative
   2. Contrasting methods for weak and strong coupling
Outline

4. Weakly and strongly correlated superconductivity
   1. Qualitative
   2. Contrasting methods

5. High Tc the view from DMFT
   1. Quantum clusters
   2. Normal state and pseudogap
   3. SC state

6. Organics

7. Methods, 2 of them: C-DMFT and TPSC

8. Conclusion
3. Strong vs weak correlations for an antiferromagnet

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

$J = \frac{4t^2}{U}$

Mott

Heisenberg

Slater

AFM
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
Antiferromagnetic phase: emergent properties

- Some broken symmetries
  - Time reversal symmetry
  - Translation by one lattice spacing
  - Unbroken Time-reversal times translation by lattice vector $\mathbf{a}$
  - Spin waves
  - Single-particle gap
Differences between weakly and strongly correlated

• Different in ordered phase (finite frequency)
  – Ordered moment
  – Landau damping
    • Spin waves all the way or not to $J$

• Different, even more, in the normal state:
  – metallic in $d = 3$ if weakly correlated
  – Insulating if strongly correlated
  – Pressure dependence of $T_N$
Strong vs weak correlations

Contrasting methods
Ordered state

- Mean-field (Hartree-Fock) for AFM

Schrieffer, Wen, Zhang, PRB 1989
More methods for ordered states, $n=1$

- Numerically, stochastic series expansion,
- High-temperature series expansion,
- Quantum Monte Carlo
- World-line
- Worm algorithms
- Variational methods

• Ground state of $S=1/2$ in $d=2$ is AFM, not spin liquid
In paramagnetic state
Theory difficult even at weak to intermediate correlation!

- RPA (OK with conservation laws)
  - Mermin-Wagner
  - Pauli
- Moryia (Conjugate variables HS $\phi^4 = \langle \phi^2 \rangle \phi^2$)
  - Adjustable parameters: $c$ and $U_{\text{eff}}$
  - Pauli
- FLEX
  - No pseudogap
  - Pauli
- Renormalization Group
  - 2 loops

Zanchi Schultz, (2000)
Rohe and Metzner (2004)
Two-Particle Self-Consistent (idea)

• General philosophy
  – Drop diagrams
  – Impose constraints and sum rules
    • Conservation laws
    • Pauli principle (\( <n_\sigma^2> = <n_\sigma> \))
    • Local moment and local density sum-rules

• Get for free:
  • Mermin-Wagner theorem
  • Kanamori-Brückner screening
  • Consistency between one- and two-particle \( \Sigma G = U<n_\sigma n_{-\sigma}> \)

Vilk, AMT J. Phys. I France, 7, 1309 (1997); Allen et al.in *Theoretical methods for strongly correlated electrons* also cond-mat/0110130
(Mahan, third edition)
Doped Mott insulator: strong correlations

Normal state
Emergence and slave particle approaches

\[ H = \sum_{\langle ij \rangle} J \left( \mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} n_i n_j \right) - \sum_{ij, \sigma} t_{ij}(c_{i\sigma}^{\dagger}c_{j\sigma} + \text{H.c.}) \]

\[ c_{i\sigma}^{\dagger} = f_{i\sigma}^{\dagger}b_i \]

\[ f_{i\uparrow}^{\dagger}f_{i\uparrow} + f_{i\downarrow}^{\dagger}f_{i\downarrow} + b_i^{\dagger}b_i = 1 \]

\[ \mathbf{S}_i \cdot \mathbf{S}_j = -\frac{1}{4} f_{i\alpha}^{\dagger}f_{j\alpha} f_{j\beta}^{\dagger}f_{i\beta} - \frac{1}{4} (f_{i\uparrow}^{\dagger}f_{j\downarrow} - f_{i\downarrow}^{\dagger}f_{j\uparrow})(f_{j\uparrow}f_{i\uparrow} - f_{j\downarrow}f_{i\downarrow}) + \frac{1}{4} (f_{i\alpha}^{\dagger}f_{i\alpha}). \quad (35) \]

\[ n_i n_j = (1 - b_i^{\dagger}b_i)(1 - b_j^{\dagger}b_j) \]

Lagrangian after HS transformation

\[ Z = \int Df Df^\dagger Db Db^\dagger D\lambda D\chi D\Delta \exp \left( - \int_0^\beta d\tau L_1 \right) \]

\[ L_1 = \tilde{J} \sum_{\langle ij \rangle} (|\chi_{ij}|^2 + |\Delta_{ij}|^2) + \sum_{i\sigma} f_{i\sigma}^\dagger (\partial_\tau - i\lambda_i) f_{i\sigma} \]

\[ - \tilde{J} \left[ \sum_{\langle ij \rangle} \chi_{ij}^* \left( \sum_{\sigma} f_{i\sigma}^\dagger f_{j\sigma} \right) + \text{c.c.} \right] \]

\[ + \tilde{J} \left[ \sum_{\langle ij \rangle} \Delta_{ij} (f_{i\uparrow}^\dagger f_{j\downarrow} - f_{i\downarrow}^\dagger f_{j\uparrow}) + \text{c.c.} \right] \]

\[ + \sum_i b_i^* (\partial_\tau - i\lambda_i + \mu_B) b_i - \sum_{ij} t_{ij} b_i b_j^* f_{i\sigma}^\dagger f_{j\sigma} \]
For strong correlations

- Gutzwiller
- Variational approaches
- Slave particles (Review: Lee Nagaosa RMP)
- Extremely Correlated Fermi liquids (Shastry)
See numerous papers of Carbotte and Nicol and detailed discussions in
4. Weakly and strongly correlated superconductivity (cuprates, normal state)

Analog to weakly and strongly correlated antiferromagnets
Superconducting phase: identical properties

- **Emergent:**
  - Same broken symmetry $U(1)$ for s-wave,
  - $U(1)$ and $C_{4v}$ for d-wave
  - Single-Particle gap, point or line node.
    - $T$ dependence of $C_p$ and $\kappa$ at low $T$
  - Goldstone modes (+Higgs)
Superconductivity not universal even with phonons: weak or strong coupling

• In BCS universal ratios: e.g. $\Delta/k_BT_c$
  – Would never know the mechanism for sure if only BCS!
  – N.B. Strong coupling in a different sense
Phase diagram: hole and electron doping
Strongly correlated superconductors

- $T_c$ does not scale like order parameter
- Superfluid stiffness scales like doping
- Superconductivity can be largest close to the metal-insulator transition
- Resilience to near-neighbor repulsion
h-doped are strongly correlated: evidence from the normal state
Mott-Ioffe-Regel limit

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

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

\[ \sigma_{MIR} = \frac{e^2}{\hbar d} \]
Mott-Ioffe-Regel limit

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

\[ n = \frac{1}{2\pi d} k_F^2 \]

\[ \sigma = \left( \frac{1}{2\pi d} k_F^2 \right) \frac{e^2 \tau}{m} \]

\[ \ell = \left( \frac{\hbar k_F}{m} \right) \tau \]

\[ \sigma = \frac{1}{2\pi d} k_F e^2 \left( \frac{\ell}{\hbar} \right) \]

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

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

Gurvitch & Fiory
PRL 59, 1337 (1987)

MIR limit
Mean-free path
~ Fermi wavelength

LSCO 17%, YBCO optimal

Dominic Bergeron & AMST
PRB 2011
TPSC

Optical and dc conductivity of the two-dimensional Hubbard model in the pseudogap regime and across the antiferromagnetic quantum critical point including vertex corrections
Experiment, X-Ray absorption

Meinders et al. PRB 48, 3916 (1993)

Chen et al. PRL 66, 104 (1991)
Experiment: X-Ray absorption

Chen et al. PRL 66, 104 (1991)

Peets et al. PRL 103, (2009),

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)
Density of states (STM)

Khosaka et al. *Science* **315**, 1380 (2007);
Spin susceptibility (Knight shift): Pseudogap

Underdoped Hg1223
Julien et al. PRL 76, 4238 (1996)
ARPES: (Pseudogap)

Hole-doped, 10%

F. Ronning et al. Jan. 2002, Ca$_{2-x}$Na$_x$CuO$_2$Cl$_2$

Ronning et al. (PRB 2003)
Less strongly coupled: evidence from the normal state (MIR, pseudogap)

Less strongly correlated

- MIR
- Shape of hot spots
- Pressure dependence of $T_c$
- Size of the optical gap
e-doped cuprates: precursors

NCCO


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

$z = 1$
Electron-doped and MIR limit

NCCO

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

Onose et al. 2004
TPSC vs experiment for $\xi$

Kyung et al. PRL 93, 147004 (2004)

\( \xi(T) \) at the QCP

\begin{align*}
U &= 6, \quad t' = -0.175, \quad t'' = 0.05, \quad n = 1.2007 \\
\text{z} &= 1 \quad \text{Motoyama, Nature 2007}
\end{align*}

NCCO
Matsui et al. PRB 2007

Dominic Bergeron TPSC
Hot spots from AFM quasi-static scattering

Mermin-Wagner

\[ d = 2 \]

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


Armitage et al. PRL 2001
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)
4. Weakly and strongly correlated superconductivity

Weakly correlated case
\[ \Delta_p = -\frac{1}{2V} \sum_{p'} U(p - p') \frac{\Delta_{p'}}{E_{p'}} \left( 1 - 2n\left( E_{p'} \right) \right) \]

Exchange of spin waves?
Kohn-Luttinger

T_c 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).

Results from TPSC

Satisfies Mermin-Wagner
Relation between symmetry and wave vector of AFM fluctuations

Hassan et al. PRB 2008
Organics & Pnictides

Organic

Pnictide

Bourbonnais, Sedeki, 2012

Doiron-Leyraud et al., PRB 80, 214531 (2009)
Heavy fermions

3D metals tuned by pressure, field or concentration

CeRhIn$_5$

Magnetic superconductivity

Knebel et al. (2009)

Quantum criticality

Mathur et al., Nature 1998
4. Weakly and strongly correlated superconductivity

Strong correlations point of view
A cartoon strong coupling picture


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

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

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

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

Miyake, Schmitt–Rink, and Varma
P.R. B 34, 6554-6556 (1986)
5. High-temperature superconductors
the view from dynamical mean-field theory

5.1: Quantum cluster approaches
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)
• 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
Two solvers for the cluster-in-a-bath problem
Competition AFM-dSC

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
At finite $T$, solving cluster in a bath problem

- Continuous-time Quantum Monte Carlo calculations to sum all diagrams generated from expansion in powers of hybridization.
  
  
5.2 Normal state and pseudogap
The view from quantum clusters
Phase diagram, hole-doped (YBCO)

Laliberté, …. Taillefer (2016)
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?
Underdoped metal very sensitive to anisotropy

Okamoto, Sénéchal, Civelli, AMST
Phys. Rev. B 82, 180511R 2010

D. Fournier et al. Nature Physics
Link to Mott transition up to optimal doping

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

Correlated metal

PG
First order transition at finite doping

$n(\mu)$ 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)
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 $T \rightarrow T_p$.
- 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

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 $K_z$ to the $^{89}$Y NMR Knight shift [11] for YBCO$_{5.6}$ permit to define the PG onset $T^*$. Here $K_z$ 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.)
Spin susceptibility
Two crossover lines

Sordi et al. PRL 108, 216401 (2012)
PRB 87, 041101(R) (2013)
c-axis resistivity

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)
Fratino et al.
Sci. Rep. 6, 22715
An organizing principle
3 bands, charge transfer insulator


FIG. 2. (a) Noninteracting Fermi surface for the model parameter investigated in Fig. 1a of main text, namely $e_p = 9$, $t_{pp} = 1$, $t_{pd} = 1.5$, which gives a total occupation $n_{tot}$ equal to five. (b) Non-interacting band structure for the same model parameter along with the resulting total density of states. Color corresponds to the d-character of the hybridised bands. The band crossing the Fermi level has mostly oxygen character.

Giovanni Sordi

Lorenzo Fratino
3 bands, charge transfer insulator

3 bands, charge transfer insulator


**$T_{\text{pair}}$**

**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. PRL 106, 047006 (2011)
Magnetoresistance, LSCO
Fluctuating vortices

• 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

Gull, Millis, arxiv.org:1304.6406
Gaussian amplitude fluctuations in Eu-LSCO

Chang, Doiron-Leyraud et al.
Effect of disorder

Superconductivity in underdoped vs BCS
First-order transition leaves its mark
Schematic $T$ dependence of the gap

$T$ dependence of the gap underdoped

Alexis Reyembaut
$\Delta/T_c$

c-axis Superfluid stiffness \( U = 9t, \ T = 1/100 \)

Fratino, Sordi, unpublished

Panagopoulos et al. PRB 2000

See also, Gull Millis, PRB, 2013
FIG. 8. Superfluid stiffness $\rho_s$ determined in the superconducting state at $T = t/60$ from Eq. 15, as a function of doping.
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
$T = 0$ phase diagram: superconductivity

Mechanism in the presence of strong correlation
Dome vs Mott (CDMFT)

Kancharla, Kyung, Civelli, Sénéchal, Kotliar AMST
CDMFT global phase diagram

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

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

Kyung, Sénéchal, Tremblay, Phys. Rev. B
80, 205109 (2009)

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.

Frequencies important for pairing

for $\omega \rightarrow \infty$

Resilience to near-neighbor repulsion $V$

In mean-field, $J - V$

$J = 130\text{ meV}$

$V = 400\text{ meV}$

The $\ln(E_F/\omega_D)$ necessary to screen $V$, for $\mu^*$ not enough

Weak-coupling: $V < U (U/W)$ for survival of d-wave

Resilience to near-neighbor repulsion

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

Sénéchal, Day, Bouliane, AMST PRB 87, 075123 (2013)
Effect of $V$, finite temperature, $U = 9t$
6. Superconductivity in the organics
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 \((X = \text{Cu[N(CN)₂]Cl})\)


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

\(B_{g}\) for \(C_{2h}\) and \(B_{2g}\) for \(D_{2h}\)

Powell, McKenzie cond-mat/0607078
Perspective
Phase diagram BEDT

\[ t' = 0.6t \]

\[ X = Cu_2(CN)_3 \quad (t' \sim t) \]

Y. Kurisaki, et al.  

Theoretical phase diagram BEDT

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


Sénéchal, Sahebsara, Phys. Rev. Lett. 97, 257004
### Other compounds (R. Valenti et al.)

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<th>Hueckel</th>
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<td>Br</td>
<td>0.68</td>
<td>7.2</td>
</tr>
</tbody>
</table>

- Kandpal et al. PRL (2009)
- Nakamura et al. JPSJ (2009)
- Komatsu et al. JPSJ (1996)
- Kyung, Tremblay PRL (2006)
- Tocchio, Parola, Gros, Becca PRB (2009)
Doped organic: experiment
Doped BEDT

Doped BEDT

Organics: Phase diagram, finite T

Made possible by algorithmic improvements

P. Sémon et al.
PRB 85, 201101(R) (2012)
PRB 90 075149 (2014);
and PRB 89, 165113 (2014)
$t' = 0.4t$ overview

Compare: T. Watanabe, H. Yokoyama and M. Ogata
First order and Widom line in organics

G. Sordi et al. Scientific Reports, 2, 547 (2012)

Compare: T. Watanabe, H. Yokoyama and M. Ogata
JPS Conf. Proc.
3, 013004 (2014)

C.-D. Hébert, P. Sémon, A.-M.S. T PRB 92, 195112 (2015)
Signatures of Widom line in the superconducting state
\[ t' = 0.8 \, t \]
Generic case highly frustrated case
AFM quantum critical point in heavy fermions (with same category of methods)

Heavy fermions

\[ H = \sum_{k,\sigma} \epsilon_k c_{k,\sigma}^\dagger c_{k,\sigma} + \sum_{k,\sigma} \epsilon_f f_{k,\sigma}^\dagger f_{k,\sigma} + \sum_{k,\sigma} V_k (f_{k,\sigma}^\dagger c_{k,\sigma} + H.c.) + \sum_i U \left( n_{f_i} - \frac{1}{2} \right) \left( n_{f_i} - \frac{1}{2} \right) \]

\[ V_k = V + 2V' \left[ \cos(k_x) + \cos(k_y) \right] \]

U=4

AFM: antiferro-magnetism
SC: superconducting

\( V'/V = 2 \): more frustrated case
\( V'/V = 5 \): less frustrated 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 an AFM QCP. Extension of Mott
  – SC from short range $J$.
  – $T_c$ decreases at Widom line
Perspective
Perspective
Perspective
Perspective
Perspective
Perspective
Main collaborators

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Maxime Charlebois

Alexandre Day

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Further references

For references, September 2013 Julich summer school
Strongly Correlated Superconductivity

http://www.cond-mat.de/events/correl13/manuscripts/tremblay.pdf

Lecture notes

Merci

Thank you
Methods
Measurable quantities: Green’s functions

\[ \langle O \rangle \equiv \frac{Tr\left[ e^{-\beta(H-\mu N)}O \right]}{Tr\left[ e^{-\beta(H-\mu N)} \right]} \]

\[ G_{k\sigma}(\tau) = -\langle T_\tau [c_{k\sigma}(\tau)c_{k\sigma}^\dagger] \rangle \]

\[ = -\theta(\tau)\langle c_{k\sigma}(\tau)c_{k\sigma}^\dagger \rangle + \theta(-\tau)\langle c_{k\sigma}^\dagger c_{k\sigma}(\tau) \rangle. \]

\[ c_{k\sigma}(\tau) = e^{(H-\mu N)\tau}c_{k\sigma}e^{-(H-\mu N)\tau} \]

\[ G_{k\sigma}(i\omega_n) = \int_0^\beta d\tau e^{i\omega_n\tau}G_{k\sigma}(\tau) \]

\[ \omega_n = (2n + 1)\pi T \]
Green’s function: free electrons, atomic limit

\[ H = -\sum_{<ij>\sigma} t_{ij} \left( c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma} \right) \]

\[ G_{k\sigma}(i\omega_n) = \frac{1}{i\omega_n - (\epsilon_k - \mu)} \]

\[ H = \sum_i n_{i\uparrow} n_{i\downarrow} + U \sum_i n_{i\uparrow} n_{i\downarrow} \]

\[ \langle n \rangle = 1 \quad G_{\sigma}(i\omega_n) = \frac{1/2}{i\omega_n + U/2} + \frac{1/2}{i\omega_n - U/2} \]
Self-energy and all that

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

\[
G_{k\sigma}(i\omega_n) = \frac{1}{i\omega_n - (\varepsilon_k - \mu) - \Sigma_{k\sigma}(i\omega_n)}
\]

\[
G^{-1}_{k\sigma}(i\omega_n) = G^{0-1}_{k\sigma}(i\omega_n) - \Sigma_{k\sigma}(i\omega_n)
\]

Self-energy in the atomic limit for \( n = 1 \)

\[
G_{\sigma}(i\omega_n) = \frac{1/2}{i\omega_n + \frac{U}{2}} + \frac{1/2}{i\omega_n - \frac{U}{2}}
\]

\[
G_{\sigma}(i\omega_n) = \frac{1}{i\omega_n + \frac{U}{2} - \Sigma(i\omega_n)}
\]

\[
\Sigma(i\omega_n) = \frac{U}{2} + \frac{U^2}{i\omega_n}
\]
Dynamical “variational” principle

\[ \Omega_t[G] = \Phi[G] - Tr[(G_0^{-1} - G^{-1})G] + Tr \ln(-G) \]

\[ \Phi[G] = \bigcirc + \bigcirc \quad + \quad \bigcirc \bigcirc + \quad .... \quad \text{Universality} \]

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

\[ \frac{\delta \Omega_t[G]}{\delta G} = \Sigma - G_0^{-1} + G^{-1} = 0 \]

Then \( \Omega \) is grand potential

Related to dynamics (cf. Ritz)

Luttinger and Ward 1960, Baym and Kadanoff (1961)

H.F. if approximate \( \Phi \) by first order

FLEX higher order
Self-consistency condition

• Obtain Green’s function for the « impurity » (cluster) in a bath
• Extract $\Sigma$
• Substitute $\Sigma$ in lattice Green’s function
• Project lattice Green’s function on impurity (cluster).
• If the two Green’s functions are not equal, modify the bath until they are.
Self-consistency

\[ G_{\sigma}(i\omega_n)^{-1} = G_{\sigma}^{0-imp}(i\omega_n)^{-1} - \Sigma_{\sigma}(i\omega_n) \]

\[ N_c \int \frac{d^d\vec{k}}{(2\pi)^d} \frac{1}{G_{k\sigma}^{0}(i\omega_n)^{-1}-\Sigma_{\sigma}(i\omega_n)} = G_{\sigma}^{imp}(i\omega_n) \]
Methods of derivation

• Cavity method
• Local nature of perturbation theory in infinite dimensions
• Expansion around the atomic limit
• Effective medium theory
• Potthoff self-energy functional

DMFT as a stationary point
Another way to look at this (Potthoff)

\[
\Omega_t[G] = \Phi[G] - Tr[(G_0^{-1} - G^{-1})G] + Tr \ln(-G)
\]

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

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

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 $H_0(t')$**

CT-QMC impurity solver
Monte Carlo method


\[ Z = \int_{c} dx p(x). \]

\[ \langle A \rangle_p = \frac{1}{Z} \int_{c} dx \mathcal{A}(x) p(x). \]

\[ \langle A \rangle_p \approx \langle A \rangle_{MC} = \frac{1}{M} \sum_{i=1}^{M} \mathcal{A}(x_i). \]

\[ \langle A \rangle = \frac{1}{Z} \int_{c} dx \mathcal{A}(x) p(x) = \frac{\int_{c} dx \mathcal{A}(x) \left[ \frac{p(x)}{\rho(x)} \right] \rho(x)}{\int_{c} dx \left[ \frac{p(x)}{\rho(x)} \right] \rho(x)} \equiv \frac{\langle A(p/\rho) \rangle_p}{\langle p/\rho \rangle_p}. \]
Monte Carlo: Markov chain

- Ergodicity
- Detailed balance

\[
\frac{W_{xy}}{W_{yx}} = \frac{p(y)}{p(x)}
\]

\[
W_{xy} = W_{xy}^{\text{prop}} W_{xy}^{\text{acc}}
\]

\[
W_{xy}^{\text{acc}} = \min[1, R_{xy}]
\]

\[
R_{xy} = \frac{p(y) W_{yx}^{\text{prop}}}{p(x) W_{xy}^{\text{prop}}}
\]
Reminder on perturbation theory

\[
\exp(-\beta(H_a + H_b)) = \exp(-\beta H_a)U(\beta)
\]

\[
\frac{\partial U(\beta)}{\partial \beta} = -H_b(\beta)U(\beta)
\]

\[
U(\beta) = 1 - \int_0^\beta d\tau H_b(\tau) + \int_0^\beta d\tau \int_0^\tau d\tau' H_b(\tau)H_b(\tau') + ...
\]
Partition function as sum over configurations

\[ Z = \text{Tr}[\exp(H_a + H_b)] \]

\[ Z = \sum_{k=0}^{\infty} \sum_{\gamma \in \Gamma_k} \int_0^\beta d\tau_1 \cdots \int_{\tau_{k-1}}^\beta d\tau_k \text{Tr}[e^{-\beta H_a} H_b(\tau_k) \times H_b(\tau_{k-1}) \cdots H_b(\tau_1)] . \]

\[ x = (k, \gamma, (\tau_1, \ldots, \tau_k)), \quad p(x) = w(k, \gamma, \tau_1, \ldots, \tau_k) d\tau_1 \cdots d\tau_k, \]
Updates

\[ W_{(k, \bar{\tau})}^{\text{prop}}(k+1, \bar{\tau}^{'}) = \frac{d\tau}{\beta} \]
\[ W_{(k+1, \bar{\tau}^{'})}^{\text{prop}}(k, \bar{\tau}) = \frac{1}{k + 1}. \]

\[ R_{(k, \bar{\tau}),(k+1, \bar{\tau}^{'})} = \frac{p((k + 1, \bar{\tau}^{'})}{p((k, \bar{\tau}))} \frac{W_{(k+1, \bar{\tau}^{'})}^{\text{prop}}(k, \bar{\tau})}{W_{(k, \bar{\tau})}^{\text{prop}}(k+1, \bar{\tau}^{'})} \]
\[ = \frac{w(k + 1)d\tau^{'}}{w(k)d\tau_1 \cdots d\tau_{k+1}} \frac{\beta}{1/(k + 1)} \]
\[ = \frac{w(k + 1)}{w(k)} \frac{\beta}{k + 1}. \]

Solving cluster in a bath problem

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


Expansion in powers of the hybridization

\[ H_{\text{hyb}} = \sum_{pq} (V_p c_p^d d_j + V_p^* d_j^\dagger c_p) = \tilde{H}_{\text{hyb}} + \tilde{H}_{\text{hyb}}^\dagger \]

\[ Z = \sum_{k=0}^{\infty} \int_0^\beta d\tau_1 \cdots \int_{\tau_{k-1}}^\beta d\tau_k \int_0^\beta d\tau'_1 \cdots \int_{\tau'_{k-1}}^\beta d\tau'_k \]
\[ \times \sum_{p_1} \sum_{p'_1} \sum_{j_1, j'_1, p_1, p'_1} \cdots \sum_{j_k, j'_k, p_k, p'_k} V_{j_1}^{j'_1} V_{p_1}^{j'_1} \cdots V_{j_k}^{j'_k} V_{p_k}^{j'_k} \]
\[ \times \text{Tr}_d[T_\tau e^{-\beta H_{\text{loc}}} d_{j_k}(\tau_k) d_{j'_k}(\tau'_k) \cdots d_{j_1}(\tau_1) d_{j'_1}(\tau'_1)] \]
\[ \times \text{Tr}_c[T_\tau e^{-\beta H_{\text{bath}}} c_{p_k}^\dagger(\tau_k) c_{p'_k}(\tau'_k) \cdots c_{p_1}^\dagger(\tau_1) c_{p'_1}(\tau'_1)]. \]

\[ P_m = \frac{\langle m | e^{-\beta H_{\text{loc}}} d_{j_k}(\tau_k) d_{j'_k}(\tau'_k) \cdots d_{j_1}(\tau_1) d_{j'_1}(\tau'_1) | m \rangle}{\sum_n \langle n | e^{-\beta H_{\text{loc}}} d_{j_k}(\tau_k) d_{j'_k}(\tau'_k) \cdots d_{j_1}(\tau_1) d_{j'_1}(\tau'_1) | n \rangle} \]
Sign problem

\[ S = S_{cl}(c^\dagger, c) + \int_0^\beta d\tau d\tau' c^\dagger(\tau') \Delta(\tau' - \tau)c(\tau) \]

P. Sénon, A.-M.S. Tremblay, (unpub.)
Two-Particle Self-Consistent Approach (U < 8t) - How it works

• General philosophy
  – Drop diagrams
  – Impose constraints and sum rules
    • Conservation laws
    • Pauli principle (\( <n_\sigma^2> = <n_\sigma> \))
    • Local moment and local density sum-rules

• Get for free:
  • Mermin-Wagner theorem
  • Kanamori-Brückner screening
  • Consistency between one- and two-particle \( \Sigma G = U<n_\sigma n_{-\sigma}> \)

Vilk, AMT J. Phys. I France, 7, 1309 (1997); Allen et al. in *Theoretical methods for strongly correlated electrons* also cond-mat/0110130
(Mahan, third edition)
TPSC approach: two steps

I: Two-particle self consistency

1. Functional derivative formalism (conservation laws)
   (a) spin vertex:
   \[ U_{sp} = \frac{\delta \Sigma_{\uparrow}}{\delta G_{\downarrow}} - \frac{\delta \Sigma_{\uparrow}}{\delta G_{\uparrow}} \]
   (b) analog of the Bethe-Salpeter equation:
   \[ \chi_{sp} = \frac{\delta G}{\delta \phi} = GG + GU_{sp}\chi_{sp}G \]
   (c) self-energy:
   \[ \Sigma_{\sigma} (1, \overline{1}; \{ \phi \}) G_{\sigma} (\overline{1}, 2; \{ \phi \}) = -U \left< c_{-\sigma}^\dagger (1^+) c_{-\sigma} (1) c_{\sigma} (1) c_{\sigma}^\dagger (2) \right>_{\phi} \]
   \[ \approx A_{\{ \phi \}} G_{-\sigma}^{(1)} (1, 1^+; \{ \phi \}) G_{\sigma}^{(1)} (1, 2; \{ \phi \}) \]

2. Factorization
TPSC…

Kanamori-Brückner screening

\[ U_{sp} = U \frac{\langle n_\uparrow n_\downarrow \rangle}{\langle n_\uparrow \rangle \langle n_\downarrow \rangle} \]

\[ \chi_{sp}^{(1)}(q) = \frac{\chi_0(q)}{1 - \frac{1}{2} U_{sp} \chi_0(q)} \]

3. The F.D. theorem and Pauli principle

\[ \langle (n_\uparrow - n_\downarrow)^2 \rangle = \langle n_\uparrow \rangle + \langle n_\downarrow \rangle - 2 \langle n_\uparrow n_\downarrow \rangle \]

\[ \frac{T}{N} \sum_q \chi_{sp}^{(1)}(q) = n - 2 \langle n_\uparrow n_\downarrow \rangle \]

II: Improved self-energy

Insert the first step results into exact equation:

\[ \Sigma_\sigma (1, \bar{1}; \{ \phi \}) G_\sigma (\bar{1}, 2; \{ \phi \}) = -U \langle c_\bar{\sigma}^\dagger (1^\uparrow) c_{-\sigma} (1) c_{\sigma} (1) c_\sigma^\dagger (2) \rangle_\phi \]

\[ \Sigma_{\sigma}^{(2)}(k) = U n_\sigma + \frac{U T}{8 N} \sum_q \left[ 3 U_{sp} \chi_{sp}^{(1)}(q) + U_{ch} \chi_{ch}^{(1)}(q) \right] G_\sigma^{(1)}(k + q) \]
A better approximation for single-particle properties (Ruckenstein)

\[ \sum_1^3 2 = - \sum_1^3 2 + \]

Y.M. Vilk and A.-M.S. Tremblay, Europhys. Lett. 33, 159 (1996);

N.B.: No Migdal theorem
Benchmarks for TPSC
$n = 1$

\[ \xi \sim \exp\left(\frac{C(T)}{T}\right) \]

**Calc.:** Vilk et al. P.R. B 49, 13267 (1994)


Check on accuracy

Notes:
- F.L. parameters
- Self also Fermi-liquid

QMC + cal.: Vilk et al. P.R. B 49, 13267 (1994)
Proofs...

e-doped cuprates: precursors


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

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

Mermin-Wagner

$d = 2$

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

Motoyama, E. M. et al..

Armitage et al. PRL 2001
Main collaborators

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Alexandre Day
Vincent Bouliane
Further references

For references, September 2013 Julich summer school
Strongly Correlated Superconductivity

http://www.cond-mat.de/events/correl13/manuscripts/tremblay.pdf

Lecture notes

André-Marie Tremblay

Sponsors:
Mammouth
Merci

Thank you