# Strongly correlated superconductivity

#### A.-M. Tremblay







CMP in the City, London, 17th June 2013



#### How to make a metal









Courtesy, S. Julian

# Superconductivity















**—** -p'







# #1 Cooper pair, #2 Phase coherence

$$E_{P} = \sum_{\mathbf{p},\mathbf{p}'} U_{\mathbf{p}-\mathbf{p}'} \psi_{\mathbf{p}\uparrow,-\mathbf{p}\downarrow} \psi_{\mathbf{p}'\uparrow,-\mathbf{p}'\downarrow}^{*}$$

$$E_{P} = \sum_{\mathbf{p},\mathbf{p}'} U_{\mathbf{p}-\mathbf{p}'} \left( \langle \psi_{\mathbf{p}\uparrow,-\mathbf{p}\downarrow} \rangle \psi_{\mathbf{p}'\uparrow,-\mathbf{p}'\downarrow}^{*} + \psi_{\mathbf{p}\uparrow,-\mathbf{p}\downarrow} \langle \psi_{\mathbf{p}'\uparrow,-\mathbf{p}'\downarrow}^{*} \rangle \right)$$

$$|\mathrm{BCS}(\theta)\rangle = \dots + e^{iN\theta}|N\rangle + e^{i(N+2)\theta}|N+2\rangle + \dots$$



# Breakdown of band theory Half-filled band is metallic?



# Half-filled band: Not always a metal

#### NiO, Boer and Verway



Peierls, 1937



Mott, 1949 SHERBROOKE

#### « Conventional » Mott transition



Figure: McWhan, PRB 1970; Limelette, Science 2003



# Superconductivity, in the presence of strong repulsion?



#### High-temperature superconductors

#### Armitage, Fournier, Greene, RMP (2009) La<sub>2-x</sub>Sr<sub>x</sub>CuO<sub>4</sub> Re<sub>2-x</sub>Ce<sub>x</sub>CuO<sub>4</sub> ~ 300K V $T_N$ $T_N$ AF AF T $T_{c}$ 30K 0.10 0.20 0.10 0.20 Electron doping / Ce content (x) Hole doping / Sr content (x) $< \frac{1}{2}$ 1/2 Band filling $> \frac{1}{2}$

#### Mott Physics away from n = 1



# Strongly correlated SC: Layered d=2 organics



Powell, McKenzie J. Phys.: Condens. Matter 18 (2006) R827–R866



# Model



#### Hubbard model



1931-1980

Effective model, Heisenberg:  $J = 4t^2 / U$ 



# Outline

- Weak to intermediate coupling
  - TPSC
  - e-doped cuprates
- A phase at weak and at strong coupling
- h-doped cuprates as doped Mott insulators
- Cluster Dynamical Mean-Field Theory
- Strong coupling superconductivity
  - Organics
  - High Tc



# Methodology

#### Weak-coupling approaches



# Theory difficult even at weak to intermediate coupling!

- $\frac{1}{3} = \frac{1}{3} = \frac{1}$
- RPA (OK with conservation laws)
  - Mermin Wagner
  - Pauli
- Moryia (Conjugate variables HS  $\phi^4 = \langle \phi^2 \rangle \phi^2$ )

Σ

- Adjustable parameters: c and  $U_{eff}$
- Pauli
- FLEX
  - No pseudogap
  - Pauli
- Renormalization Group
  - 2 loops

Rohe and Metzner (2004) Katanin and Kampf (2004)



# Two-Particle-Self-Consistent Approach



# Benchmarks for TPSC





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# QMC benchmark for TPSC



Calc. + QMC: Moukouri et al. P.R. B 61, 7887 (2000).



# Two-Particle Self-Consistent Approach

- General philosophy
  - Drop diagrams (U < 6t)
  - 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)

# **Two-Particle Self-Consistent Approach**

A better approximation for single-particle properties (Ruckenstein)



Y.M. Vilk and A.-M.S. Tremblay, J. Phys. Chem. Solids **56**, 1769 (1995). Y.M. Vilk and A.-M.S. Tremblay, Europhys. Lett. **33**, 159 (1996);

N.B.: No Migdal theorem



#### Cartoon « BCS » weak-coupling picture

$$\Delta_{\mathbf{p}} = -\frac{1}{2V} \sum_{\mathbf{p}'} U(\mathbf{p} - \mathbf{p}') \frac{\Delta_{\mathbf{p}'}}{E_{\mathbf{p}'}} \left(1 - 2n\left(E_{\mathbf{p}'}\right)\right)$$





Exchange of spin waves? Kohn-Luttinger

 $T_c$  with pressure

Kohn, Luttinger, P.R.L. 15, 524 (1965).

P.W. Anderson Science 317, 1705 (2007)





# e-doped cuprates with TPSC



#### Hot spots from AFM quasi-static scattering

d = 2



Armitage et al. PRL 2001

# Pseudogap for e-doped curates





# Fermi surface plots

Hubbard repulsion U has to...



# d = 2 precursors, e-doped



$$\xi^{\star} = 2.6(2)\xi_{\rm th}$$

Vilk, A.-M.S.T (1997)

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

Semi-quantitative fits of both ARPES and neutron



#### Cartoon « BCS » weak-coupling picture

$$\Delta_{\mathbf{p}} = -\frac{1}{2V} \sum_{\mathbf{p}'} U(\mathbf{p} - \mathbf{p}') \frac{\Delta_{\mathbf{p}'}}{E_{\mathbf{p}'}} \left(1 - 2n\left(E_{\mathbf{p}'}\right)\right)$$





Exchange of spin waves? Kohn-Luttinger

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P.W. Anderson Science 317, 1705 (2007)



#### Superconductivity in TPSC







# BCS vs AFM mediated SC

- Symmetry from wave vector of AFM
- Dominant wave vector from shape of Fermi surface
- For given shape of FS,  $T_c$  increases with U
- *N*(*0*) not so important
- Competition with pseudogap => optimal *t*'
- $T_c$  above or below RC regime, but  $\xi > a$

Hassan, Davoudi, Kyung, A.-M.S.T. Phys. Rev. B **77**, 094501 (2008)


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### What is a phase?

#### Weak vs strong coupling



#### Local moment and Mott transition





#### Local moment and Mott transition



## Superconducting phase

- 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!



## A phase: Superconducting



#### AFM and superconductivity



L. Taillefer, Annual Reviews of CMP 2010



#### Weakly or strongly correlated?



L. Taillefer, Annual Reviews of CMP 2010



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#### Hole-doped cuprates as Mott insulators



# Mott-Ioffe-Regel limit

$$\sigma = \frac{ne^2\tau}{m}$$

$$k_F \ell = rac{2\pi}{\lambda_F} \ell \sim 2\pi$$
 $\sigma_{MIR} = rac{e^2}{\hbar d}$ 



#### Hole-doped cuprates and MIR limit



LSCO 17%, YBCO optimal

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

PHYSICAL REVIEW B 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





#### Experiment: X-Ray absorption



Peets et al. PRL **103**, (2009), Phillips, Jarrell PRL , vol. **105**, 199701 (2010)

# 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)

# Strong coupling superconductivity



#### A cartoon strong coupling picture

P.W. Anderson Science 317, 1705 (2007)

$$J\sum_{\langle i,j\rangle} \mathbf{S}_{i} \cdot \mathbf{S}_{j} = J\sum_{\langle i,j\rangle} \left(\frac{1}{2}c_{i}^{\dagger}\vec{\sigma}c_{i}\right) \cdot \left(\frac{1}{2}c_{j}^{\dagger}\vec{\sigma}c_{j}\right)$$
$$d = \langle \hat{d} \rangle = 1/N\sum_{\vec{k}} (\cos k_{x} - \cos k_{y}) \langle c_{\vec{k},\uparrow}c_{-\vec{k},\downarrow} \rangle$$
$$H_{MF} = \sum_{\vec{k},\sigma} \varepsilon(\vec{k}) c_{\vec{k},\sigma}^{\dagger} c_{\vec{k},\sigma} - 4Jm\hat{m} - Jd(\hat{d} + \hat{d}^{\dagger}) + F_{0}$$

Pitaevskii Brückner:

Pair state orthogonal to repulsive core of Coulomb interaction

Miyake, Schmitt–Rink, and Varma P.R. B **34**, 6554-6556 (1986)



#### High-temperature superconductors



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

- 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?
  - RVB: P.A. Lee Rep. Prog.
    Phys. **71**, 012501 (2008)



#### Another strongly correlated superconductor





F. Kagawa, K. Miyagawa, + K. Kanoda PRB **69** (2004) +Nature **436** (2005)

#### Phase diagram (X=Cu[N(CN)<sub>2</sub>]Cl) S. Lefebvre et al. PRL 85, 5420 (2000), P. Limelette, et al. PRL 91 (2003)

CIAR The Canadian Institute for Advanced Research



#### Layered organics ( $\kappa$ -BEDT-X family)



# Perspective





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- h-doped as doped Mott insulators
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# Method



#### Mott transition and Dynamical Mean-Field Theory. The beginnings in d = infinity

- Compute scattering rate (self-energy) of impurity problem.
- Use that self-energy (ω 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



#### Another way to look at this (Potthoff)

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

$$\Omega_{t}[\Sigma] = \begin{bmatrix} \frac{\delta \Phi[G]}{\delta G} = \Sigma \\ \Phi[G] - Tr[\Sigma G] - Tr \ln(-G_{0t}^{-1} + \Sigma) \end{bmatrix}$$
Still stationary (chain rule)  

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

M. Potthoff, Eur. Phys. J. B 32, 429 (2003).



#### SFT : Self-energy Functional Theory

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

$$\Omega_{\mathbf{t}}[\Sigma] = F[\Sigma] + \operatorname{Tr}\ln(-(G_0^{-1} - \Sigma)^{-1})$$

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

$$\Omega_{\mathbf{t}}[\Sigma] = \Omega_{\mathbf{t}'}[\Sigma] - \mathrm{Tr}\ln(-(G_0^{\prime - 1} - \Sigma)^{-1}) + \mathrm{Tr}\ln(-(G_0^{-1} - \Sigma)^{-1}).$$

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

Variation of the self-energy, through parameters in  $H_0(\mathbf{t'})$ 

M. Potthoff, Eur. Phys. J. B 32, 429 (2003).



#### + and -

- Long range order:
  - Allow symmetry breaking in the bath (mean-field)
- Included:
  - Short-range dynamical and spatial correlations
- Missing:
  - Long wavelength fluctuations



# Two solvers for the cluster-in-a-bath problem





See also, Capone and Kotliar, Phys. Rev. B 74, 054513 (2006), Macridin, Maier, Jarrell, Sawatzky, Phys. Rev. B 71, 134527 (2005).

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#### **C-DMFT**

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





EFFECTIVE LOCAL IMPURITY PROBLEM



SELF-CONSISTENCY CONDITION

Here: continuous time QMC

Mean-field is not a trivial

problem! Many impurity

solvers.

P. Werner, PRL 2006 P. Werner, PRB 2007 K. Haule, PRB 2007

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

#### 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.
  - P. Werner, A. Comanac, L. de' Medici, M. Troyer, and A. J. Millis, Phys. Rev. Lett. 97, 076405 (2006).
  - K. Haule, Phys. Rev. B **75**, 155113 (2007).



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# T = 0 phase diagram n = 1

# Phase diagram Exact diagonalization as solver for cluster-in-a bath problem (T=0).



# Theoretical phase diagram BEDT

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





Phys. Rev. Lett. 95, 177001(2005) Y. Shimizu, et al. Phys. Rev. Lett. 91, (2003)
## AFM and dSC order parameters for various t'/t

•Discontinuous jump

•Strongest superconductivity near the Mott insulator!

Cu(NCS)<sub>2</sub>

0.84

10.4

1.06

3.9

Cu[N(CN)<sub>2</sub>]Br

0.68

11.6

X

ť/t

T<sub>c</sub>



121 Kyung, A.-M.S.T. PRL 97, 046402 (2006)



## T = 0 phase diagram: cuprates

## Phase diagram Exact diagonalization as impurity solver (T=0).



#### Dome vs Mott (CDMFT)



#### Kancharla, Kyung, Civelli, Sénéchal, Kotliar AMST Phys. Rev. B (2008)



#### CDMFT global phase diagram



Kancharla, Kyung, Civelli, Sénéchal, Kotliar AMST Phys. Rev. B (2008) AND Capone, Kotliar PRL (2006)



#### Armitage, Fournier, Greene, RMP (2009)











## T = 0 phase diagram

#### The glue



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

Maier, Poilblanc, Scalapino, PRL (2008)



#### The glue



#### 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  $E_i = 140 \text{ meV}$ , open for  $E_i = 80 \text{ meV}$ ), 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)





## Frequencies important for pairing



#### Bumsoo Kyung

#### David Sénéchal

$$I_{F}(\omega) \equiv -\int_{0}^{\omega} \frac{d\omega'}{\pi} \operatorname{Im} F_{ij}^{R}(\omega') \xrightarrow{(a)}_{\beta \to 0.02} 0.01$$
Cumulative Order Parameter
$$\langle c_{i\uparrow}c_{j\downarrow} \rangle \quad \text{for } \omega \to \infty$$
B. Kyung, D. Sénéchal, and A.-M.S.T, Phys. Rev. B **80**, 205109 (2009).

#### Resilience to near-neighbor repulsion V

In mean-field, 
$$J - V$$
  
 $J = 130 meV$   
 $V = 400 meV$ 

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

S. Raghu, E. Berg, A. V. Chubukov, and S. A. Kivelson, PRB 85, 024516 (2012).
S. Onari, R. Arita, K. Kuroki, and H. Aoki, PRB 70, 094523 (2004).



# Resilience to near-neighbor repulsion

David Sénéchal



Market SHERBROOKE

## J in the presence of V



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



# Resilience to near-neighbor repulsion

David Sénéchal



Market SHERBROOKE



Giovanni Sordi



Patrick Sémon



#### Kristjan Haule

# Finite T phase diagram

## Superconductivity PRL 2012



## Unified phase diagram







#### Giovanni Sordi

## Cuprates (doping driven transition)





#### Patrick Sémon





#### SC vs pseudogap



#### Nodal gap



Pushp, Yazdani Science 26 June 2009: Vol. 324 no. 5935 pp. 1689-1693



#### Tpair



ARPES Bi2212

Kondo, Takeshi, et al. Kaminski Nature Physics **2011**, *7*, 21-25





Patrick M. Rourke, et al. Hussey Nature Physics 7, 455–458 (2011)



#### Giant proximity effect



Figure 6 | Depth profile of the local field at different temperatures. The

## Actual T<sub>c</sub> in underdoped

#### • Quantum and classical phase fluctuations

- V. J. Emery and S. A. Kivelson, Phys. Rev. Lett. 74, 3253 (1995).
- V. J. Emery and S. A. Kivelson, Nature **374**, 474 (1995).
- D. Podolsky, S. Raghu, and A. Vishwanath, Phys. Rev. Lett. 99, 117004 (2007).
- Z. Tesanovic, Nat Phys 4, 408 (2008).

#### • Magnitude fluctuations

- I. Ussishkin, S. L. Sondhi, and D. A. Huse, Phys. Rev. Lett. 89, 287001 (2002).

#### • Competing order

 E. Fradkin, S. A. Kivelson, M. J. Lawler, J. P. Eisenstein, and A. P. Mackenzie, Annual Review of Condensed Matter Physics 1, 153 (2010).

#### • Disorder

- F. Rullier-Albenque, H. Alloul, F. Balakirev, and C. Proust, EPL (Europhysics Letters) 81, 37008 (2008).
- H. Alloul, J. Bobro, M. Gabay, and P. J. Hirschfeld, Rev. Mod. Phys. 81, 45 (2009).



#### Larger clusters

- Is there a minimal size cluster where T<sub>c</sub> 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:1304.6406



#### Gaussian amplitude fluctuations in Eu-LSCO



Chang, Doiron-Leyraud et al.



#### Phase fluctuations and disorder?

#### Monolayer LSCO, field doped



A. T. Bollinger et al. & I. Božović, Nature 472, 458–460

Figure 2 | Superconductor-insulator transition driven by electric field. a, Temperature dependence of normalized resistance  $r = R_{\Box}(x,T)/R_Q$  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  $R_{\Box}(x_{\odot}T) = R_Q = 6.45$  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  $r_x(T)$  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  $R_c = 6.45 \pm 0.10 \,\mathrm{k\Omega}$ . c, Scaling of the same data with respect to a single variable  $u = |x - x_c| T^{-1/zv}$ , with zv = 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  $T^{-2/3}$ . For 4.3 K < T < 10 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



F. Rullier-Albenque, H. Alloul, and G.Rikken, Phys. Rev. B **84**, 014522 (2011).



# Superconductivity in underdoped vs BCS



#### Summary



#### Summary



## Rutherford



- 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



## Conclusions

- Tools for Hubbard model,
  - weak to intermediate coupling
  - Strong coupling
- The influence of Mott Physics extends way beyond half-filling



#### Main collaborators



Giovanni Sordi







David Sénéchal



#### Bumsoo Kyung



Patrick Sémon



Dominic Bergeron



Sarma Kancharla



Marcello Civelli





Massimo Capone





#### André-Marie Tremblay





#### Le regroupement québécois sur les matériaux de pointe



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CREATING KNOWLEDGE DRIVING INNOVATION BUILDING THE DIGITAL ECONOMY

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CRÉER LE SAVOIR ALIMENTER L'INNOVATION BÂTIR L'ÉCONOMIE NUMÉRIQUE Calcul Québec




