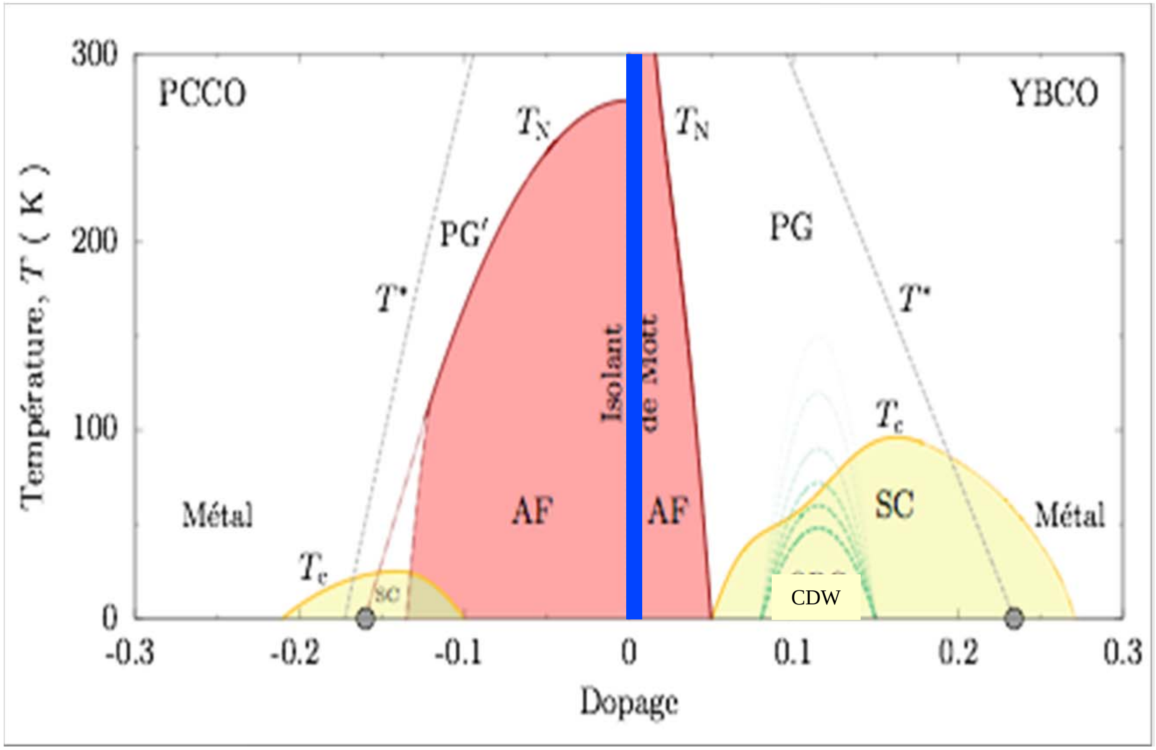
d-wave superconductivity in the one-band Hubbard model, the Cluster Dynamical-Mean-Field point of view (mostly)

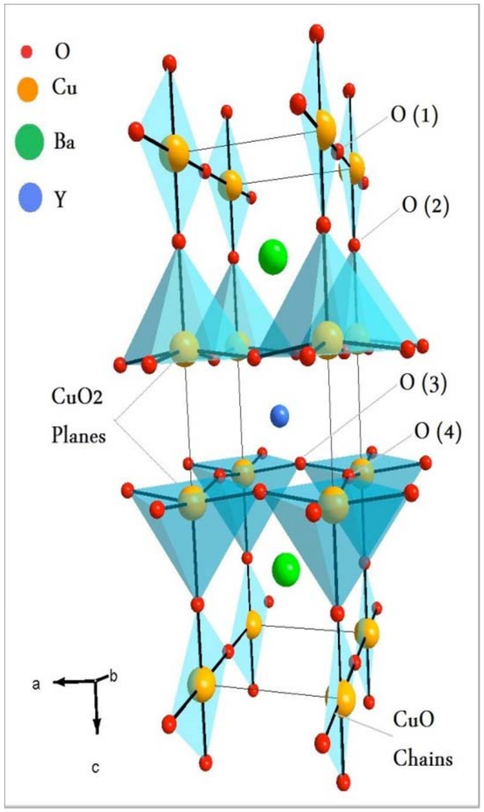
A.-M. Tremblay

Strongly correlated systems: from models to materials
11 January 2014

Our road map

Thèse de Francis Laliberté,
Université de Sherbrooke





Many methods show d-wave superconductivity

For references, September 2013 Julich summer school

Strongly Correlated Superconductivity

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

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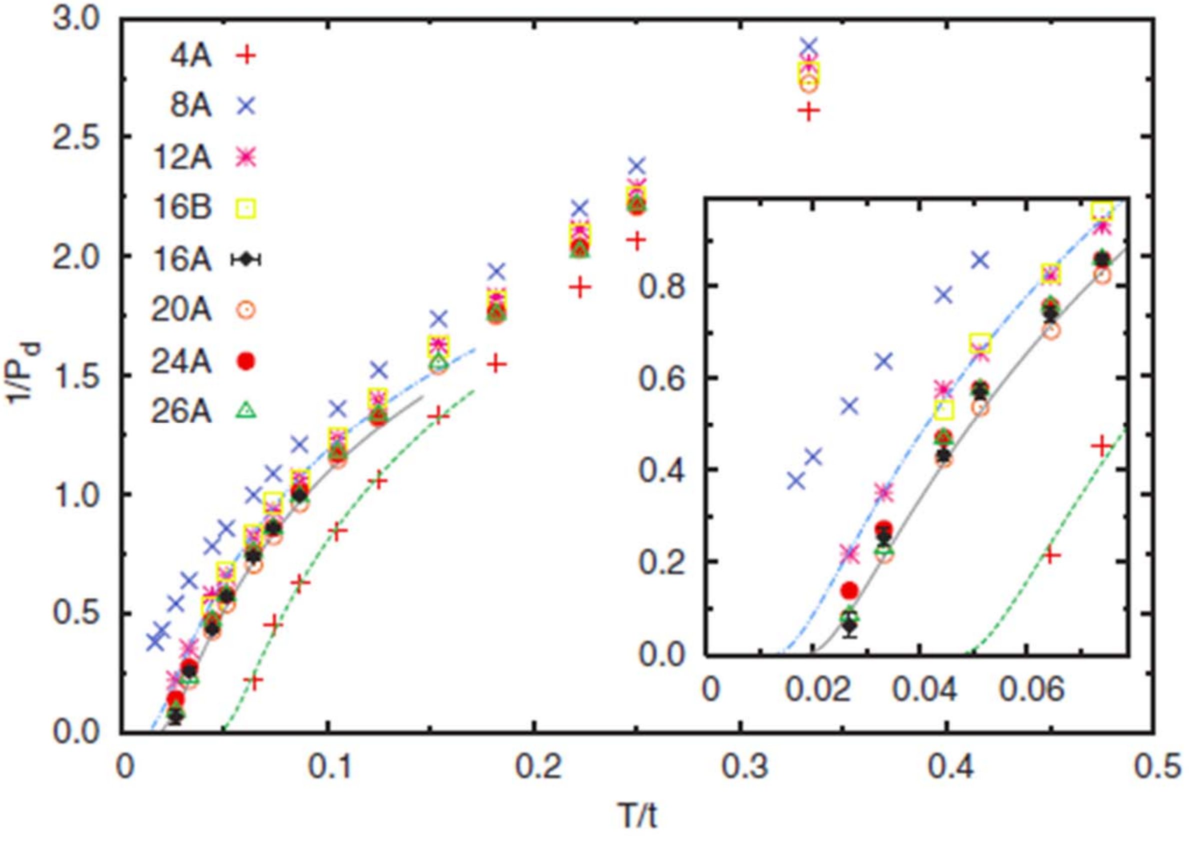
DCA: There is d-wave superconductivity

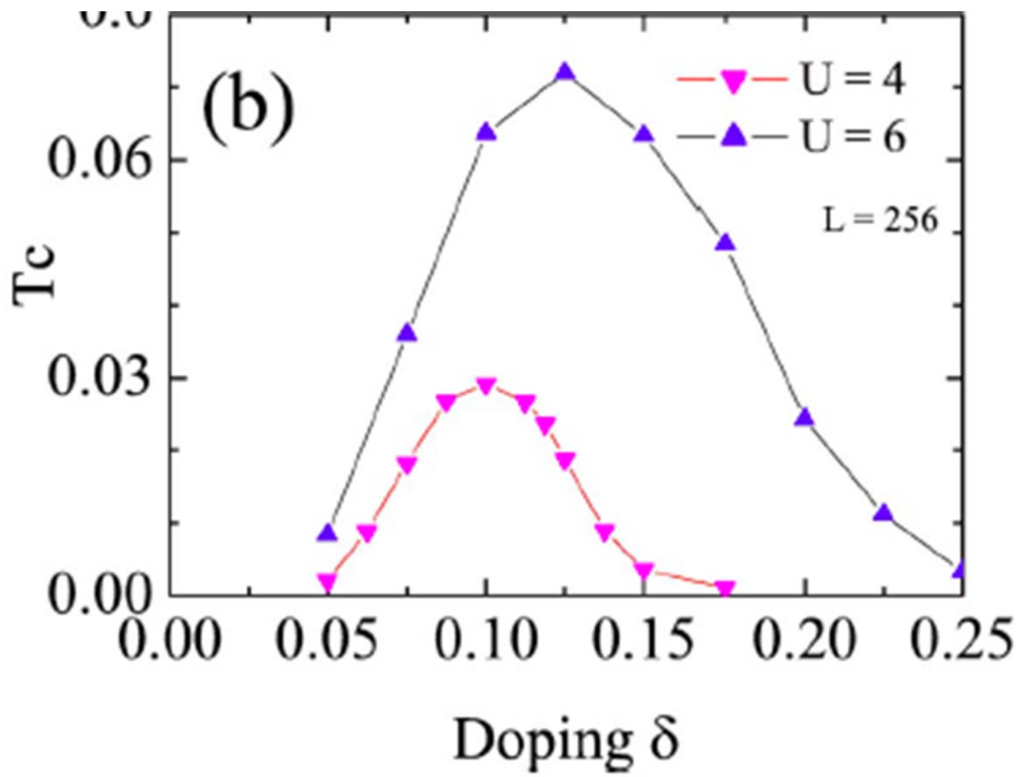


PRL 95, 237001 (2005) PHYSICAL REVIEW LETTERS week ending 2 DECEMBER 2005

Systematic Study of *d*-Wave Superconductivity in the 2D Repulsive Hubbard Model

T. A. Maier,[1] M. Jarrell,[2] T. C. Schulthess,[1] P. R. C. Kent,[3] and J. B. White[1]

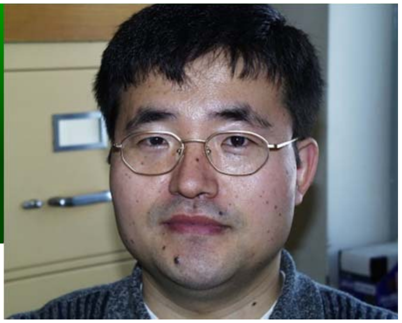
Tc from TPSC



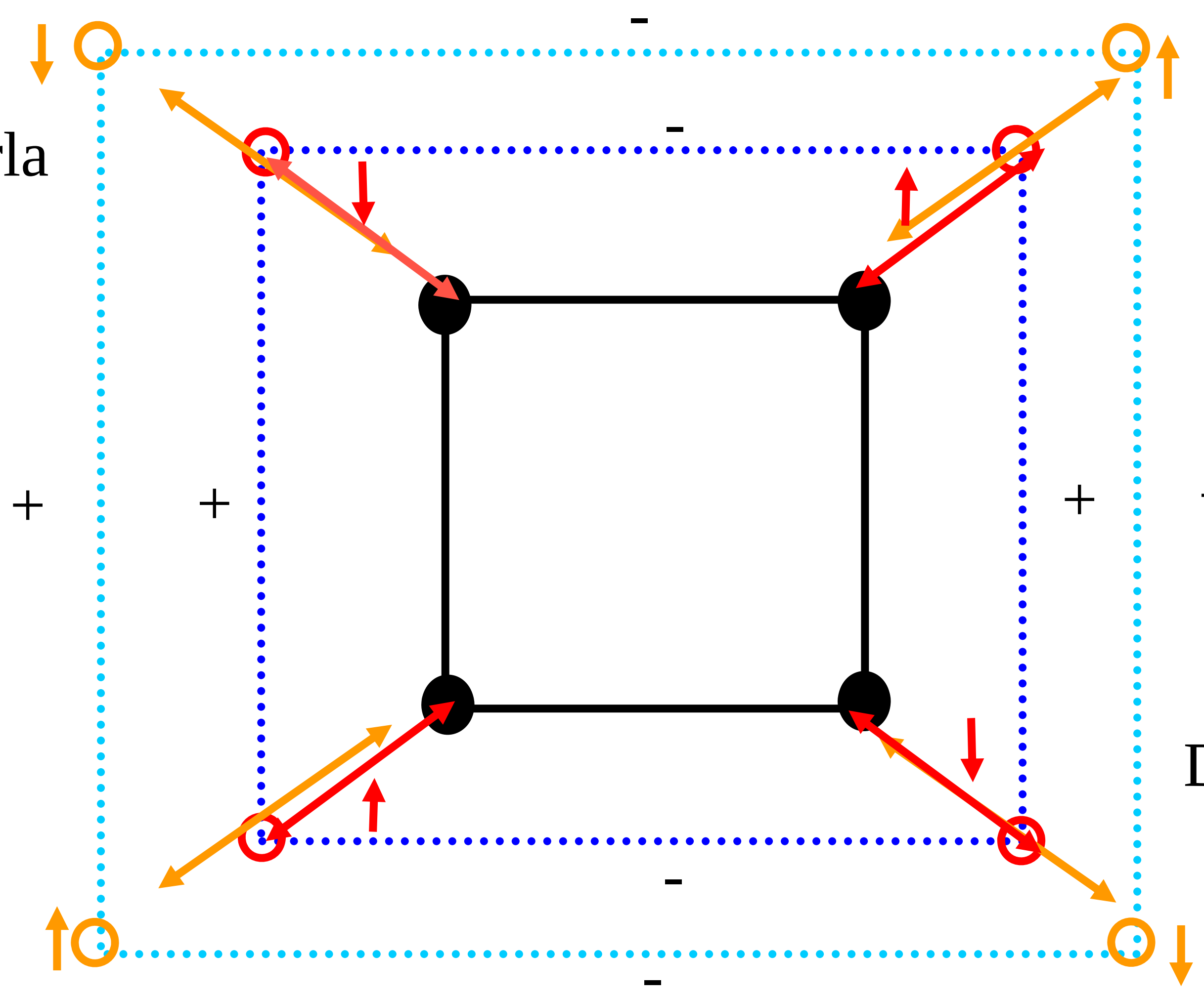
Kyung et al. PRB **68** (2003)

Competition AFM-dSC

S. Kancharla



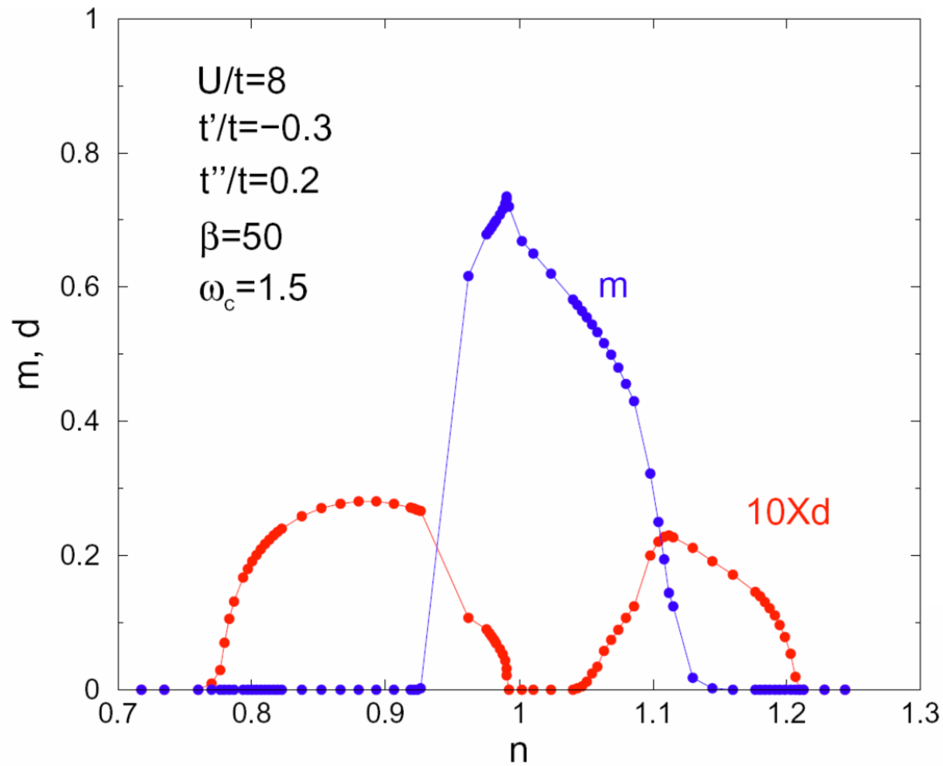
B. Kyung



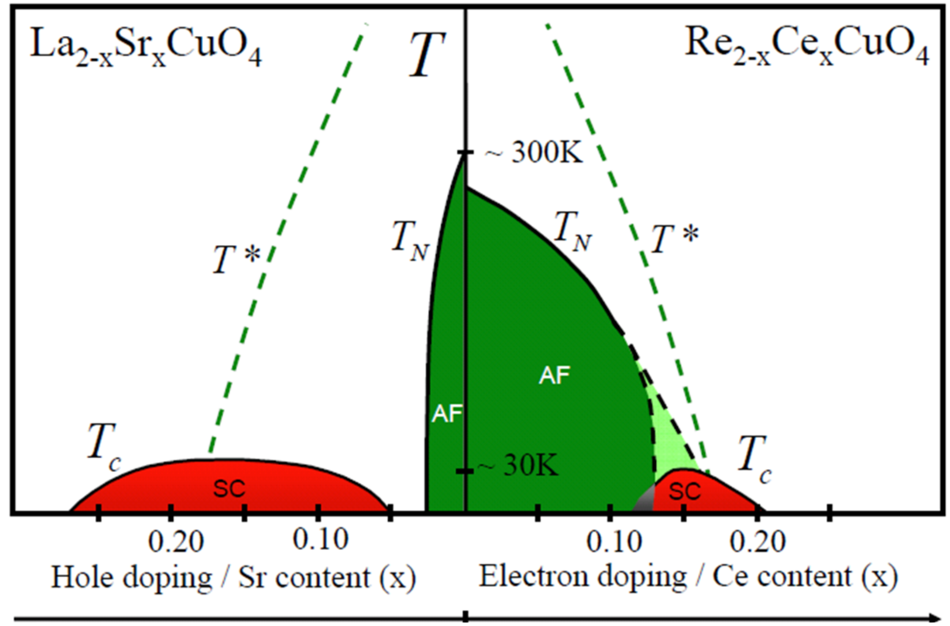
David Sénéchal

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

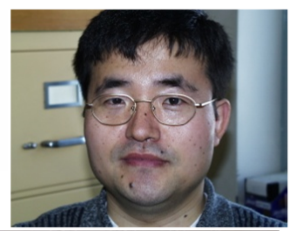
CDMFT global phase diagram



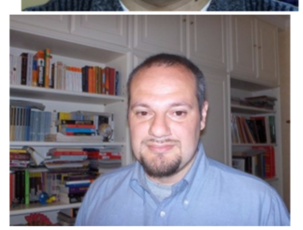
Kancharla, Kyung, Civelli, Sénéchal, Kotliar AMST Phys. Rev. B (2008)
AND Capone, Kotliar PRL (2006)



Armitage, Fournier, Greene, RMP (2009)





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The Hubbard model captures much of the physics

$$\hat{\mathcal{H}}_{Hubbard} = -t \sum_{\langle i,j \rangle \, \sigma} \left(\hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + c.h \right) + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} - \mu \sum_{i \, \sigma} \hat{n}_{i\sigma}$$

- Mott insulator
- Antiferromagnetism
- Superconductivity
- Pseudogap
- Spectral weight transfer
- Asymmetric DOS

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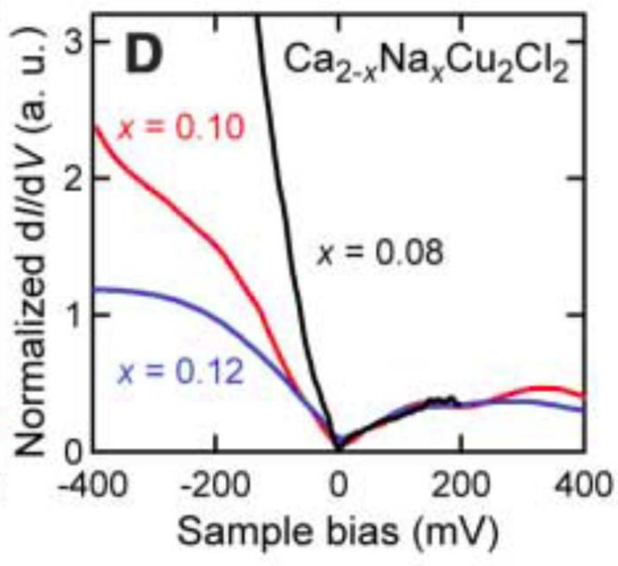
h-doped are strongly correlated: evidence from the normal state

Density of states (STM)



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

e-doped cuprates

Less strongly correlated: evidence from the normal state (MIR, pseudogap)

Sénéchal, A.-M.S. T. PRL (2004)

C. Weber, K. Haule, and G. Kotliar, Nature Physics 6, 574 (2010)

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3. Weakly and strongly correlated antiferromagnets

What is a phase?

« 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
  - Often hard to « derive » from first principles (fractionalization - gauge theories)

Antiferromagnetic phase: emergent properties

- Some broken symmetries
    - Time reversal symmetry
    - Translation by one lattice spacing
    - Unbroken Time-reversal times translation by lattice vector **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

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3. Strong vs weak correlations for an antiferromagnet

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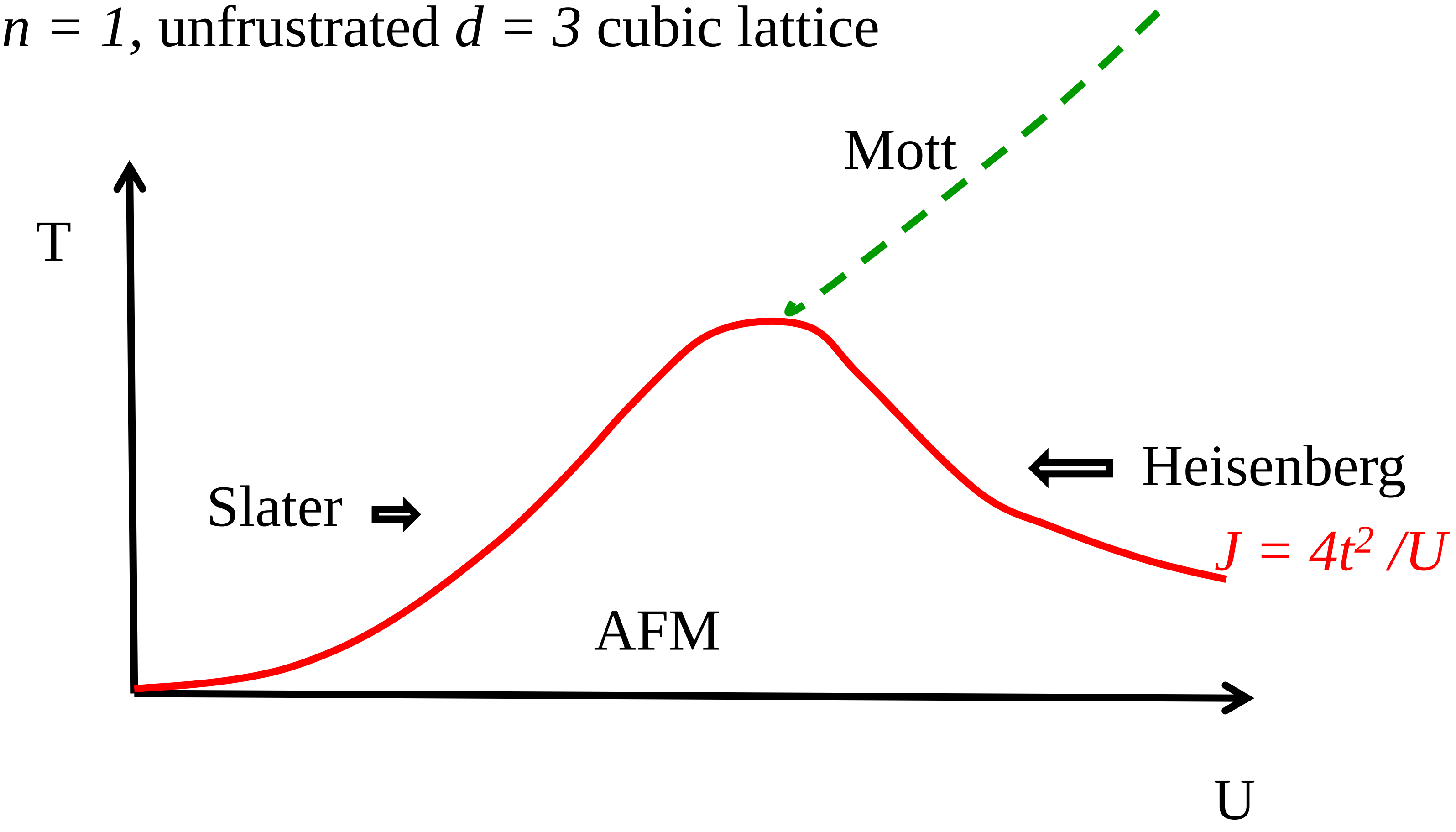
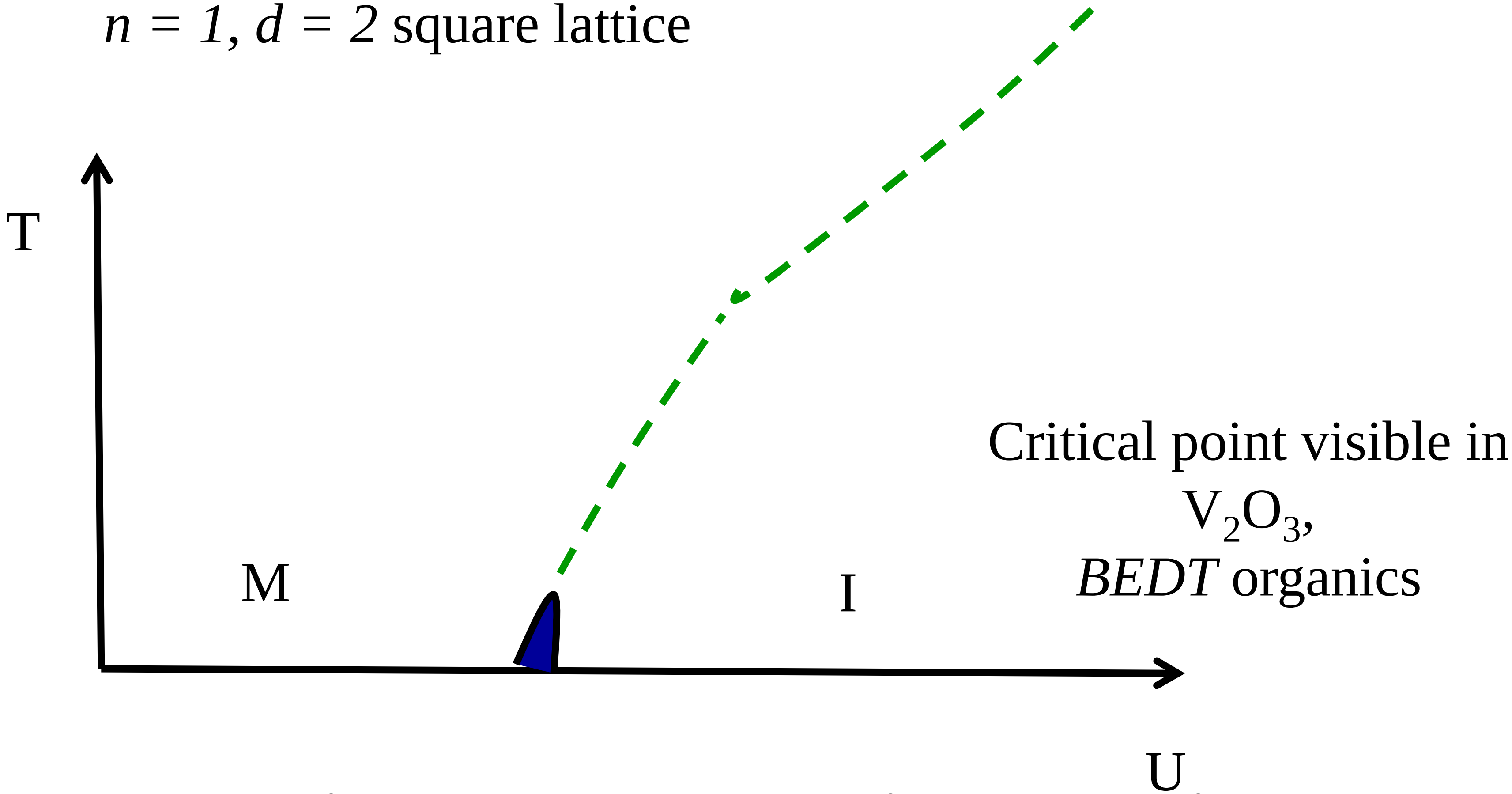
Local moment and Mott transition

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



Local moment and Mott transition

n = 1, *d = 2* square lattice



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

4. Weakly and strongly correlated superconductivity

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 κ at low *T*
  - – Goldstone modes (+Higgs)

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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

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4. Weakly and strongly correlated superconductivity

Weakly correlated case

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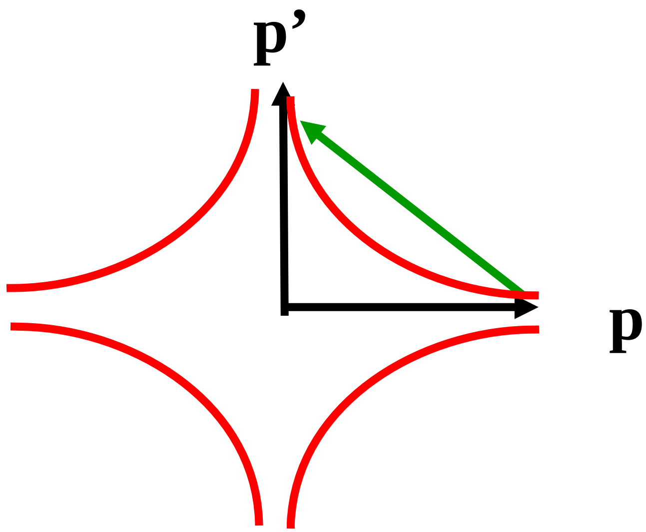
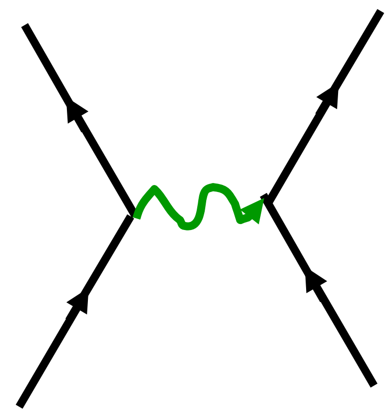
Cartoon « BCS » weak-coupling picture

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





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).

Exchange of spin waves?
Kohn-Luttinger
T_c with pressure

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

Results from TPSC

Satisfies Mermin-Wagner

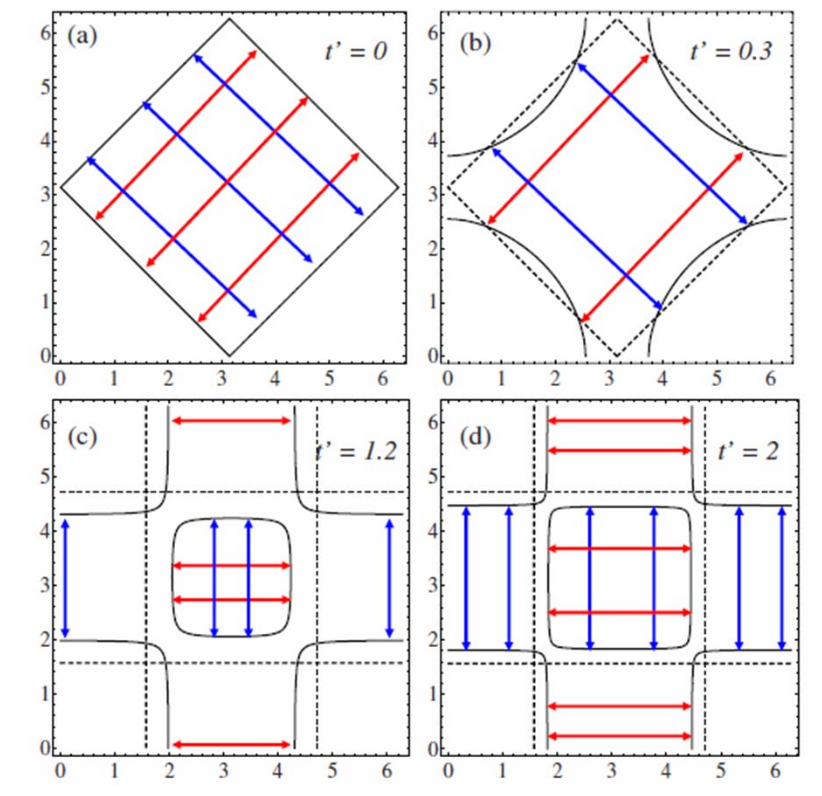
Conservation laws

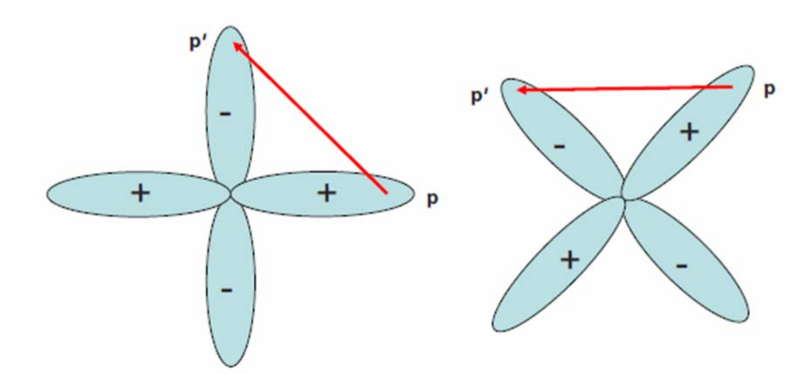
Pauli principle

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

A.-M.S.T. Review, Mancini, 2011

Relation between symmetry and wave vector of AFM fluctuations





Hassan et al. PRB 2008

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T_c depends on t'

Syed Hassan

ξ_{AFM}
~ 10 at optimal Tc

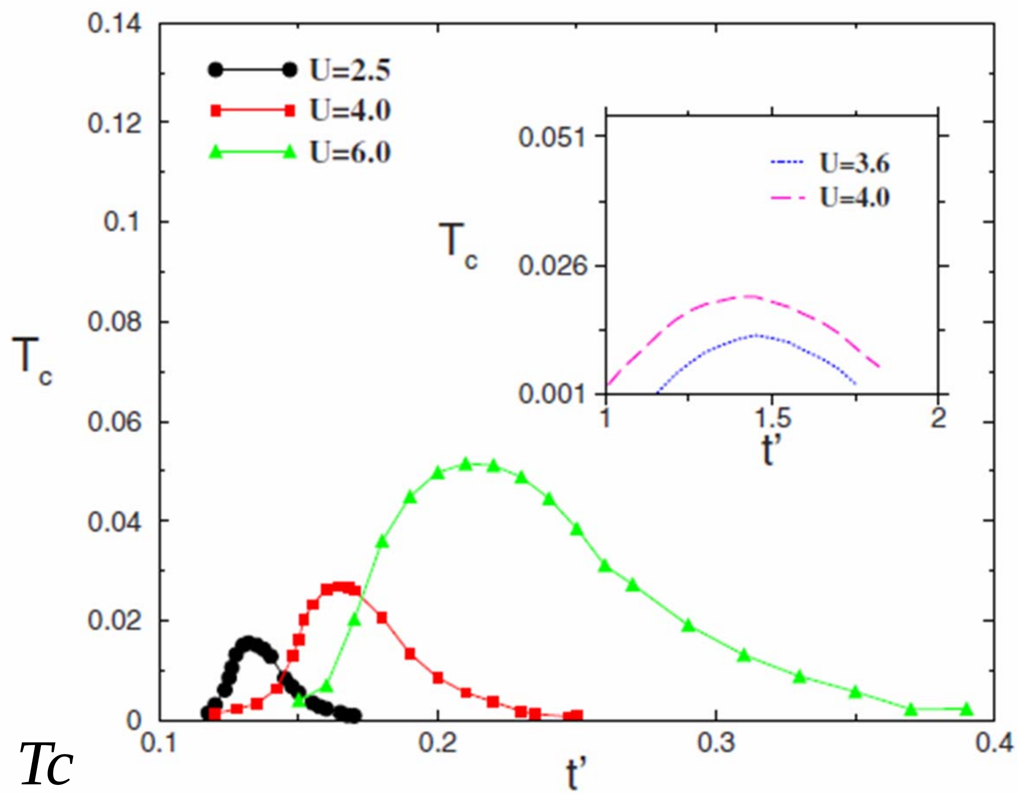

FIG. 5. (Color online) The $d_{x^2-y^2}$ superconducting critical temperature T_c as a function of t' at U=2.5, 3, and 4 for n=1. The inset shows the d_{xy} superconducting critical temperature T_c as a function of t' for U=3.6 and 4.

Bumsoo Kyung

Bahman Davoudi

Hassan et al. PRB 2008

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4. Weakly and strongly correlated superconductivity

Strongly correlated point of view

A cartoon strong coupling picture

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

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

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

Pitaevskii Brückner:

Pair state orthogonal to repulsive core of Coulomb interaction

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

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

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5. High-temperature superconductors
the view from dynamical mean-field theory

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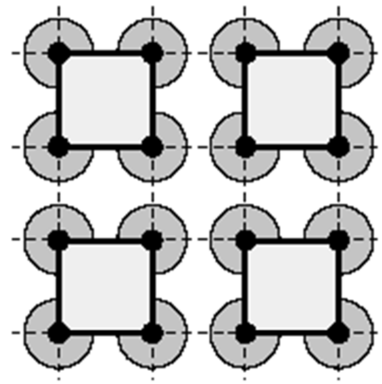
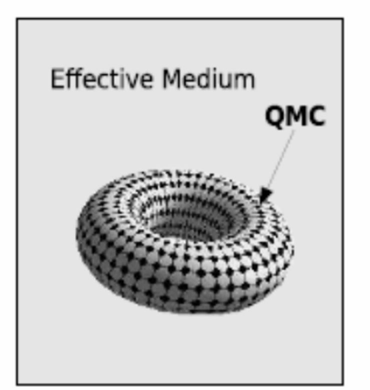
2d Hubbard: Quantum cluster method

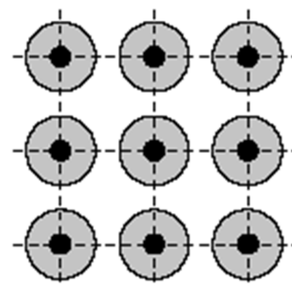
C-DMFT





DCA

DMFT



Hettler …Jarrell…Krishnamurty PRB **58** (1998)
Kotliar et al. PRL **87** (2001)
M. Potthoff *et al.* PRL **91,** 206402 (2003).

REVIEWS
Maier, Jarrell et al., RMP. (2005)
Kotliar *et al.* RMP (2006)
AMST *et al.* LTP (2006)

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+ and -

- 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

$T = 0$ phase diagram: superconductivity

Mechanism at strong coupling

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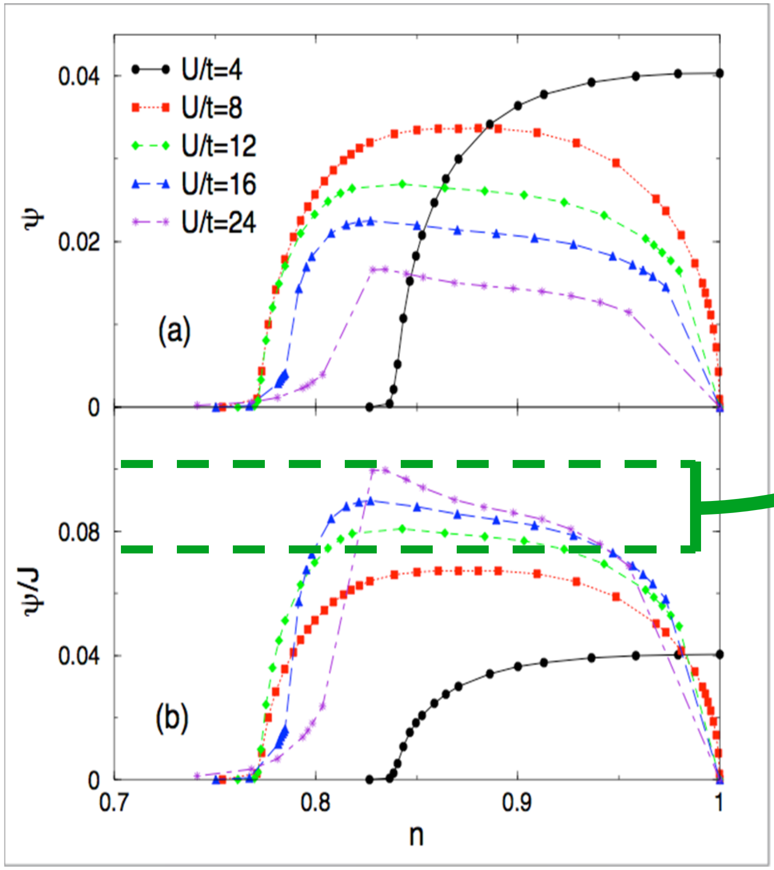
Strength of pairing



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

The superconducting order parameter scales like *J*

The glue

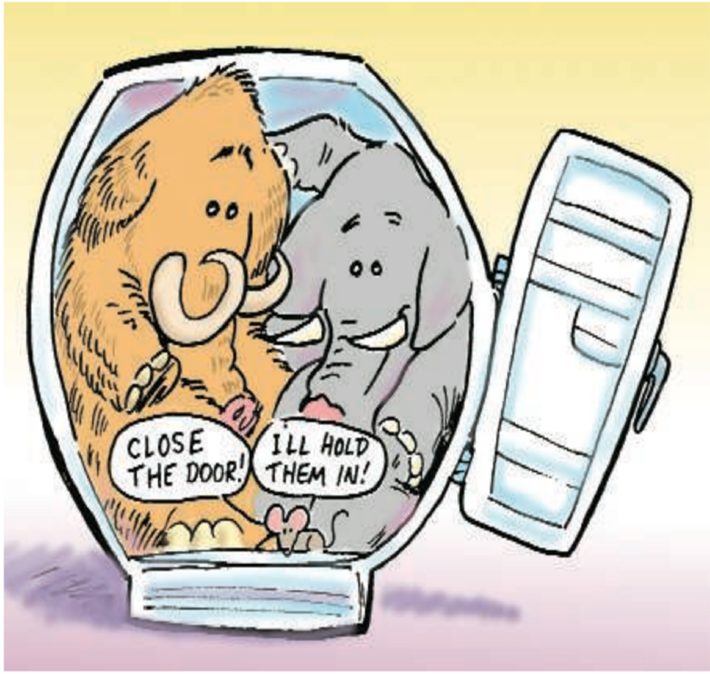
Raising the question

Is There Glue in Cuprate Superconductors?
Philip W. Anderson
Science **316**, 1705 (2007);
DOI: 10.1126/science.1140970

Is There Glue in Cuprate Superconductors?

Philip W. Anderson

Many theories about electron pairing in cuprate superconductors may be on the wrong track.



"We have a mammoth and an elephant in our refrigerator—do we care much if there is also a mouse?"

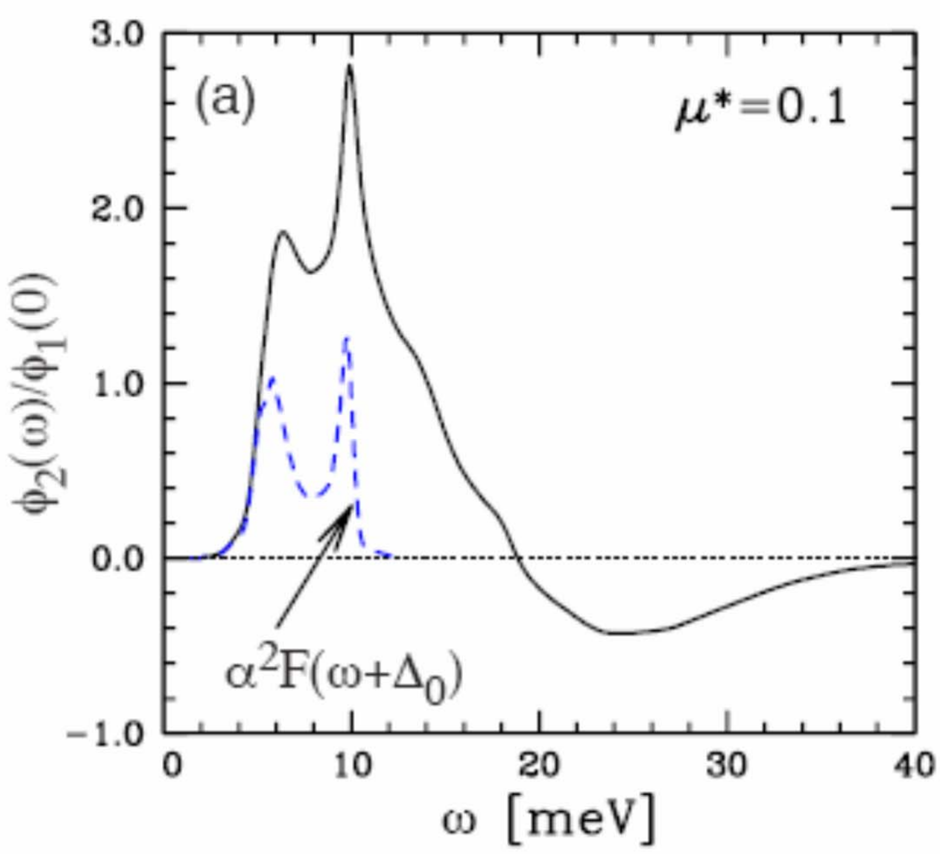
Retardation

$$V^{eff}_{él-ph}(\vec{q},\omega) = \frac{e^2}{4\pi\varepsilon_0(q^2+k_{TF}^2)}\left[1+\frac{\omega_{ph}^2(\vec{q})}{\omega^2-\omega_{ph}^2(\vec{q})}\right]$$

Université de Sherbrooke

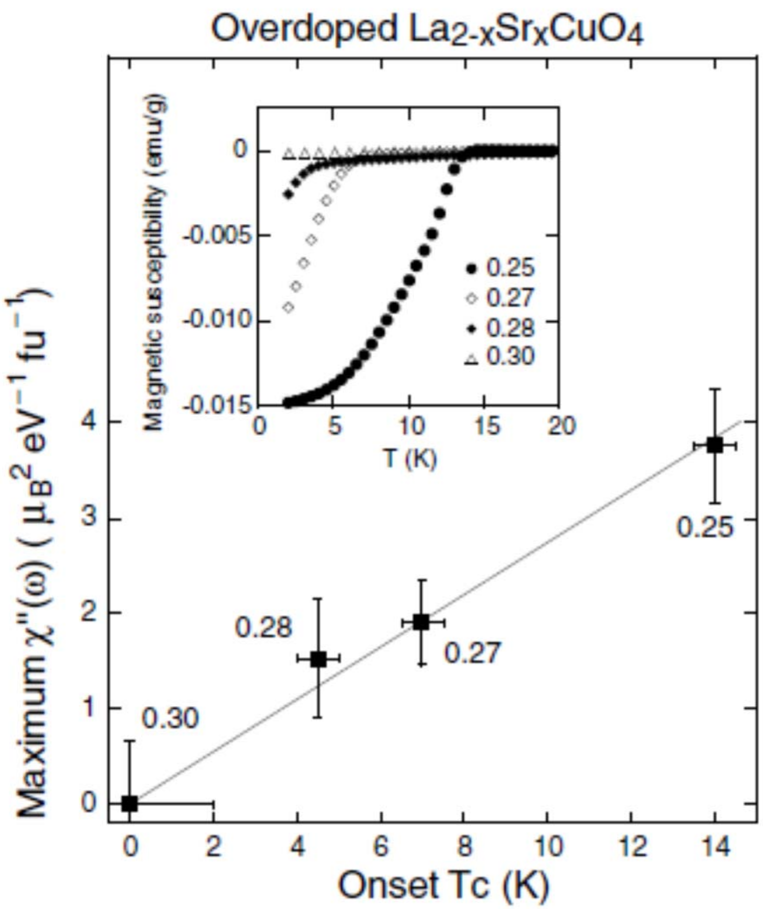
Im Σ_{an} and electron-phonon in Pb

Maier, Poilblanc, Scalapino, PRL (2008)

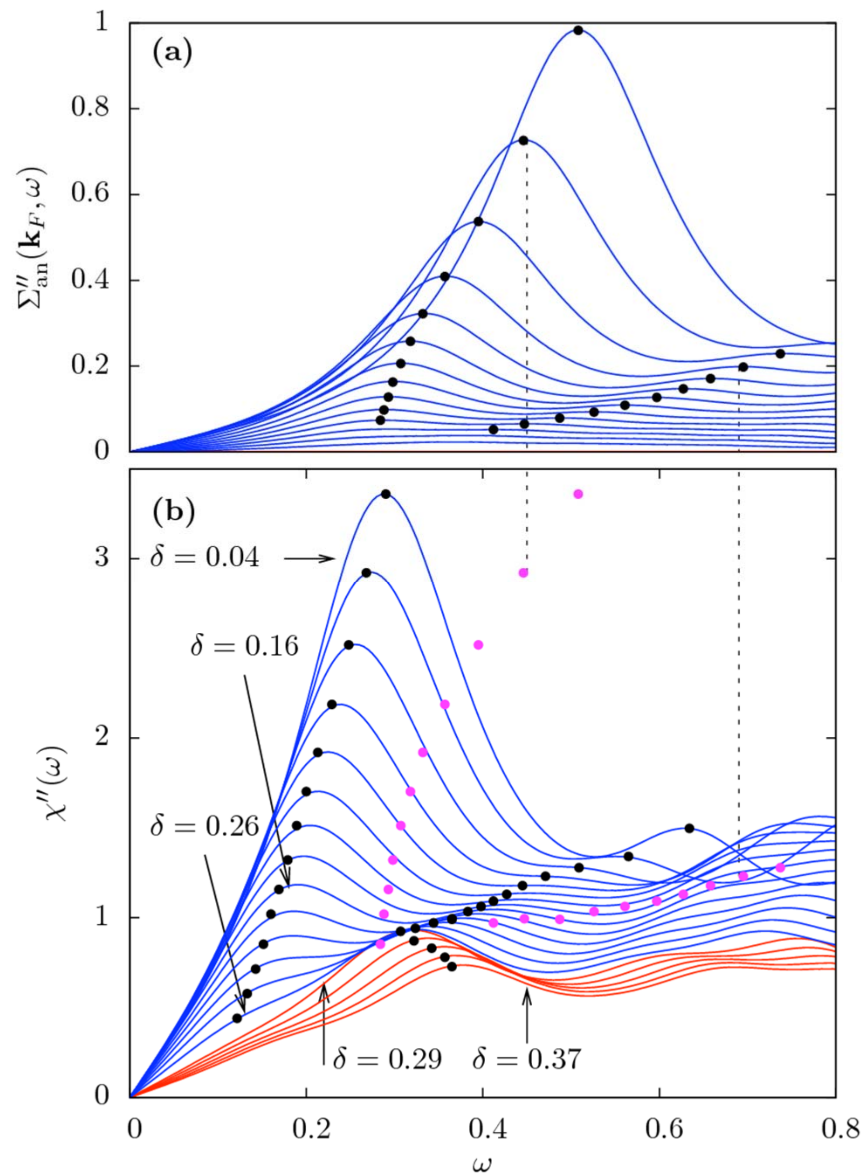


The glue

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



Wakimoto … Birgeneau PRL (2004)



The glue and neutrons

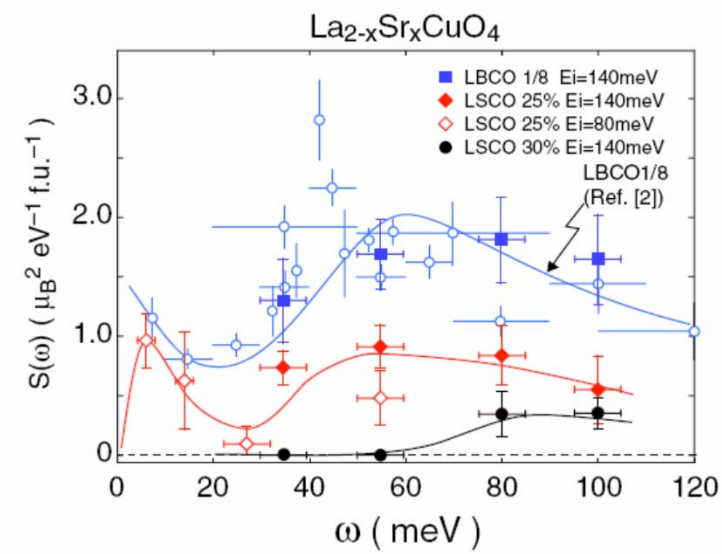
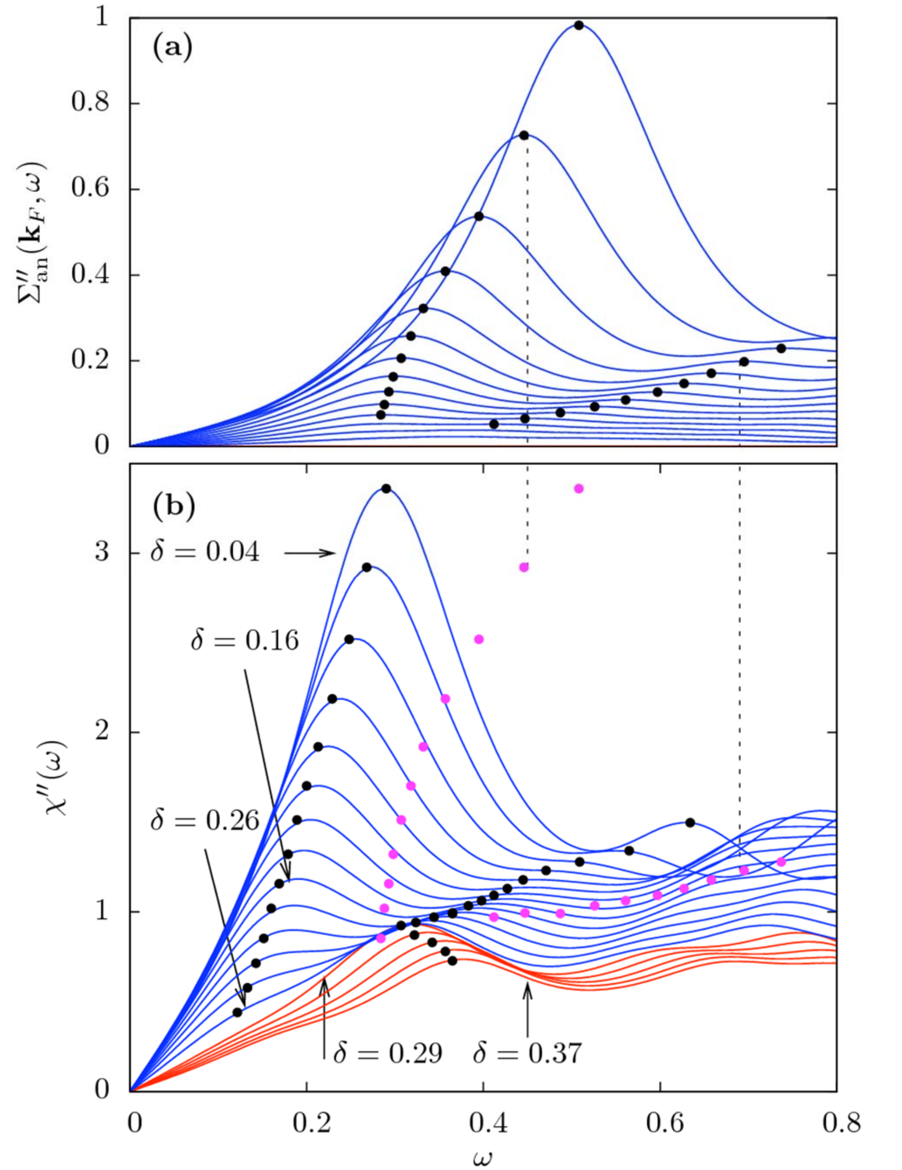


FIG. 3 (color online). **Q**-integrated dynamic structure factor $S(\omega)$ which is derived from the wide-H integrated profiles for LBCO 1/8 (squares), LSCO $x = 0.25$ (diamonds; filled for E_i = 140 meV, open for E_i = 80 meV), and $x = 0.30$ (filled circles) plotted over $S(\omega)$ for LBCO 1/8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



Wakimoto … Birgeneau PRL (2007);
PRL (2004)

Frequencies important for pairing

Bumsoo Kyung
David Sénéchal

Anomalous Green function

$$[\mathcal{F}_{an}(t)]_{lm} = -i\theta(t)\left\langle\{\hat{c}_{l\uparrow}(t), \hat{c}_{m\downarrow}(0)\}\right\rangle_{\mathcal{H}_{AIM}}$$

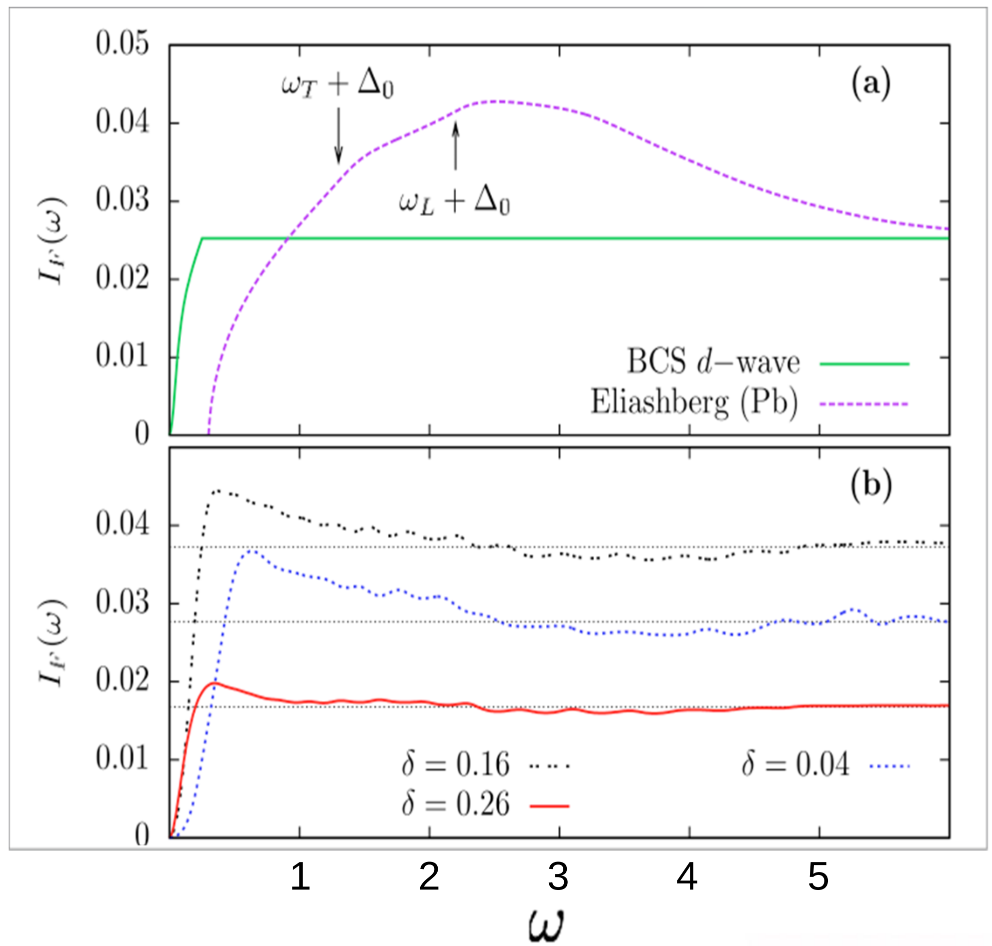
Anomalous spectral function

$$[\mathcal{A}_{an}(\omega)]_{lm} = -\frac{1}{\pi}\,\mathrm{Im}\,[\mathcal{F}_{an}(\omega)]_{lm}$$

Cumulative order parameter:

$$I_{\mathcal{F}}(\omega) = -\int_0^{\omega}\frac{\mathrm{d}\omega'}{\pi}\,\mathrm{Im}\,[\mathcal{F}_{an}(\omega')]_{lm}$$

$$I_{\mathcal{F}}(\omega) \xrightarrow[\omega\to+\infty]{} \langle\hat{c}_{l\uparrow}\hat{c}_{m\downarrow}\rangle_{\mathcal{H}_{AIM}}$$



Resilience to near-neighbor repulsion *V*

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

$YBa_2Cu_3O_7$: $t = 1$ $t' = -0.3$ $t'' = 0.2$

We expect superconductivity to disappear when:

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

$V > J$ **In mean-field strongly correlated case**

In cuprates:

$V = 400\,\mathrm{meV}$

$J = 130\,\mathrm{meV}$

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

S. Onari, R. Arita, K. Kuroki et H. Aoki, PRB **70**, 094523 (2004)
S. Raghu, E. Berg, A. V. Chubukov et S. A. Kivelson, PRB **85**, 024516 (2012)
S. Sorella, et al. Phys. Rev. Lett. 88, 117002 (2002)

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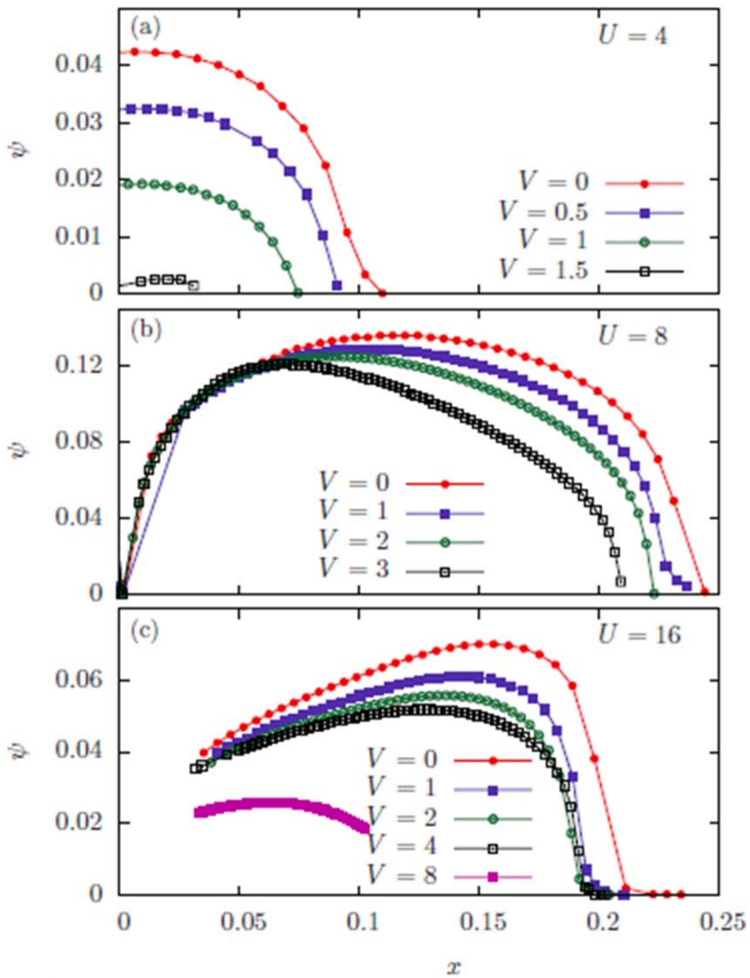
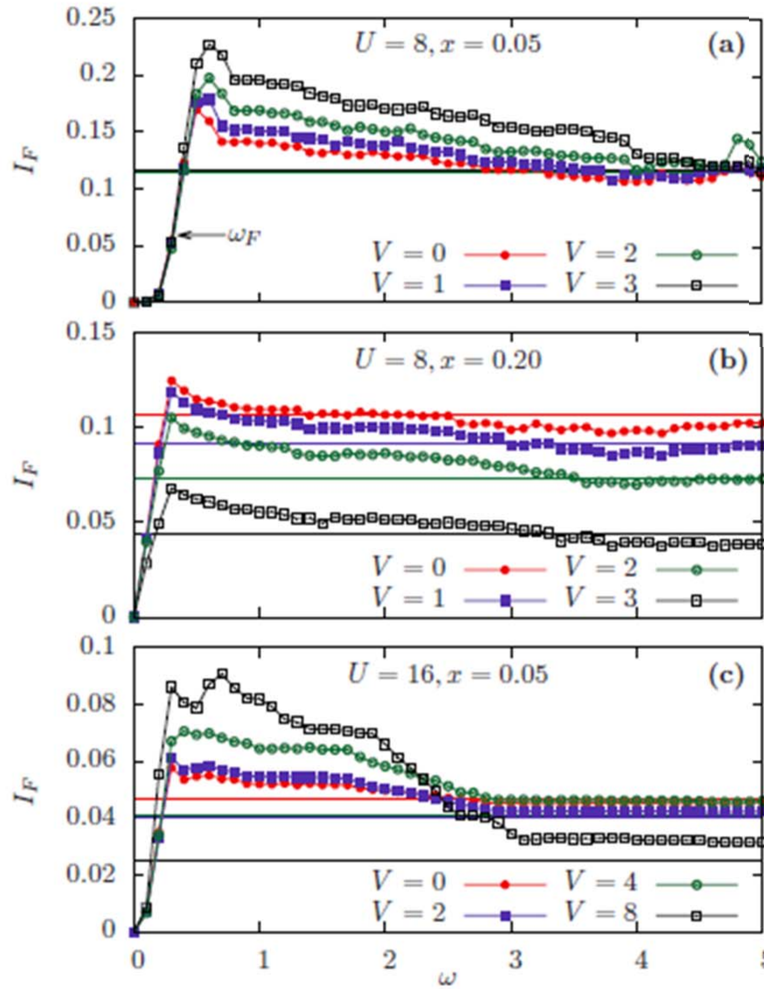
Resilience to near-neighbor repulsion

David Sénéchal

Alexandre Day

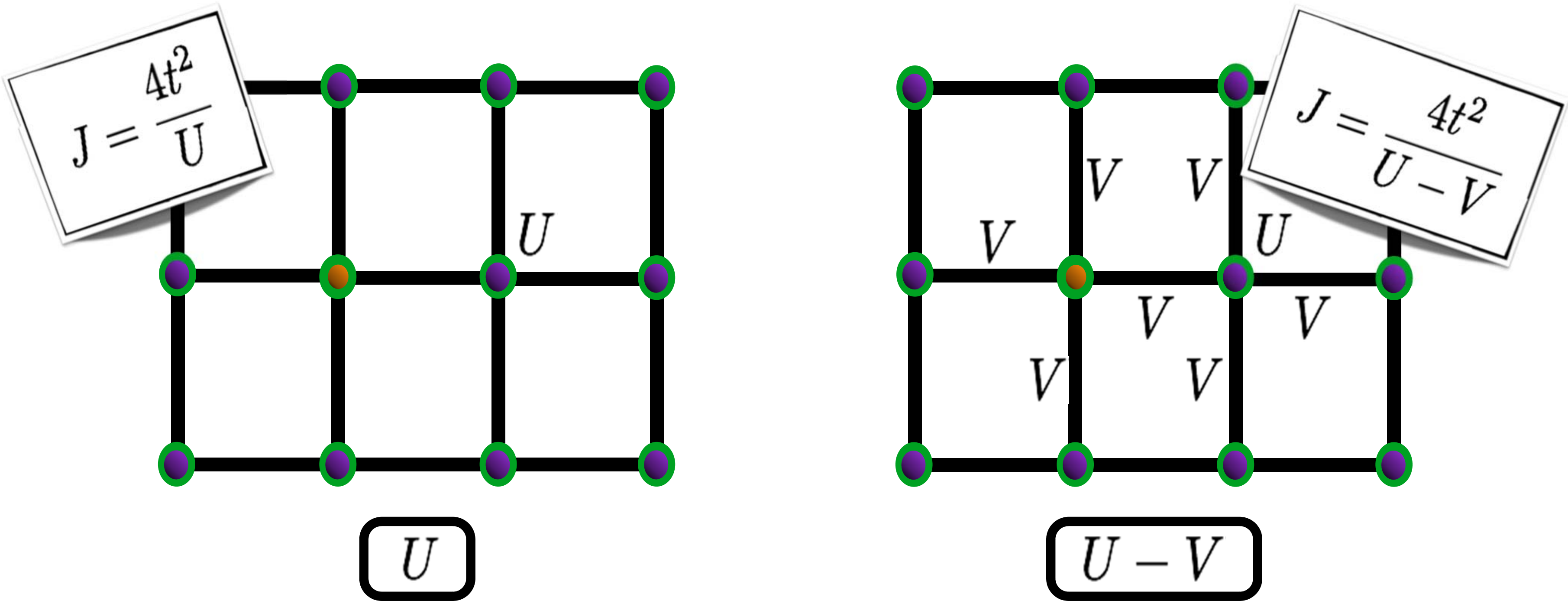
Vincent Bouliane





Sénéchal, Day, Bouliane, AMST PRB **87**, 075123 (2013)

V also increases J

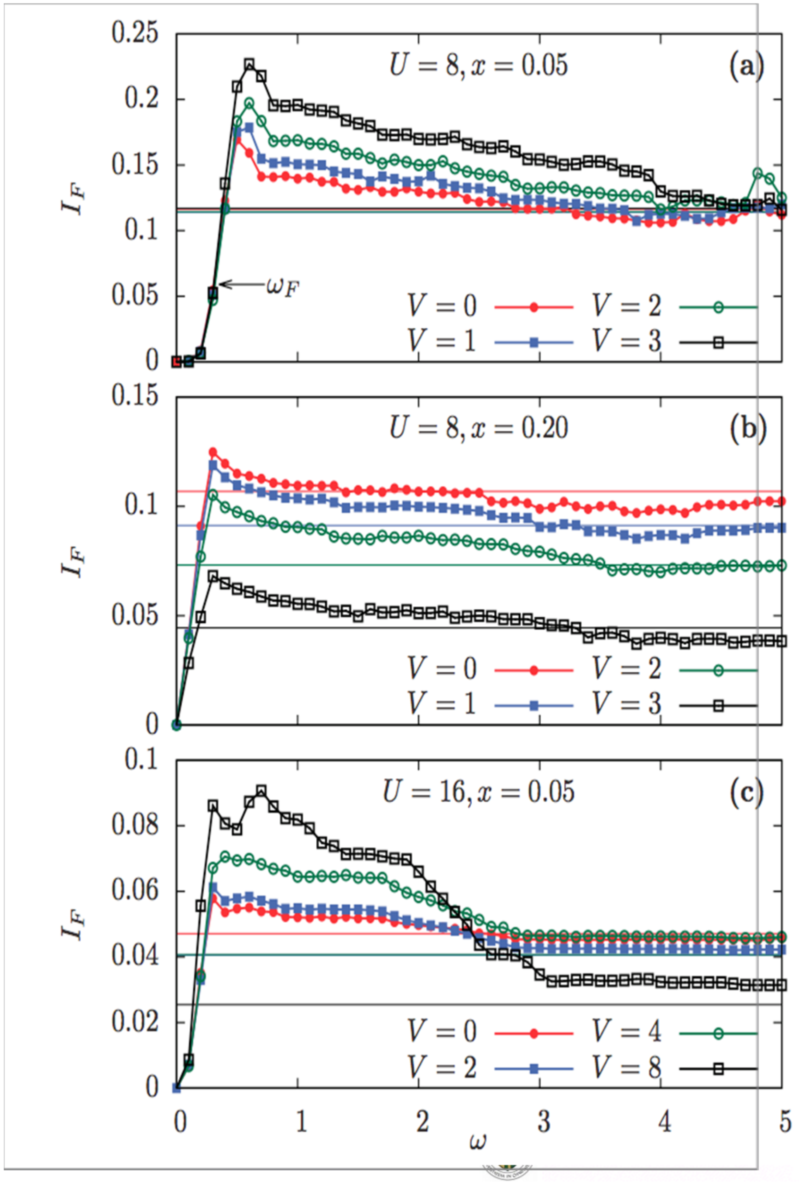


Binding aspects of V

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

***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



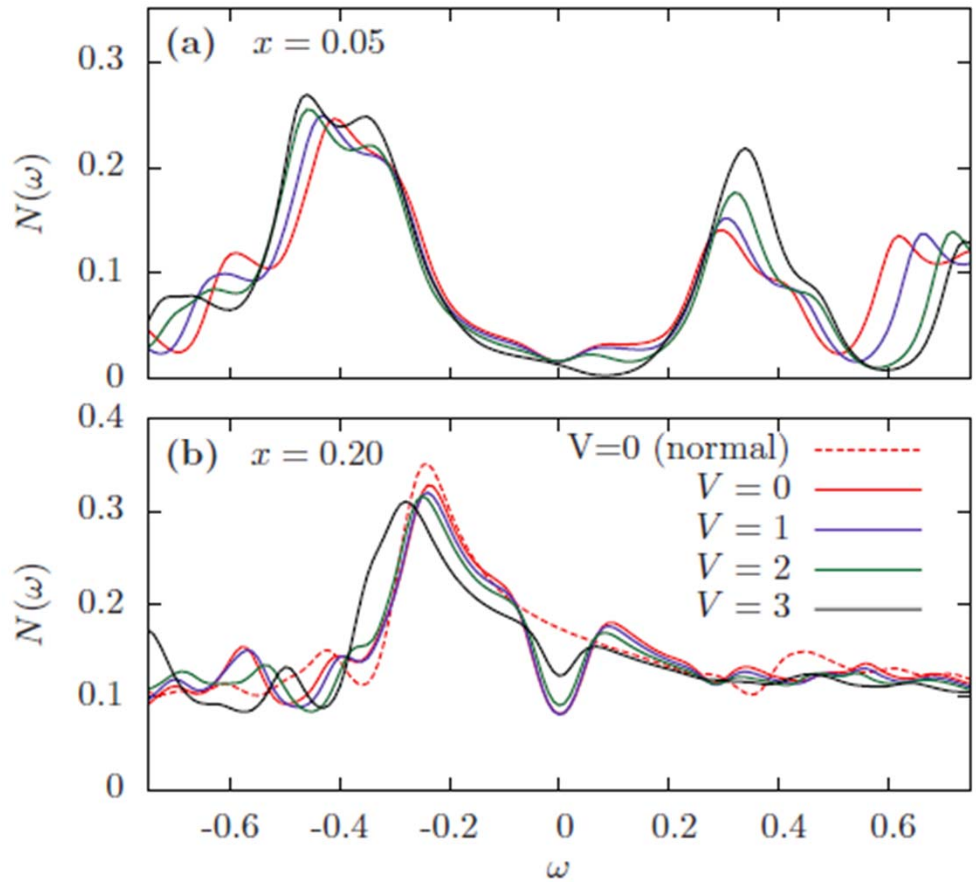
Resilience to near-neighbor repulsion

David Sénéchal

Alexandre Day

Vincent Bouliane

$U = 8t$



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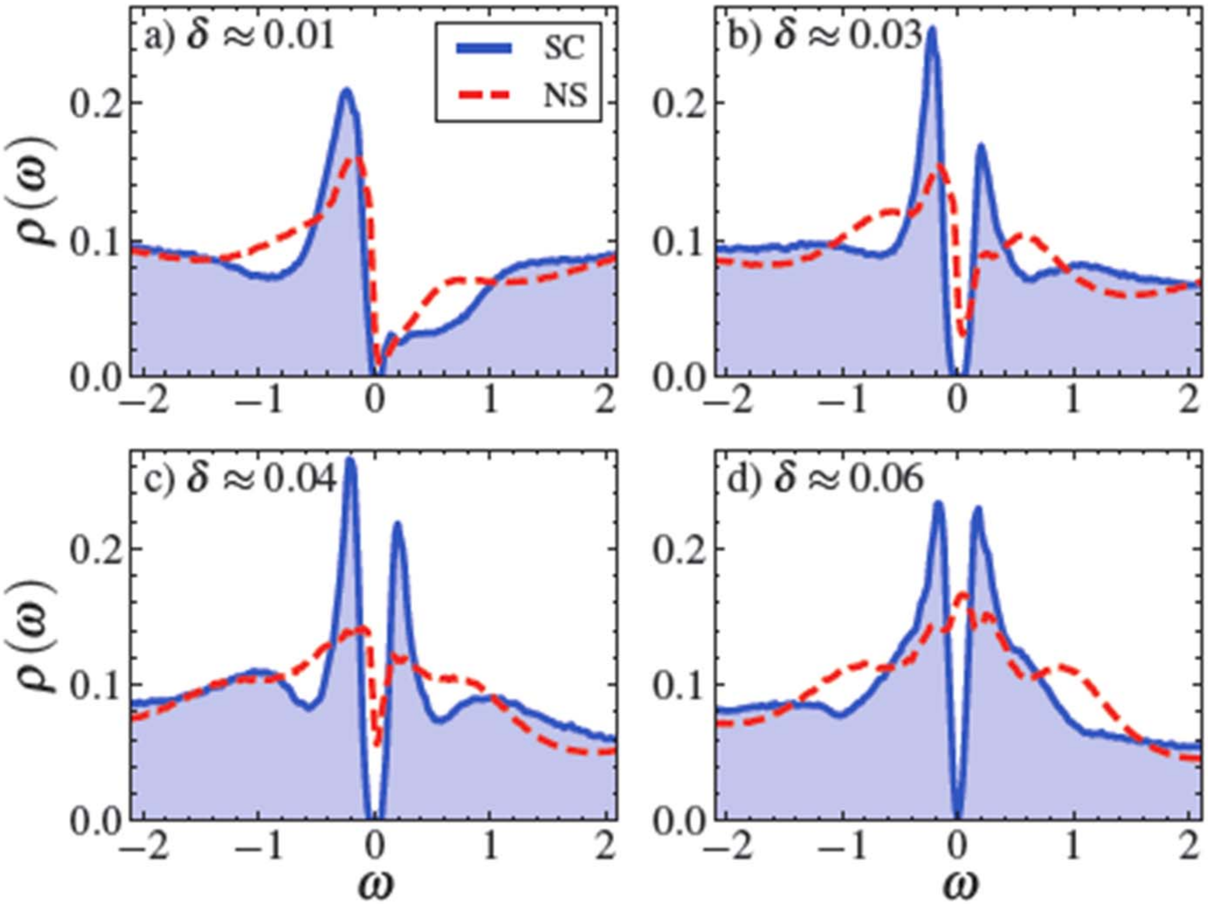
First-order transition leaves its mark



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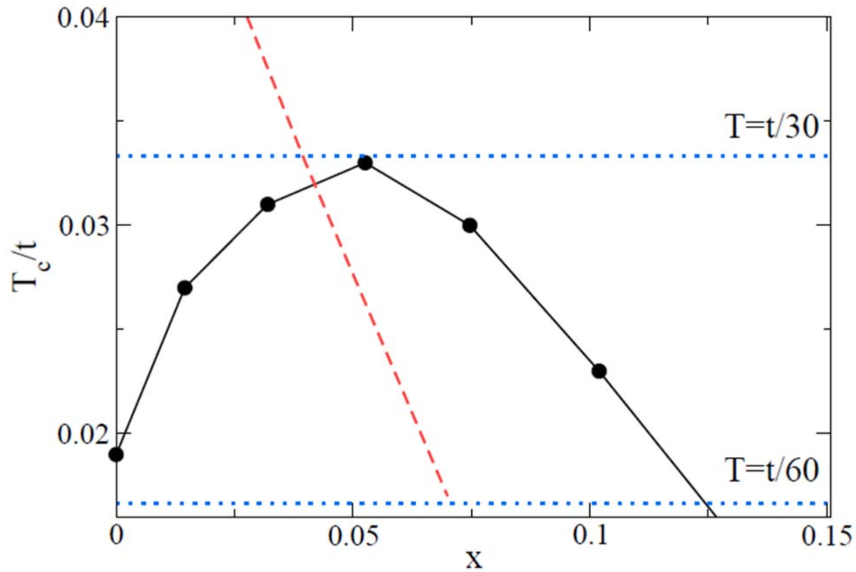
Larger cluster 8 site DCA



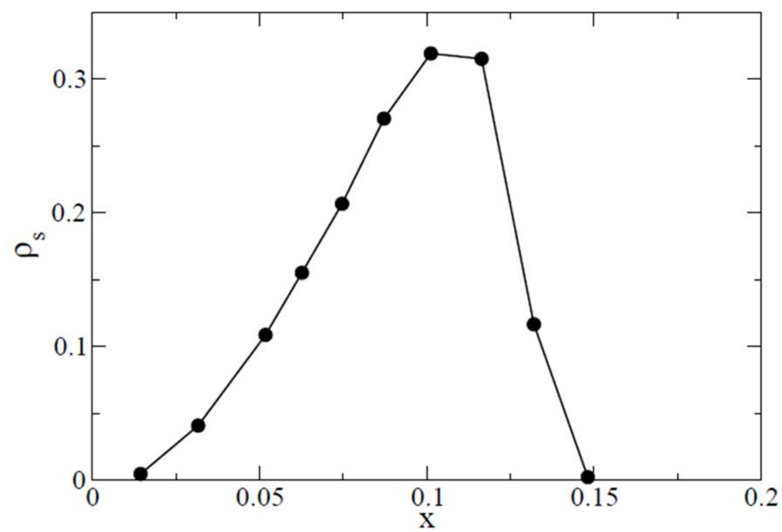


FIG. 8. Superfluid stiffness ρ_s determined in the superconducting state at $T = t/60$ from Eq. 15, as a function of doping.

Gull, Millis, arxiv.org:304.6406

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Summary

- Quantum cluster methods excellent tool to understand strongly correlated superconductivity (including strange metal)
  - 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

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

Main collaborators


Giovanni Sordi


Kristjan Haule


David Sénéchal


Bumsoo Kyung


Alexandre Day


Marcello Civelli


Syed Hassan


Vincent Bouliane


Patrick Sémon


Dominic Bergeron


Sarma Kancharla


Massimo Capone


Gabriel Kotliar

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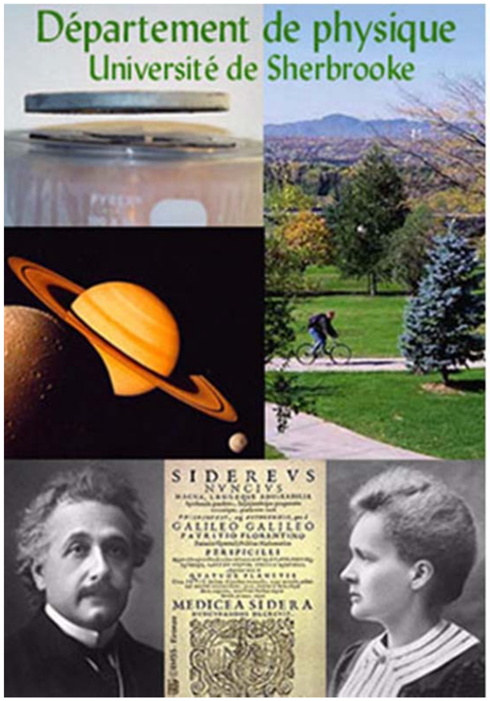

André-Marie Tremblay

CANADA RESEARCH CHAIRS
CHAIRES DE RECHERCHE DU CANADA

RQMP
Le regroupement québécois sur les matériaux de pointe

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High Performance Computing
CREATING KNOWLEDGE
DRIVING INNOVATION
BUILDING THE DIGITAL ECONOMY

Le calcul de haute performance
CRÉER LE SAVOIR
ALIMENTER L'INNOVATION
BÂTIR L'ÉCONOMIE NUMÉRIQUE

Calcul Québec

UNIVERSITÉ DE
SHERBROOKE

Merci

Thank you