Supraconductivité à haute température dans les cuprates et les organiques: Où en est-on?

André-Marie Tremblay

UNIVERSITÉ DE SHERBROOKE

Collège de France, 9, 16, 23 et 30 mars 2015
17h00 à 18h30

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…

Breakdown of band theory
Half-filled band is metallic?

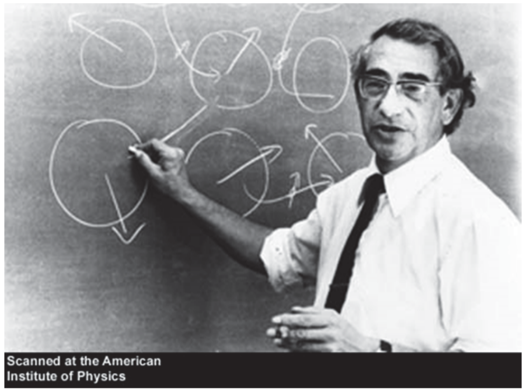
Half-filled band: Not always a metal

NiO, Boer and Verway

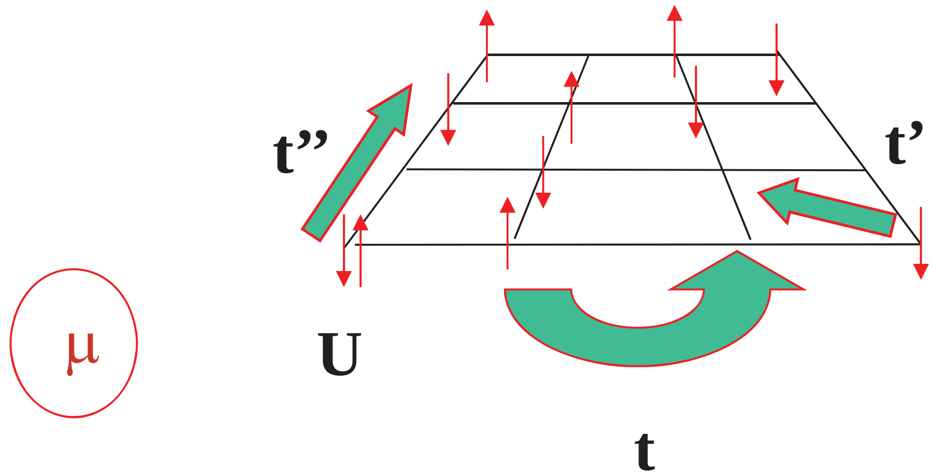
Peierls, 1937

Mott, 1949

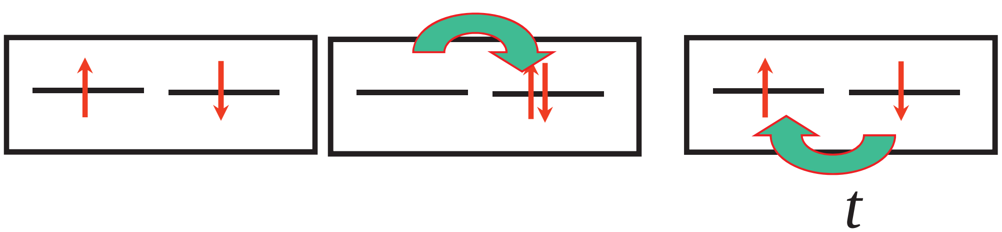
Hubbard model



1931-1980



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



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

High temperature superconductors and layered organic superconductors

Failure of

BCS theory

Band structure

and more

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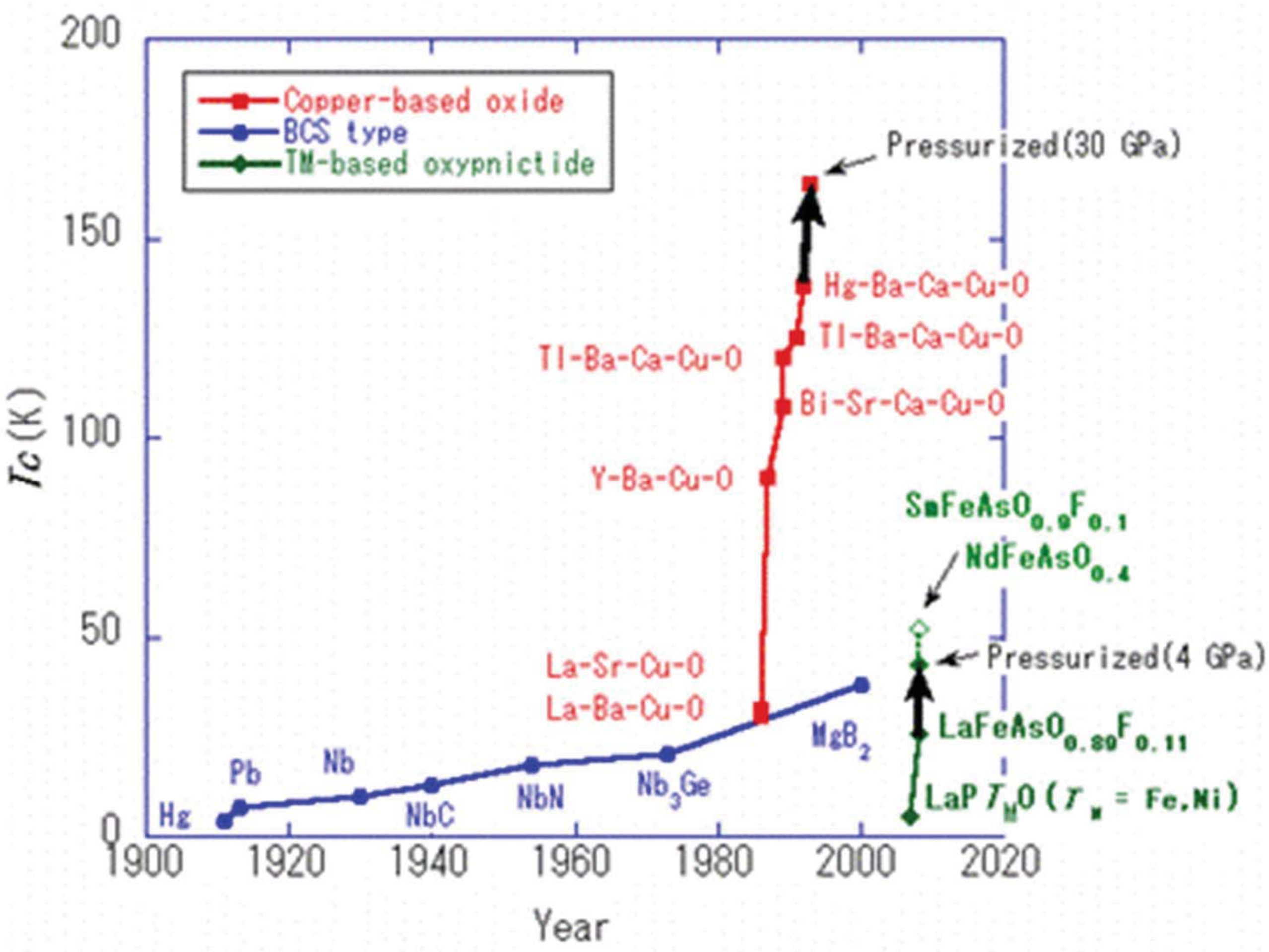
New and old superconductors



H. Takahashi: JPSJ Online—News and Comments [June 10, 2008]

March meeting APS, 1987

- New York Times headlines
"The Woodstock of Physics"

"They began lining up outside the New York Hilton Sutton Ballroom at 5:30PM for an evening session that would last until 3:00 AM"

15-18 Aug. 1969
500,000 participants

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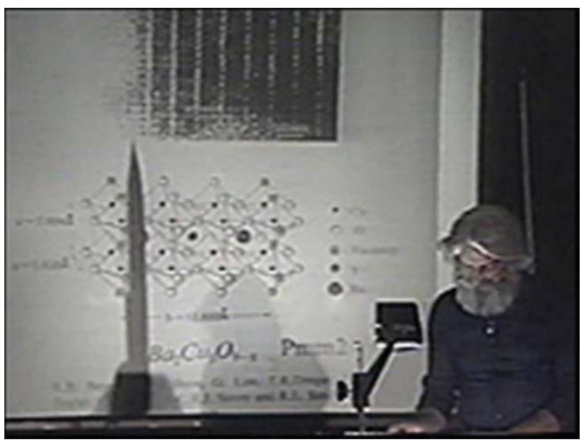

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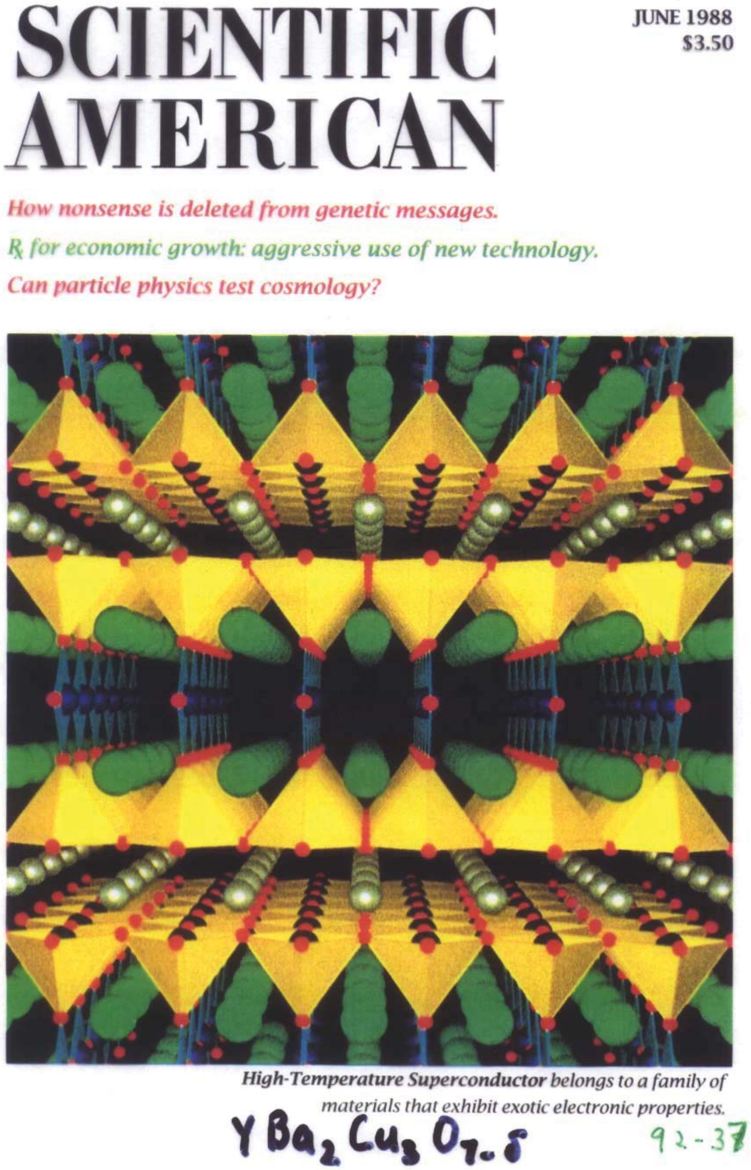
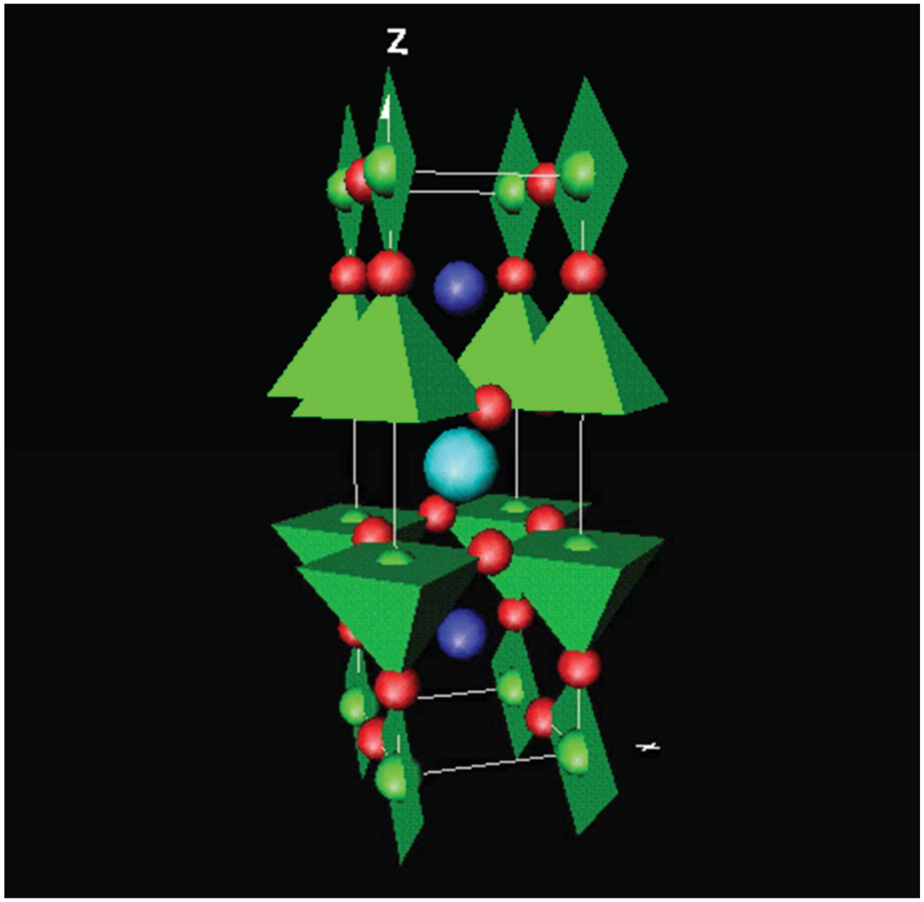
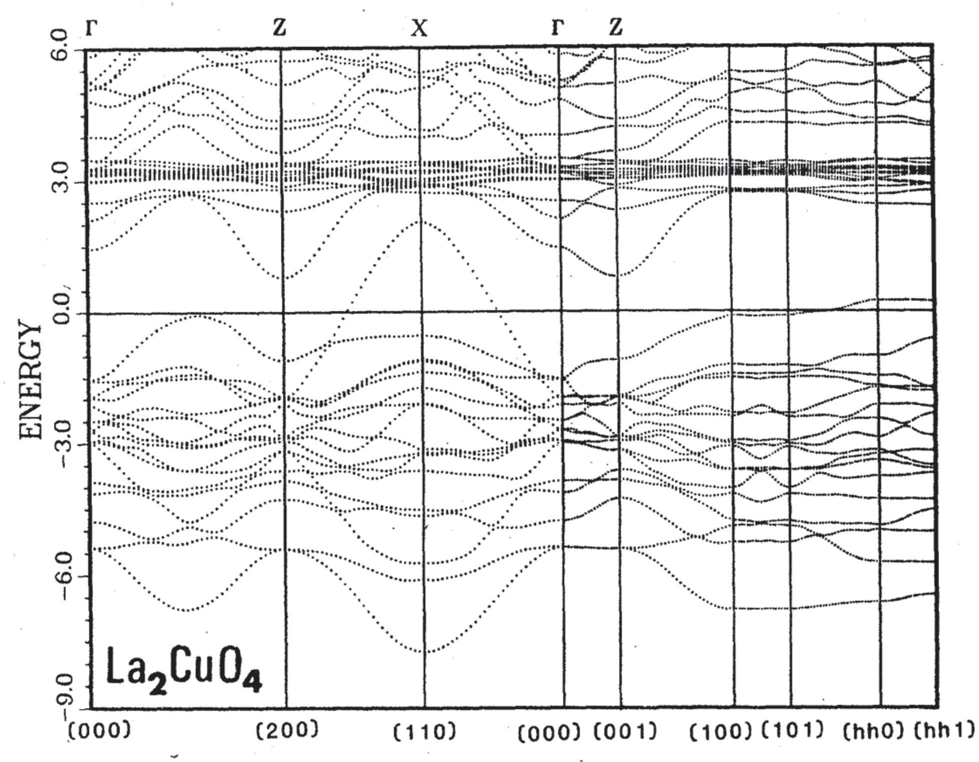
Atomic structure





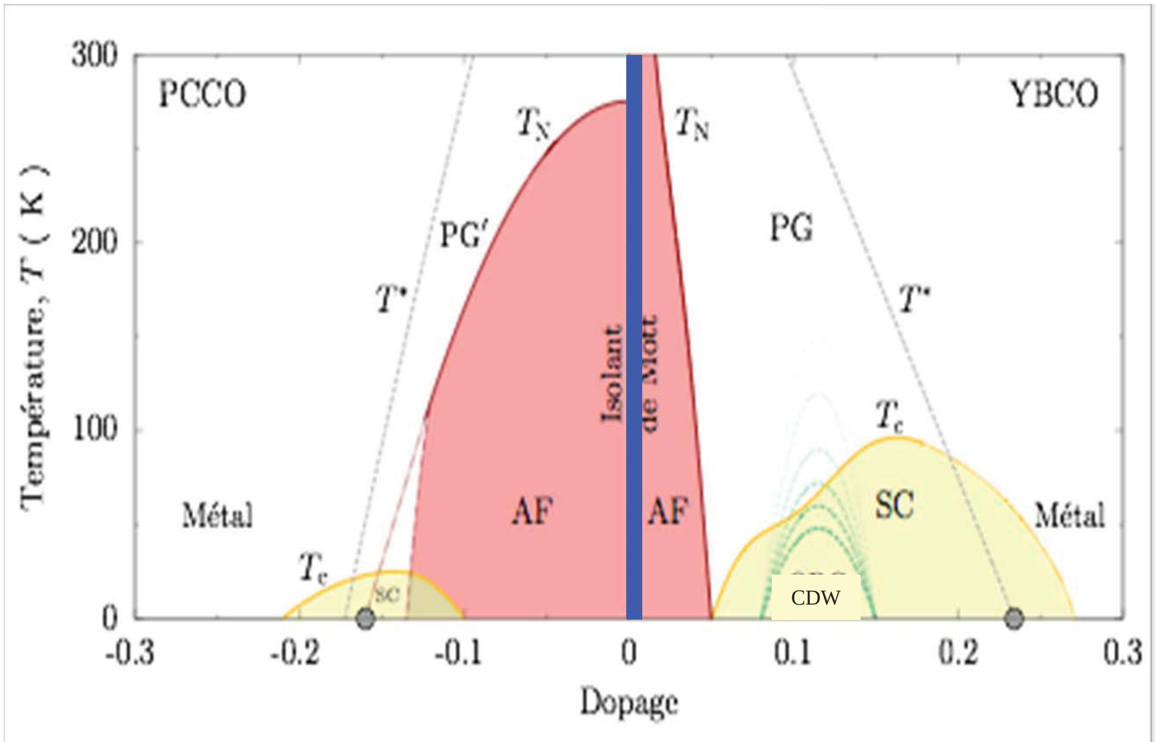
Band structure for high Tc

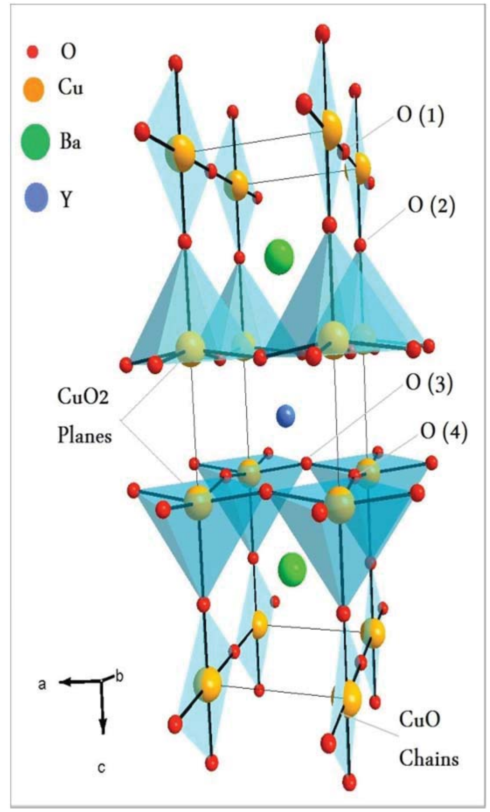


W. Pickett, Rev. Mod. Phys. 1989

Our road map

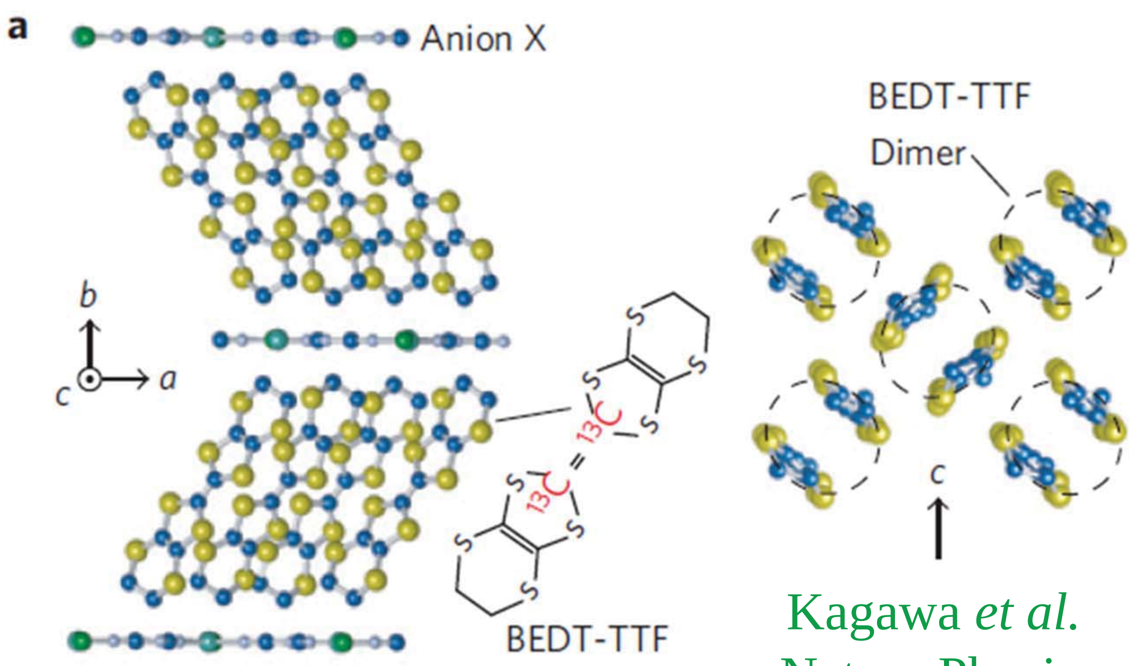
Thèse de Francis Laliberté,
Université de Sherbrooke





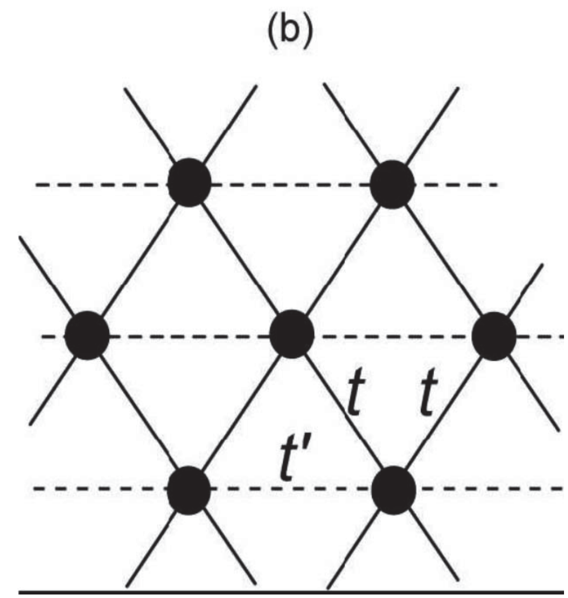
Hubbard on anisotropic triangular lattice

H. Kino + H. Fukuyama, J. Phys. Soc. Jpn **65** 2158 (1996),
R.H. McKenzie, Comments Condens Mat Phys. **18**, 309 (1998)



n=1, varying *t'/t*

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



$t \approx 50\,\text{meV}$

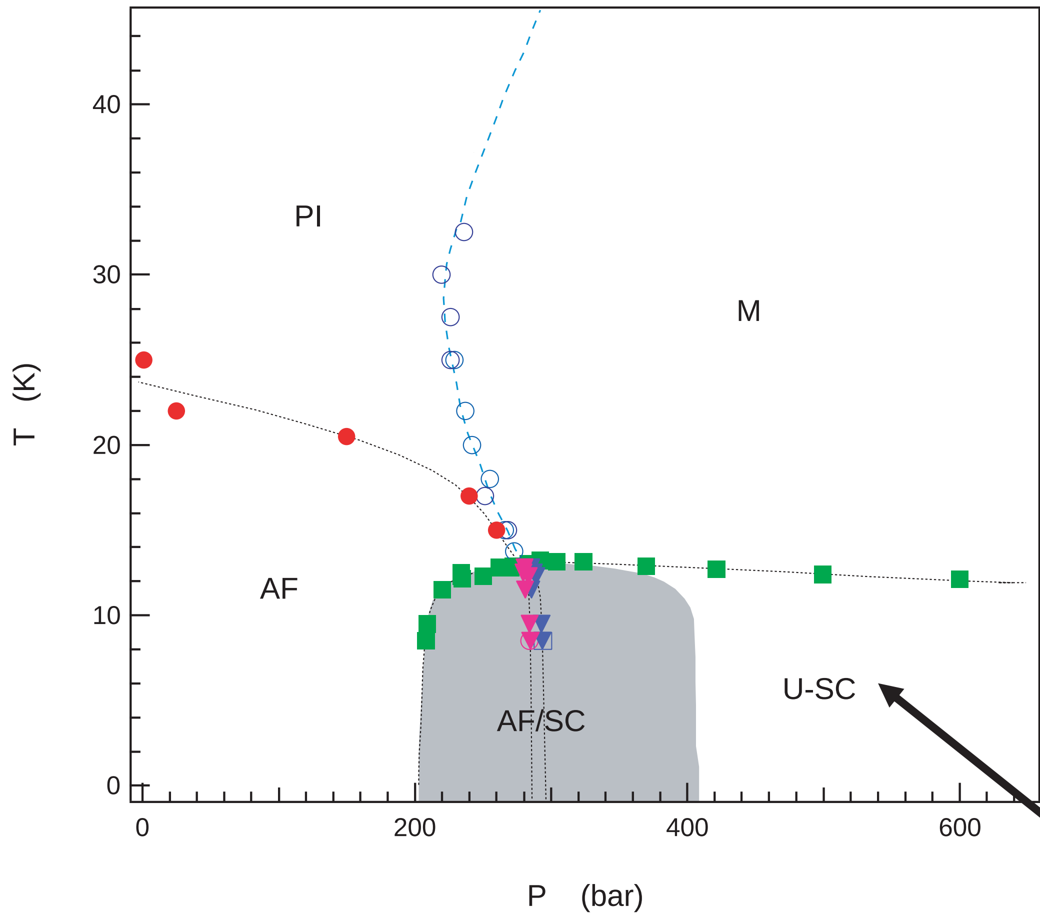
$\Rightarrow U \approx 400\,\text{meV}$

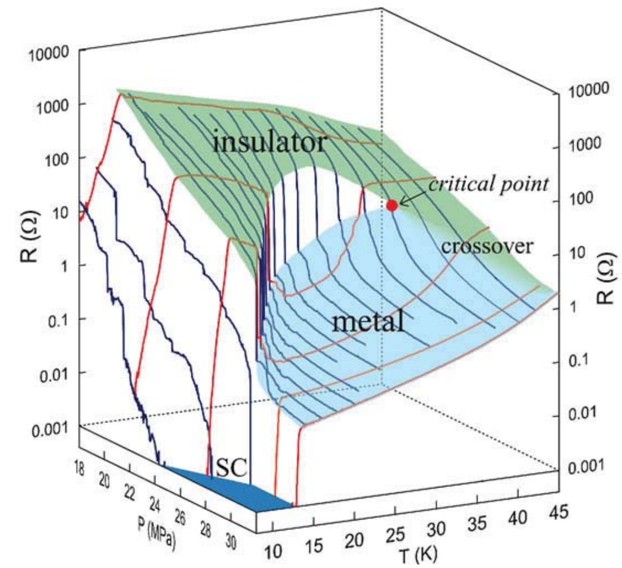
t'/t ~ 0.6 - 1.1

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

Université de Sherbrooke

Phase diagram for organics





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

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

Powell, McKenzie cond-mat/0607078

Phase diagram (X=$Cu[N(CN)_2]Cl$)

S. Lefebvre et al. PRL **85**, 5420 (2000), P. Limelette, et al. PRL 91 (2003)

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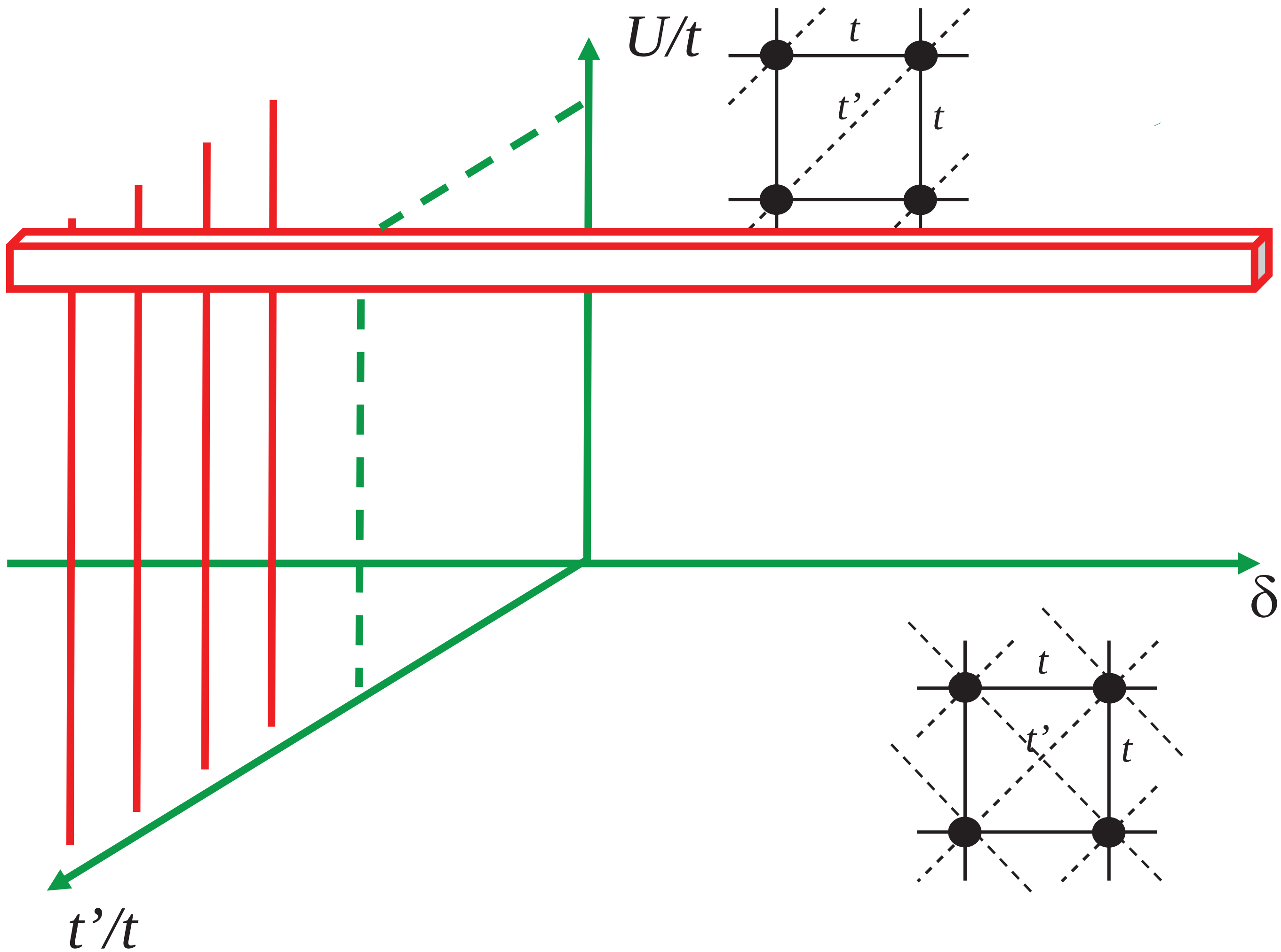
Perspective



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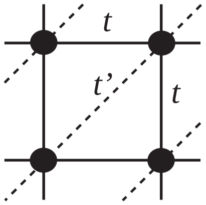
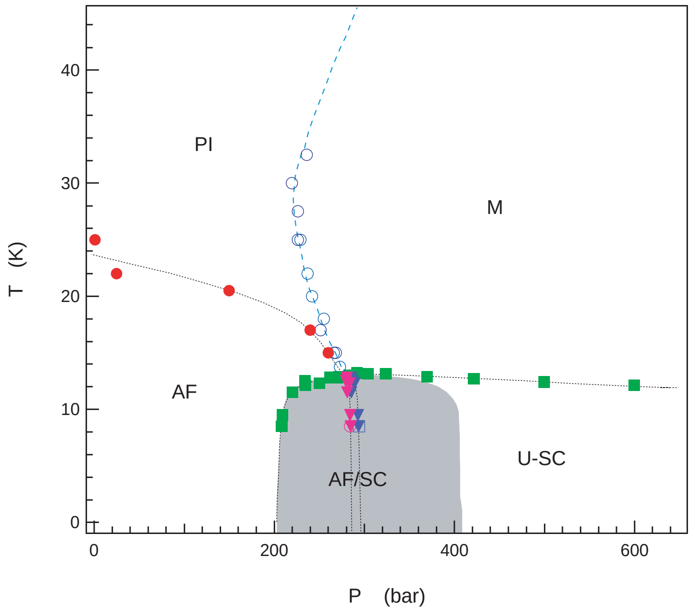
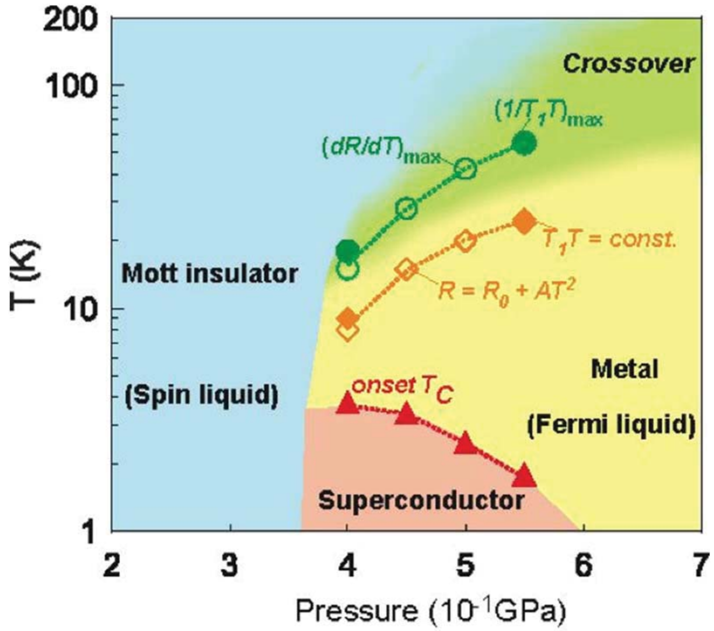
Phase diagram BEDT

$t' = 0.6t$



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





Y. Kurisaki, et al.
Phys. Rev. Lett. **95**, 177001(2005)

Y. Shimizu, et al. Phys. Rev. Lett. **91**, (2003)

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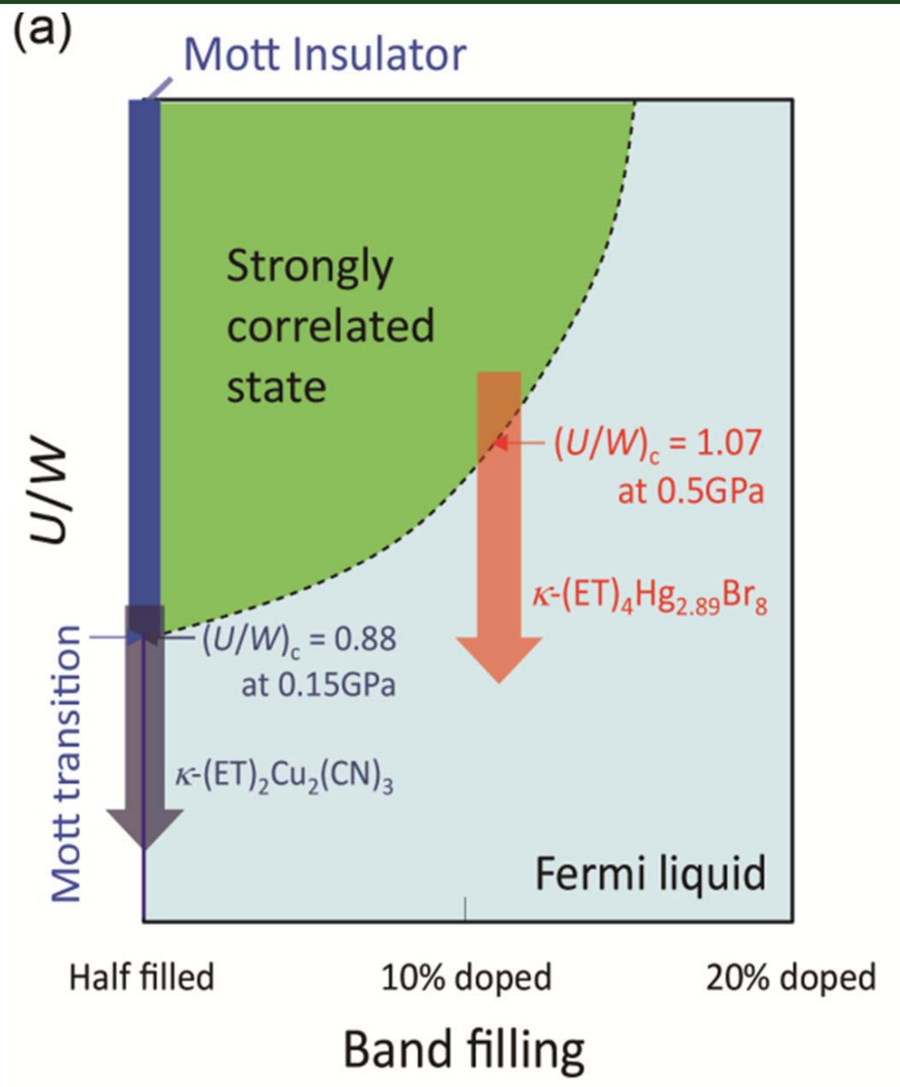
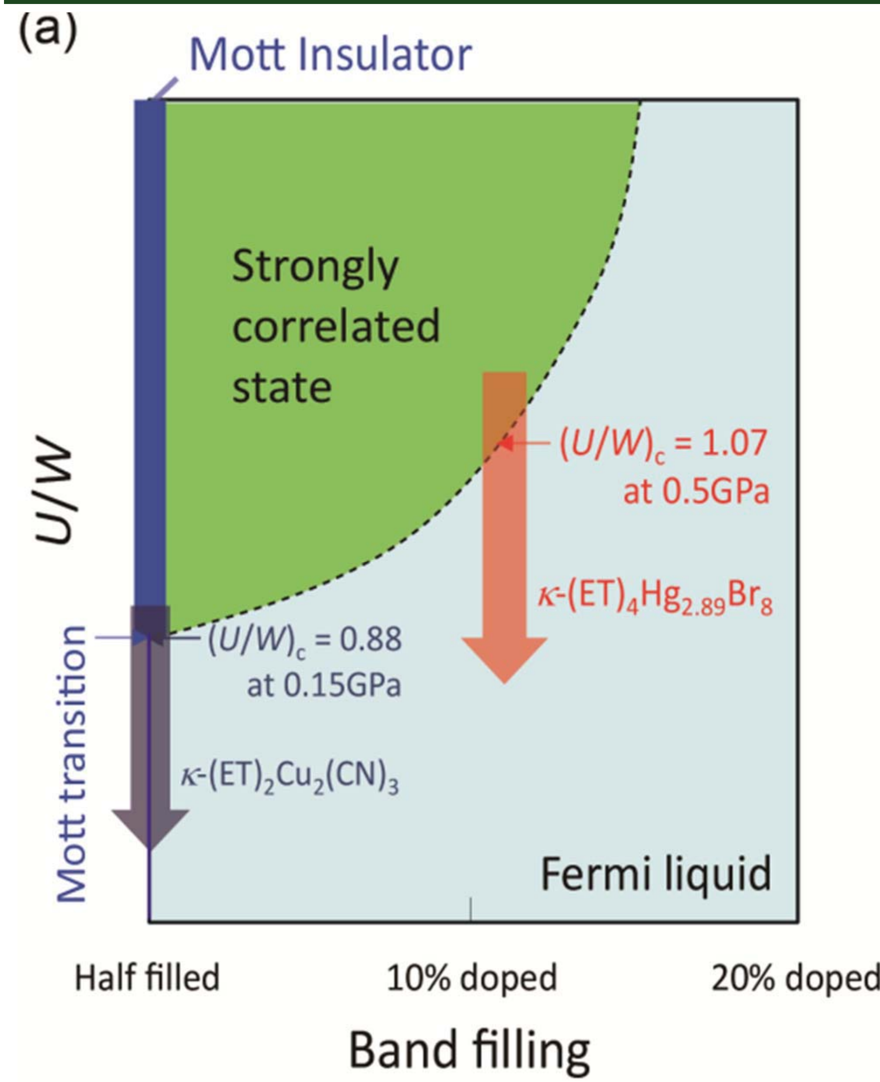
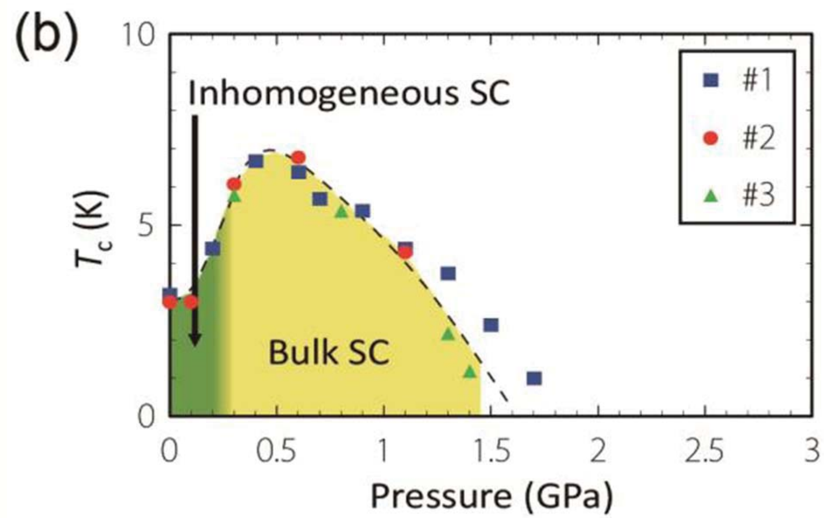
Doped organic

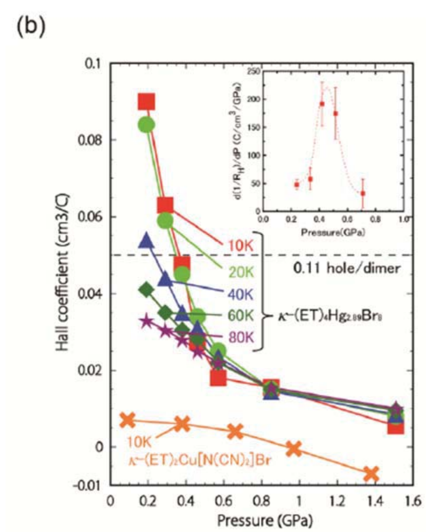


H. Oike, K. Miyagawa, H. Taniguchi, K. Kanoda PRL **114**, 067002 (2015)

Doped BEDT







H. Oike, K. Miyagawa, H. Taniguchi, K. Kanoda PRL **114**, 067002 (2015)

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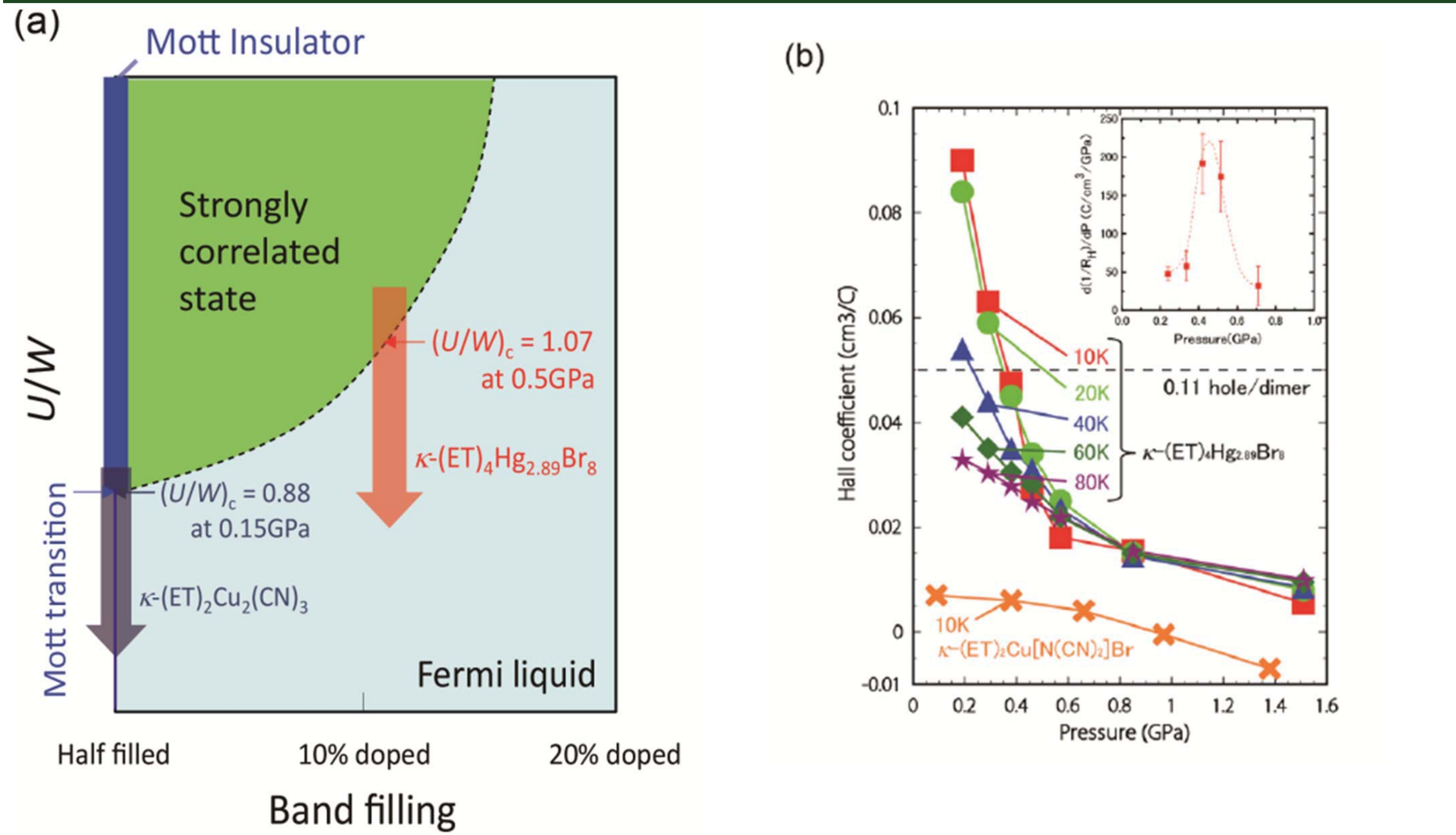
Crossover to doped Mott insulator

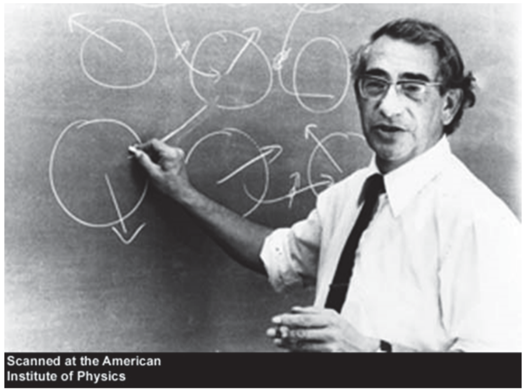


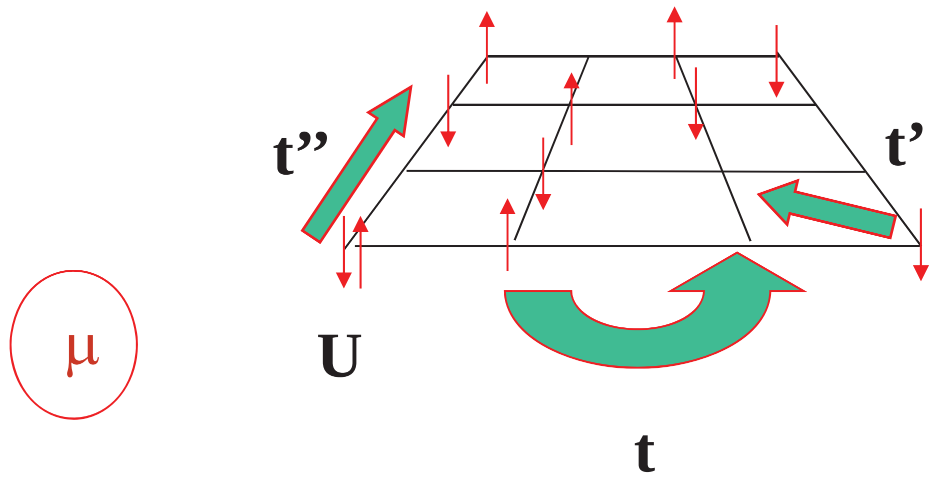
H. Oike, K. Miyagawa, H. Taniguchi, K. Kanoda PRL **114**, 067002 (2015)

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

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

Attn: Charge transfer insulator

P.W. Anderson

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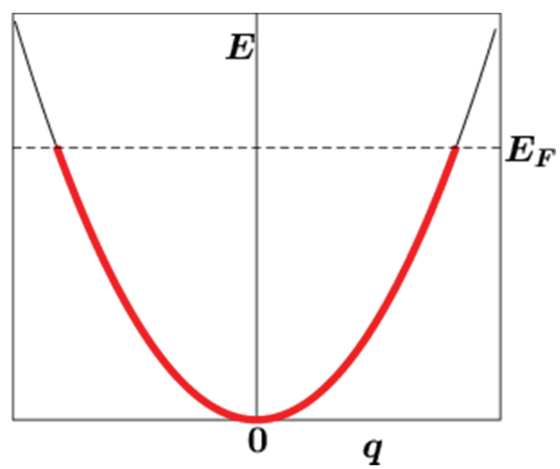
$U = 0$

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

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

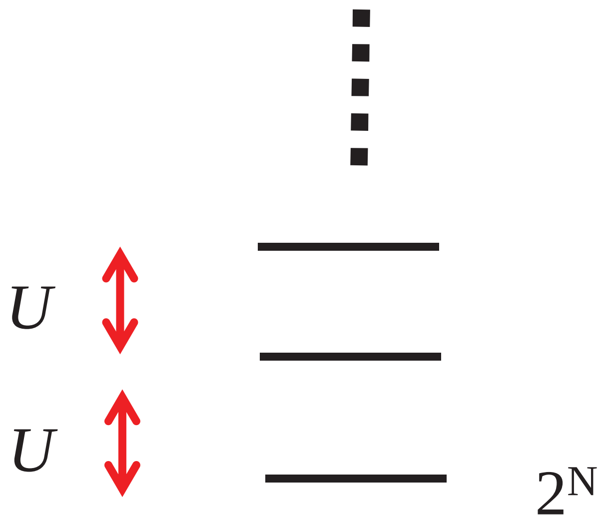
$$H = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}$$

$$|\Psi\rangle = \prod_{\mathbf{k},\sigma} c^{\dagger}_{\mathbf{k}\sigma}|0\rangle$$



$t_{ij} = 0$

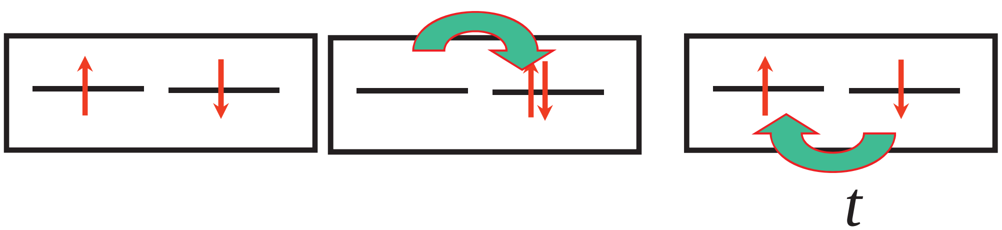
$$H = U \sum_i n_{i\uparrow} n_{i\downarrow}$$



$$|\Psi\rangle = \prod_{\mathbf{i}} c^{\dagger}_{\mathbf{i}\uparrow} \prod_{\mathbf{j}} c^{\dagger}_{\mathbf{j}\downarrow} |0\rangle$$

Interesting in the general case

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



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

Outline

- Lecture 1: overview
  - What is the problem
  - Possible approaches and answers for organics
- Lecture 2 : h-doped
  - Strongly correlated superconductivity
  - Normal phase (pseudogap)
- Lecture 3: e-doped cuprates
  - Spin wave exchange (TPSC)
  - AFM quantum critical point
- Lecture 4
  - More on cluster generalizations of DMFT

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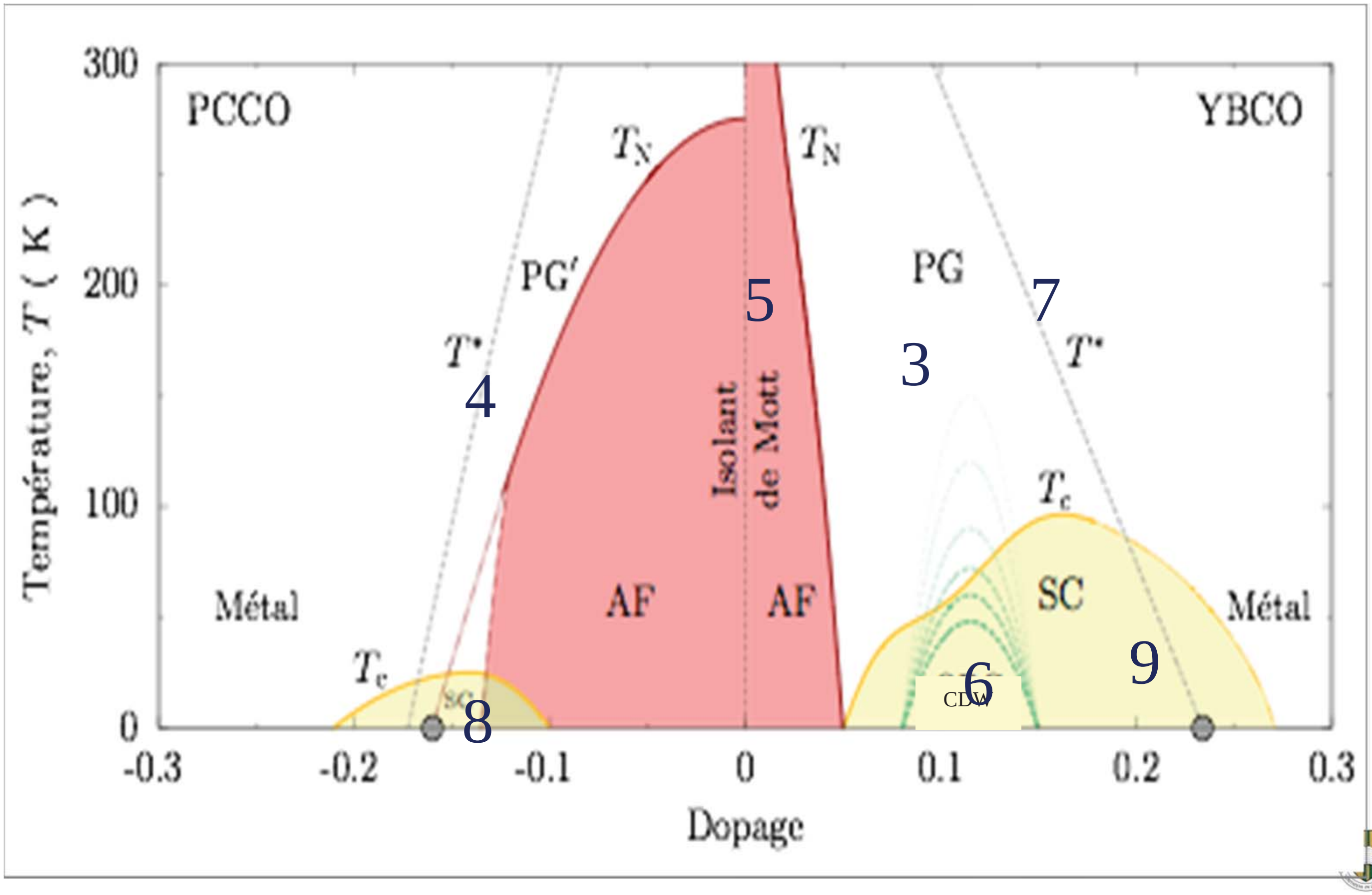
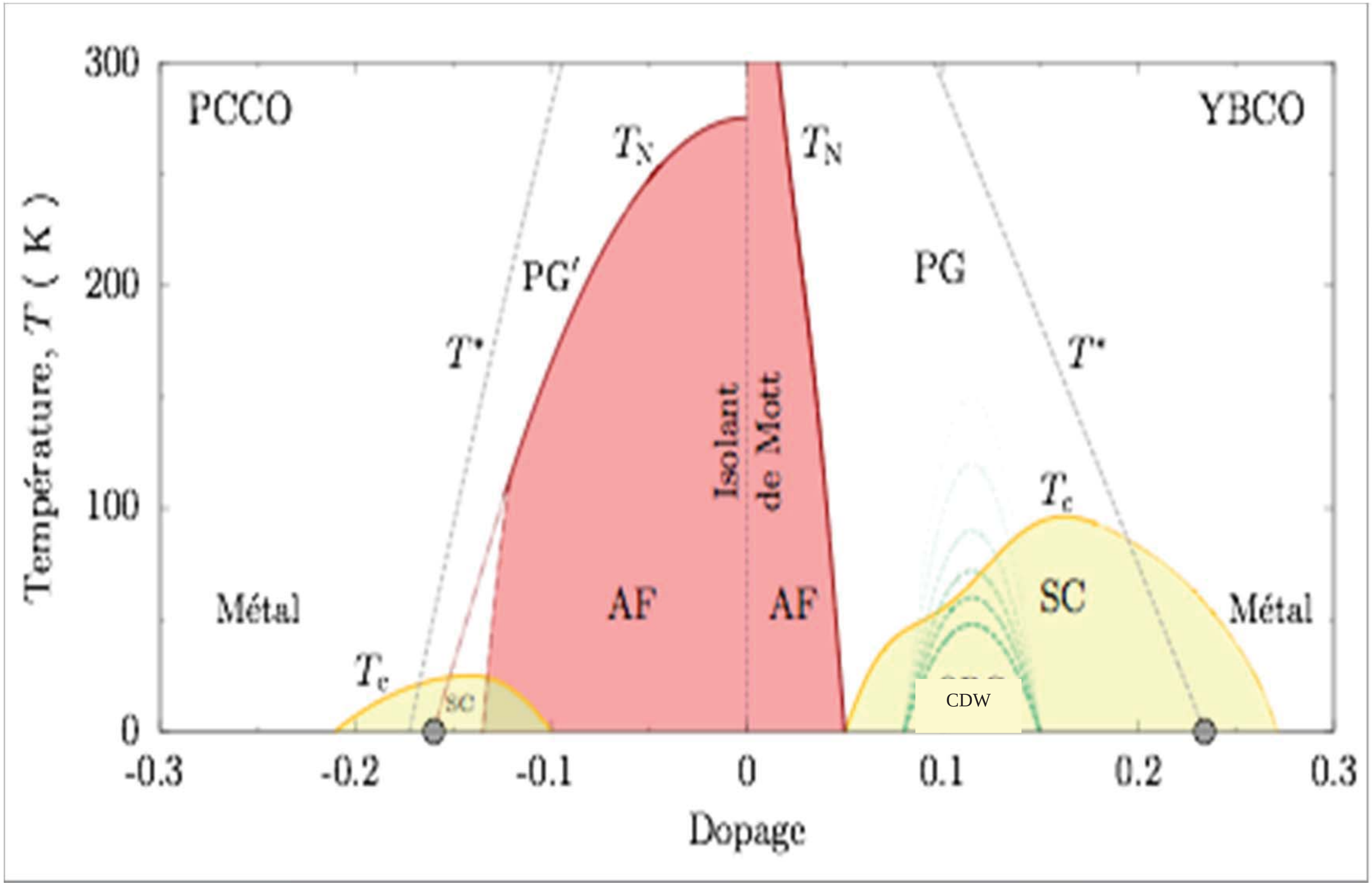
Outline

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



3. A normal, normal state?

Our road map



Thèse de Francis Laliberté, Université de Sherbrooke

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

Mott-Ioffe-Regel limit

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

$$k_F\ell = \frac{2\pi}{\lambda_F}\ell \sim 2\pi$$

$$\sigma_{MIR} = \frac{e^2}{\hbar d}$$

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Mott-Ioffe-Regel limit

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

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

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

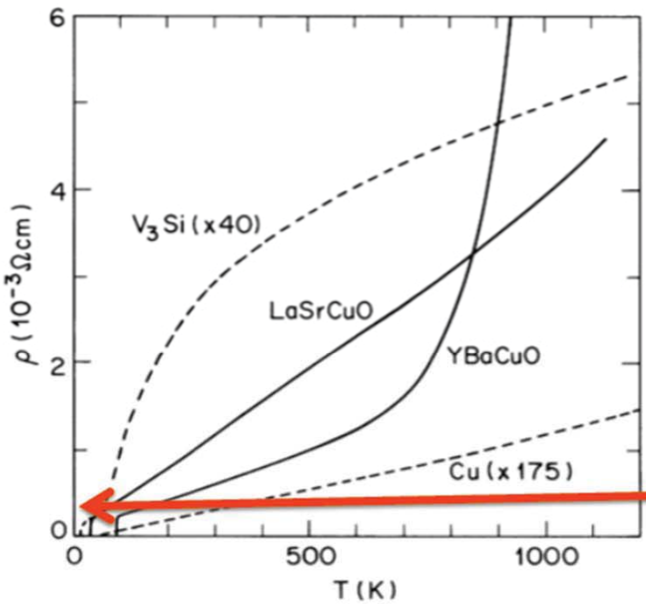
$$\ell = \left(\frac{\hbar k_F}{m}\right)\tau$$

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

$$k_F\ell = \frac{2\pi}{\lambda_F}\ell \sim 2\pi$$

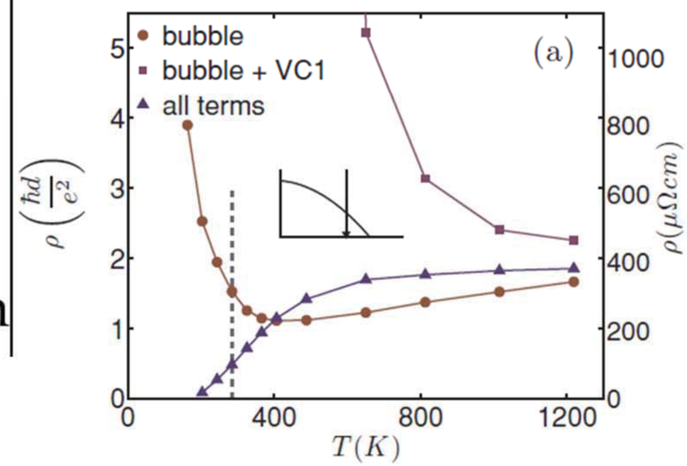
$$\sigma_{MIR} = \frac{e^2}{\hbar d}$$

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

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

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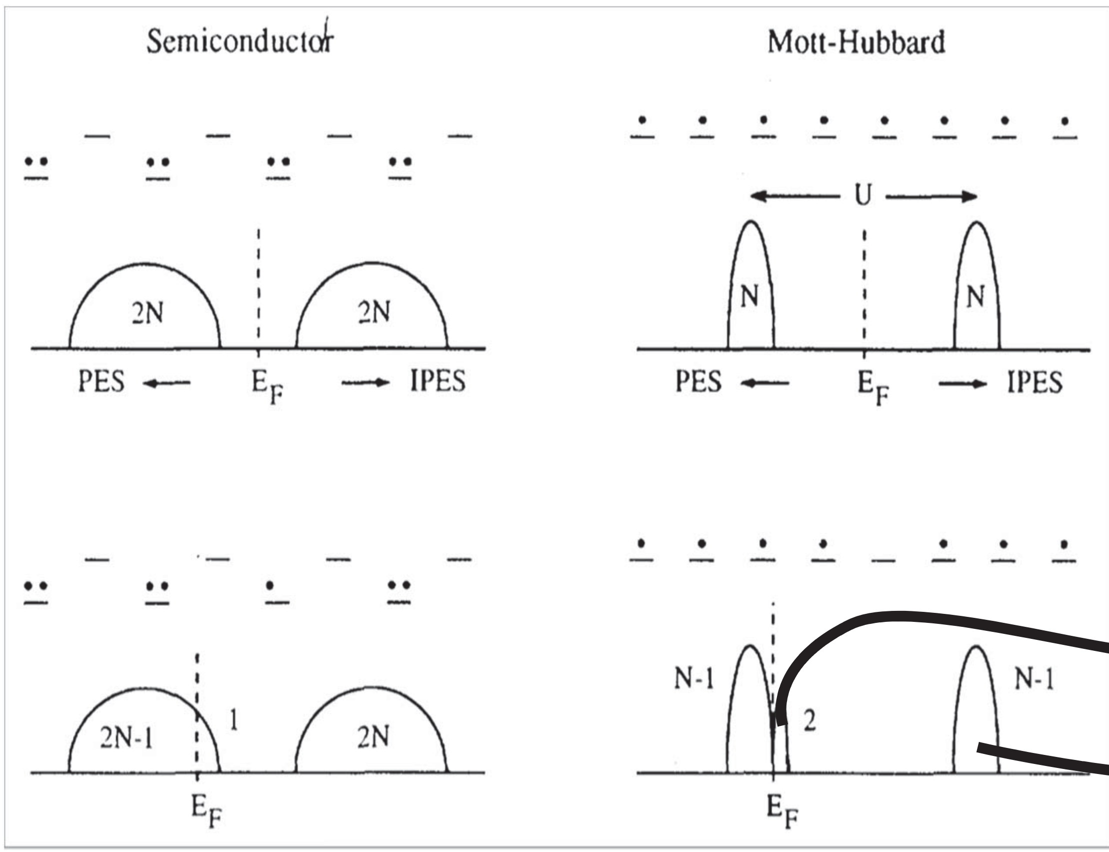
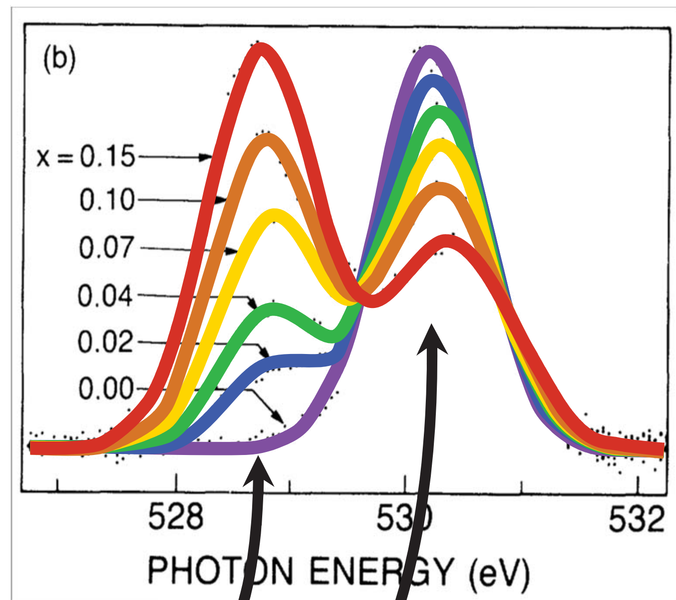
Experiment, X-Ray absorption

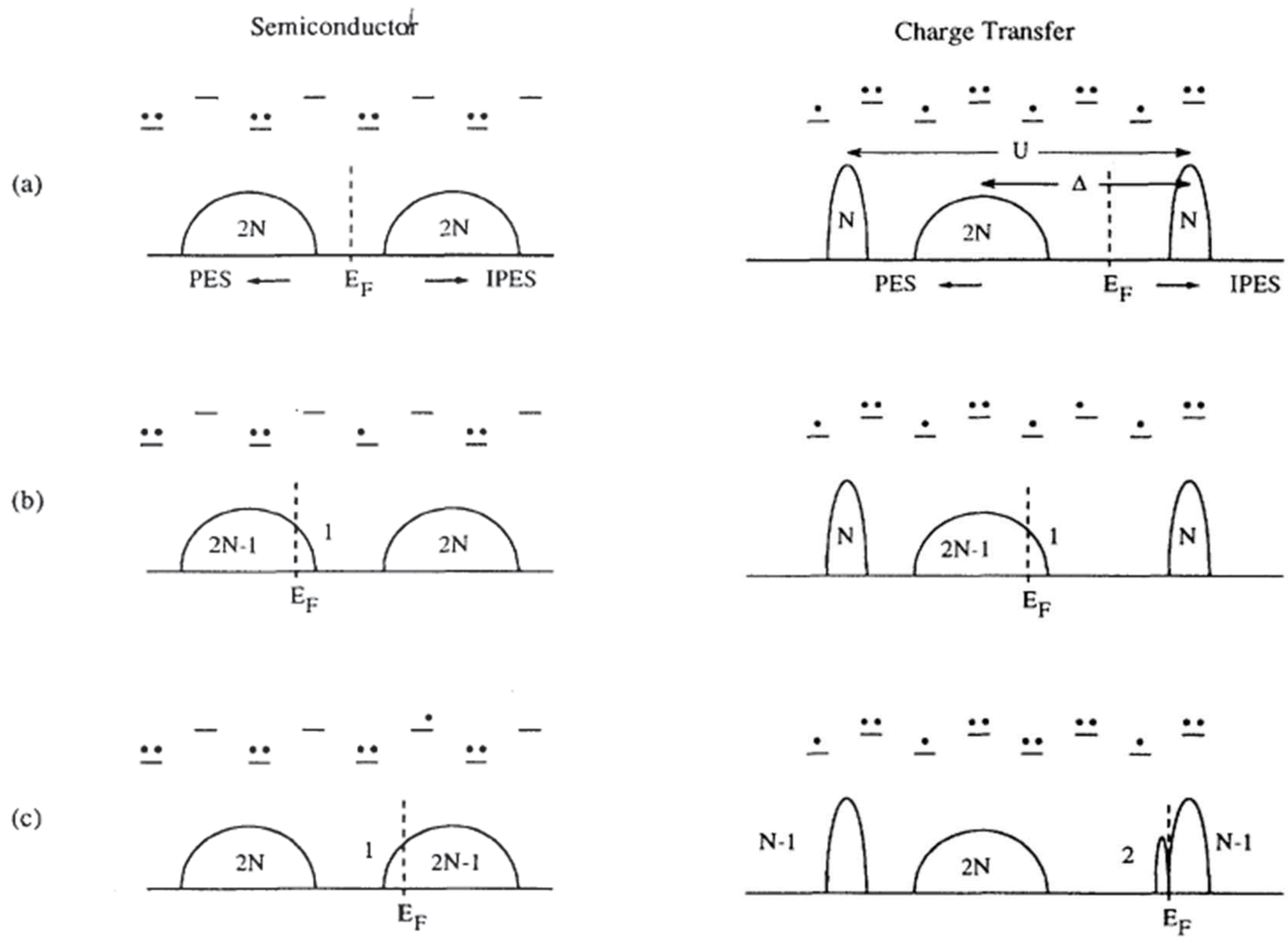
Meinders *et al.* PRB **48**, 3916 (1993)





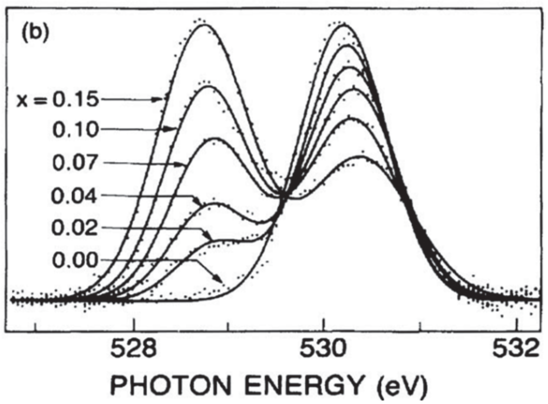
Chen et al. PRL **66**, 104 (1991)

Not obvious: Charge transfer insulator

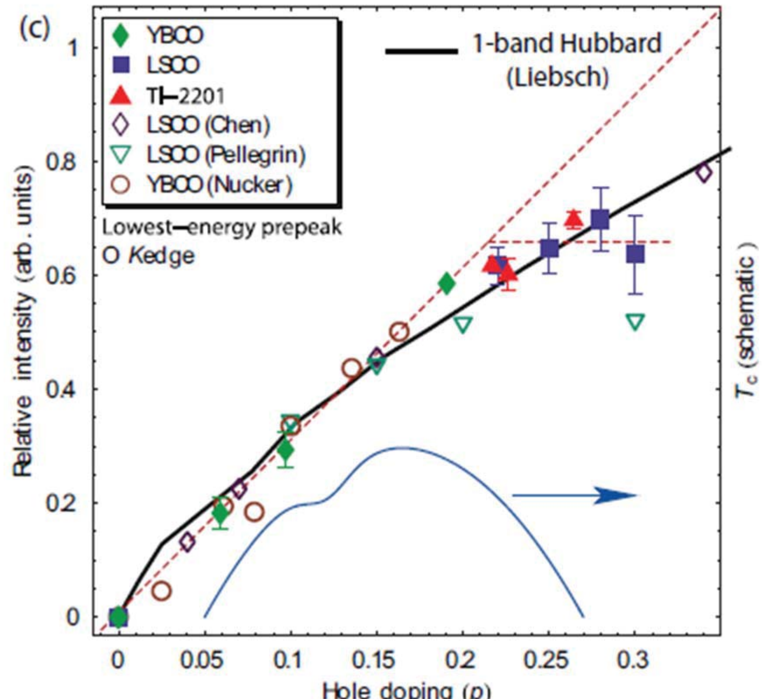


Meinders *et al.* PRB **48**, 3916 (1993)

Experiment: X-Ray absorption



Chen et al. PRL **66**, 104 (1991)



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

Number of low energy states above ω = 0 scales as *2x* +
Not as 1+x as in Fermi liquid

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

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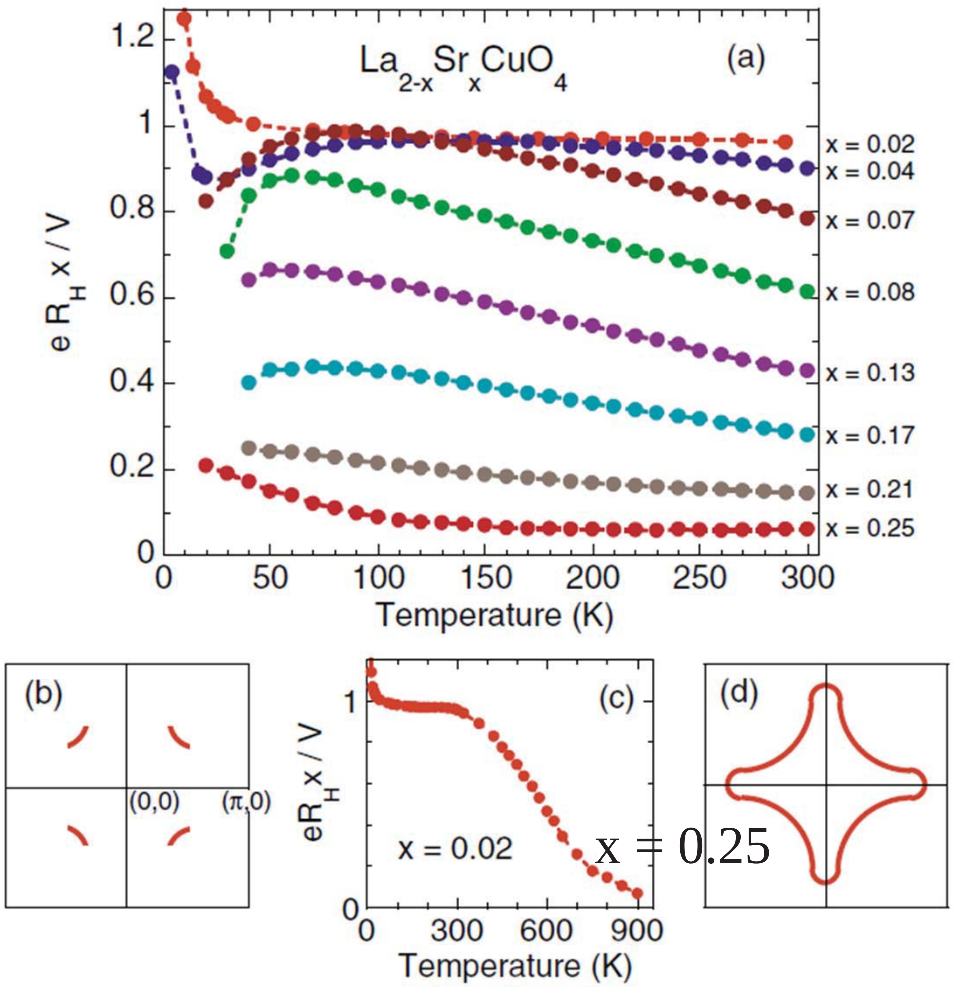
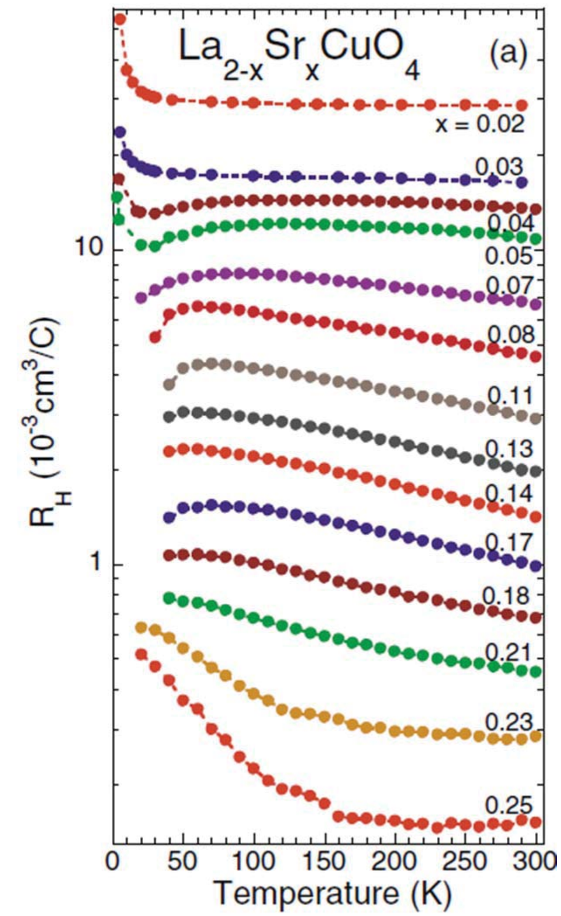
Hall coefficient





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

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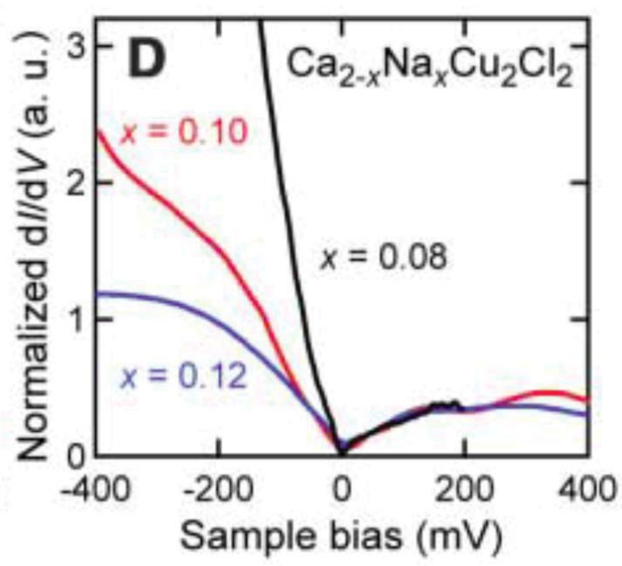
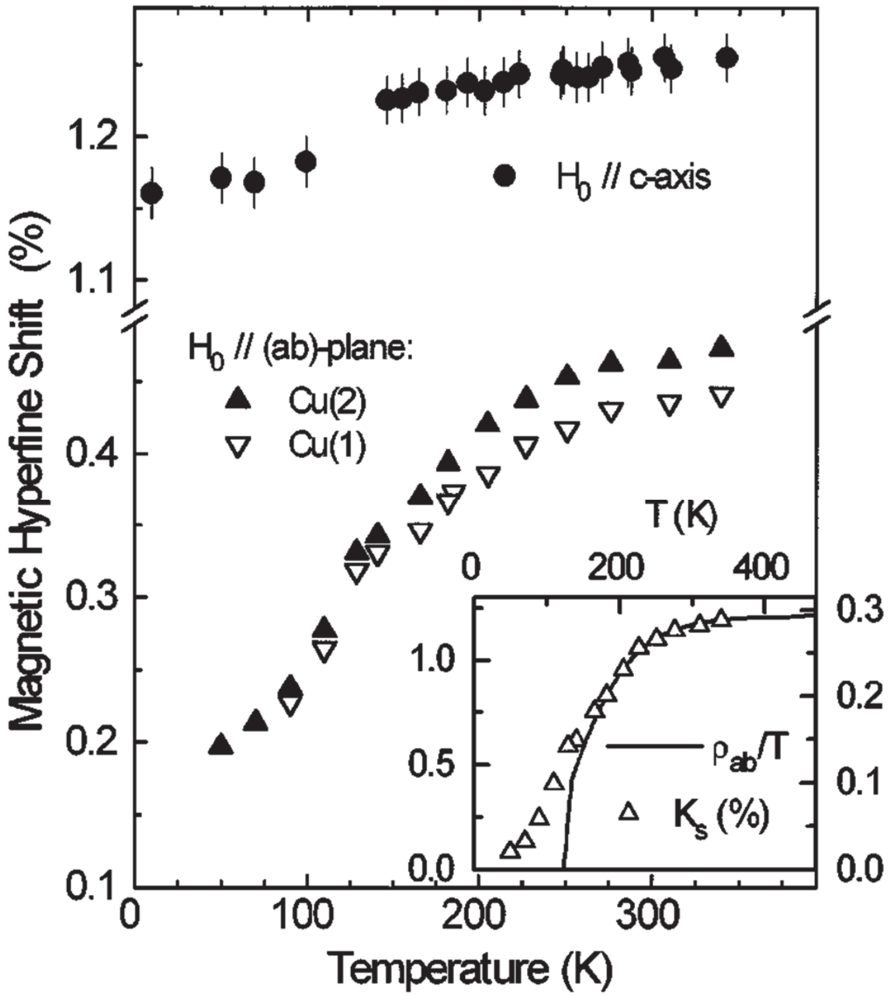
Density of states (STM)



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

Spin susceptibility (Knight shift): Pseudogap

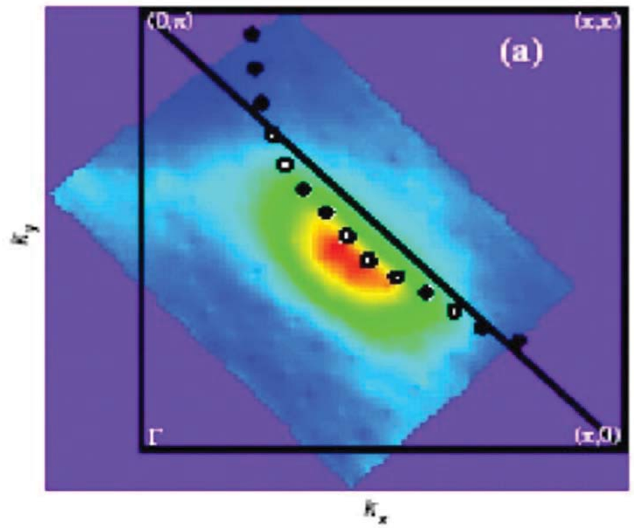


Underdoped Hg1223

Julien et al. PRL **76,** 4238 (1996)

ARPES: (Pseudogap)

Hole-doped, 10%



F. Ronning et al. Jan. 2002, $Ca_{2-x}Na_xCuO_2Cl_2$

Ronning *et al.* (PRB 2003)

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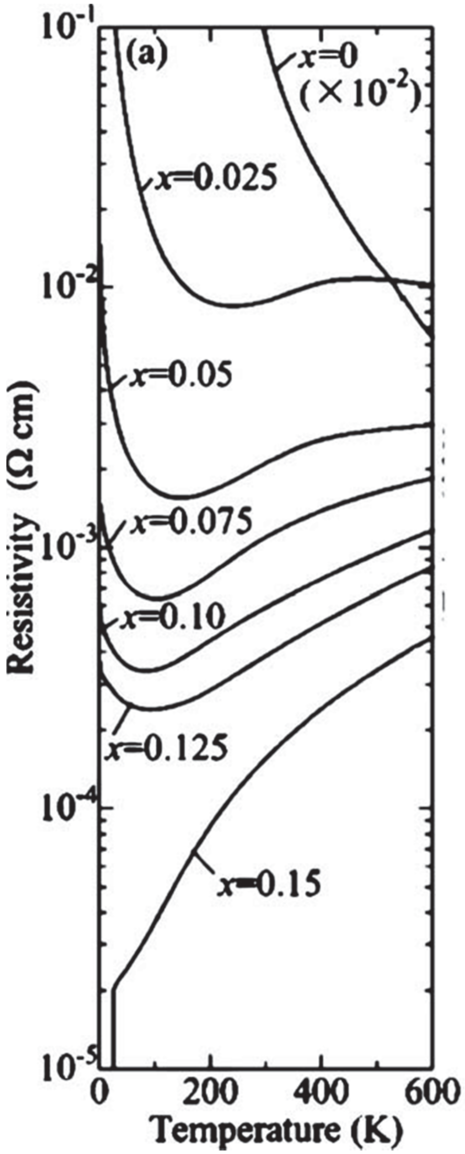
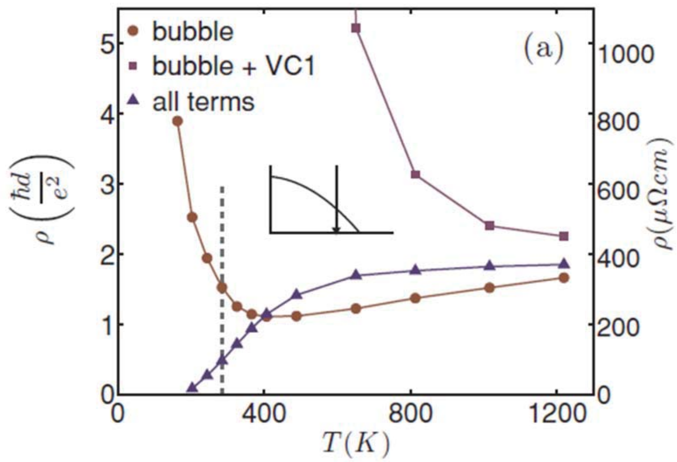
4. e-doped cuprates

Less strongly coupled: evidence from the normal state

Electron-doped and MIR limit



NCCO



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

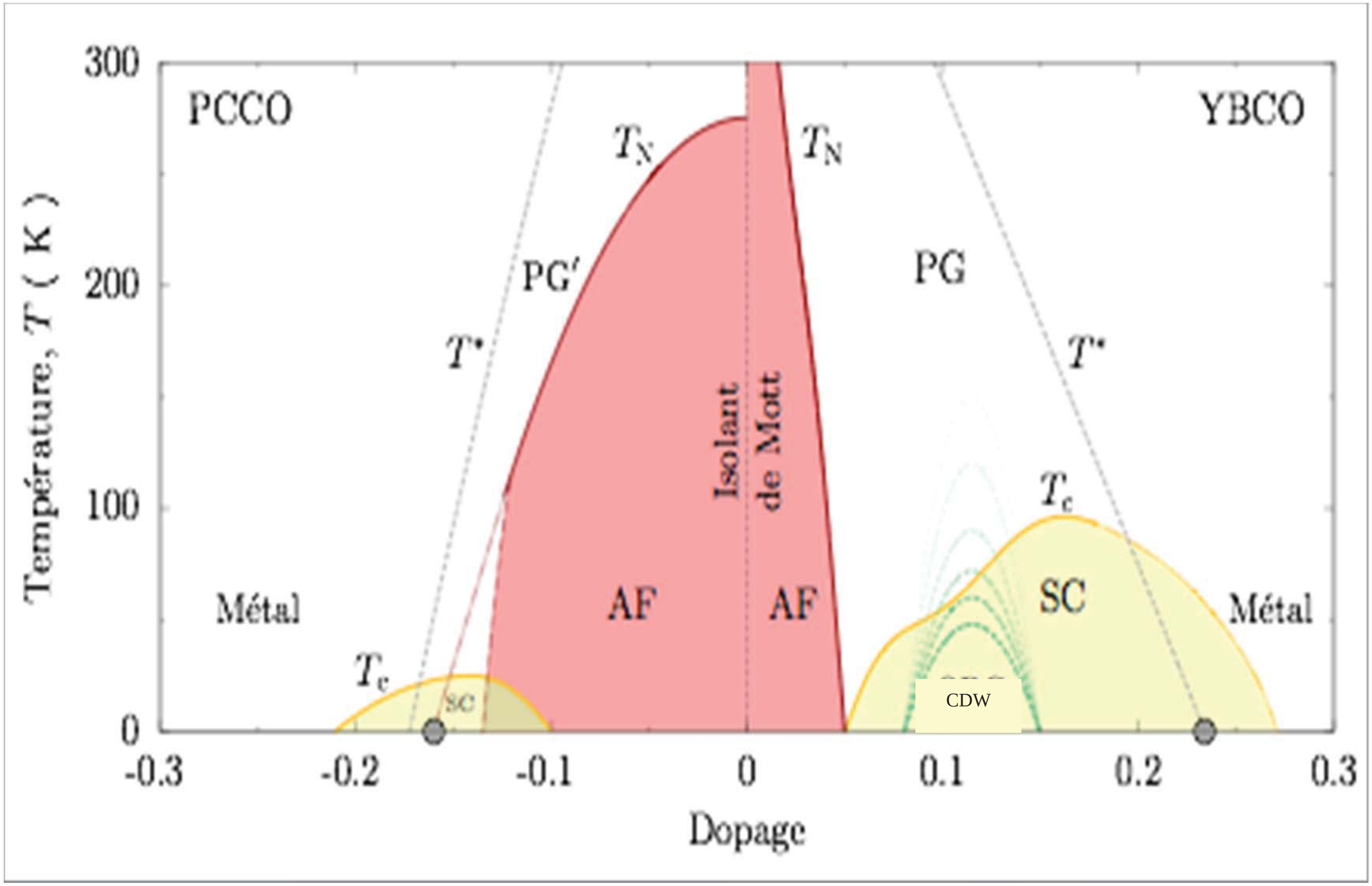
Onose et al. 2004

5. Weakly and strongly correlated antiferromagnets

What is a phase?

Our road map

Thèse de Francis Laliberté, Université de Sherbrooke



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

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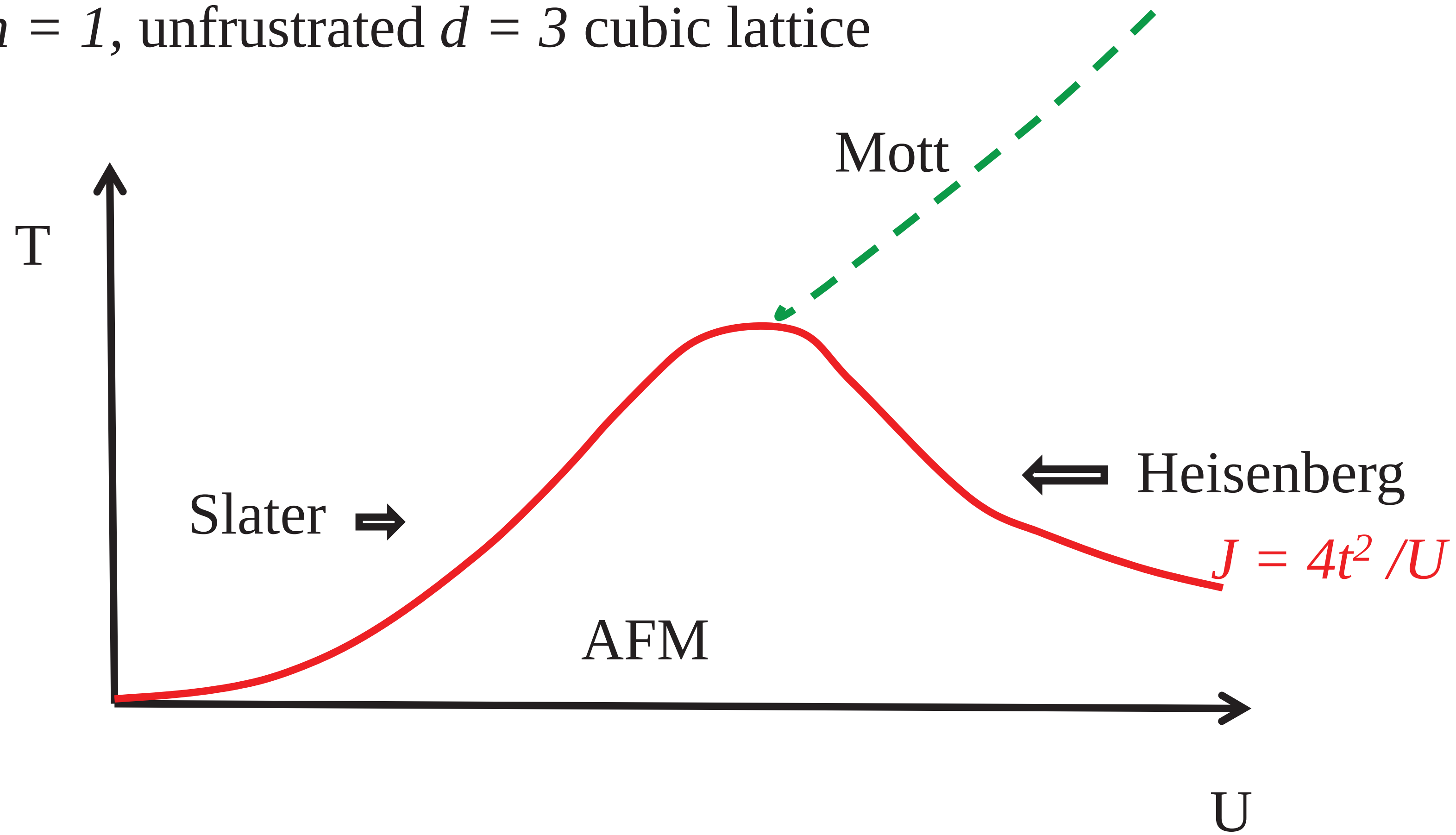
Differences between weakly and strongly correlated

- 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

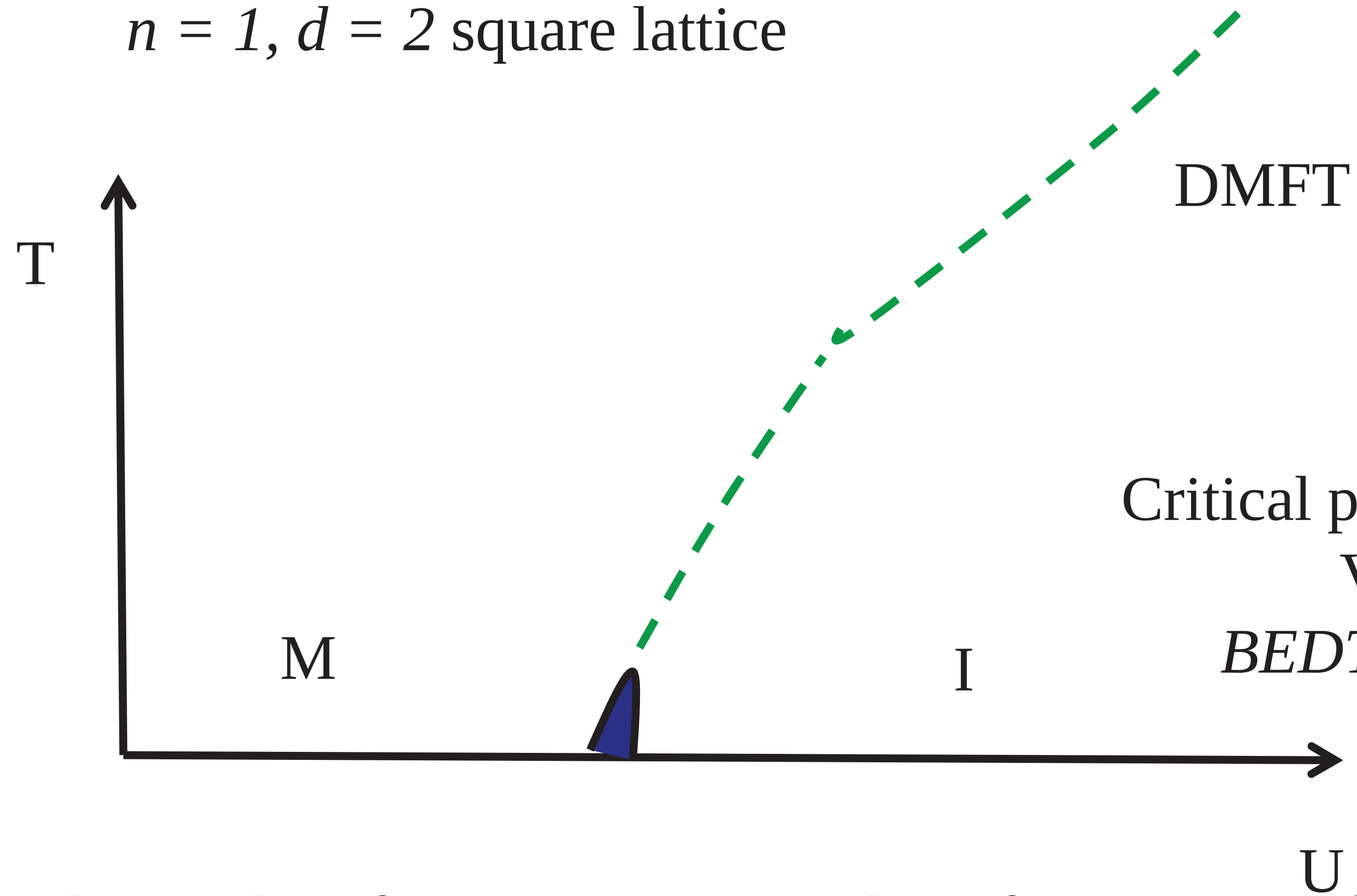
Local moment and Mott transition

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



Local moment and Mott transition

n = 1, d = 2 square lattice



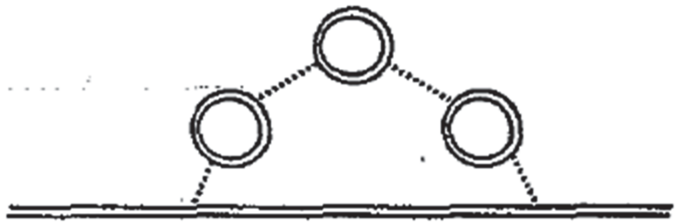
Understanding finite temperature phase from a *mean-field theory* down to *T = 0*

Strong vs weak correlations

Contrasting methods

Ordered state

- Mean-field (Hartree-Fock) for AFM



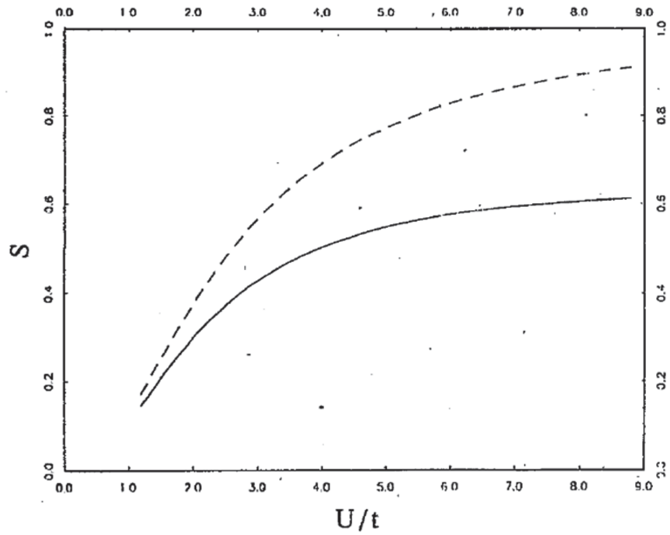


FIG. 7. The solid line represents the sublattice magnetization including the fluctuation effects. The dashed line is the mean-field result.

Schrieffer, Wen, Zhang, PRB 1989

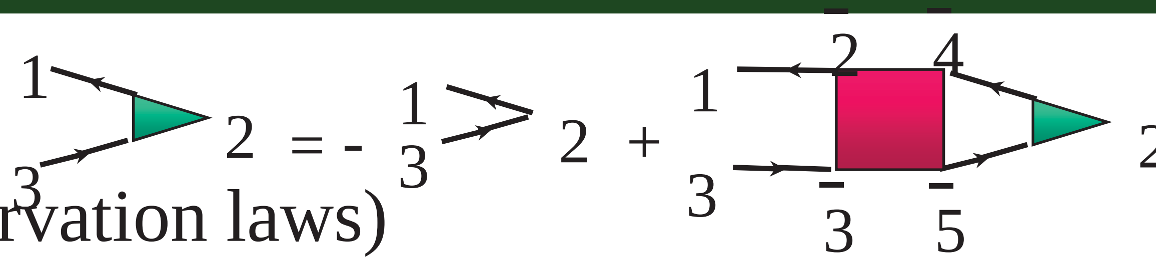
More methods for ordered states, n=1

- 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

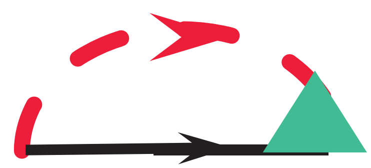
In paramagnetic state

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_{eff}
  - Pauli
- FLEX
  - No pseudogap
  - Pauli
- Renormalization Group
  - 2 loops

Σ =



Zanchi Schultz, (2000)
Rohe and Metzner (2004)
Katanin and Kampf (2004)

Two-Particle Self-Consistent (idea)

- General philosophy
  - Drop diagrams
  - Impose constraints and sum rules
    - Conservation laws
    - Pauli principle ($\langle n_\sigma^2 \rangle = \langle n_\sigma \rangle$)
    - Local moment and local density sum-rules
- Get for free:
    - Mermin-Wagner theorem
    - Kanamori-Brückner screening
    - Consistency between one- and two-particle $\Sigma G = U\langle n_\sigma n_{-\sigma} \rangle$

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)

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Doped Mott insulator : strong correlations

Normal state

At strong coupling

- Gutzwiller
- Variational approaches
- Slave particles (Review: Lee Nagaosa RMP)
- Extremely Correlated Fermi liquids (Shastry)

YRZ

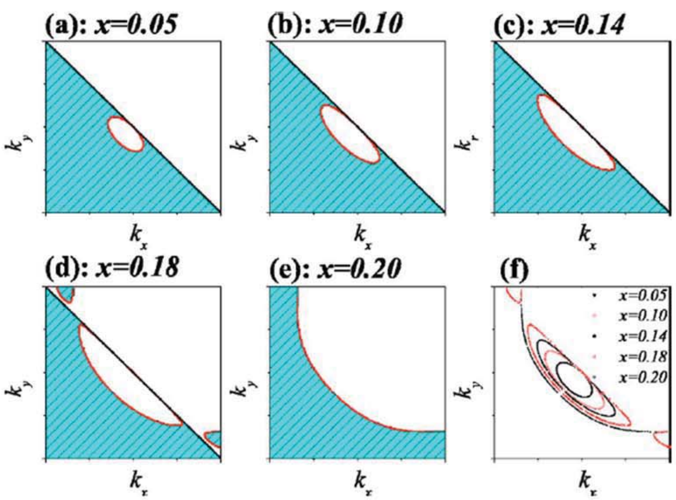
$$G^{RVB}(\boldsymbol{k},\omega) = \frac{g_t}{\omega - \xi(\boldsymbol{k}) - \Delta_R^2/[\omega + \xi_0(\boldsymbol{k})]} + G_{inc},$$

where $\boldsymbol{k} = (k_x, k_y)$,

$$\xi_0(\boldsymbol{k}) = -2t(x)(\cos k_x + \cos k_y),$$

$$\Delta_R(\boldsymbol{k}) = \Delta_0(x)(\cos k_x - \cos k_y),$$

$$\xi(\boldsymbol{k}) = \xi_0(\boldsymbol{k}) - 4t'(x)\cos k_x \cos k_y - 2t''(x)(\cos 2k_x + \cos 2k_y) - \mu_p.$$



K.-Y. Yang, T.M. Rice, and F.-C. Zhang, Phys. Rev. B 73, 174501 (2006)
See numerous papers of Carbotte and Nicol and detailed discussions in
K. Le Hur and T.M. Rice, Annals of Physics **324**, 1452 (2009)

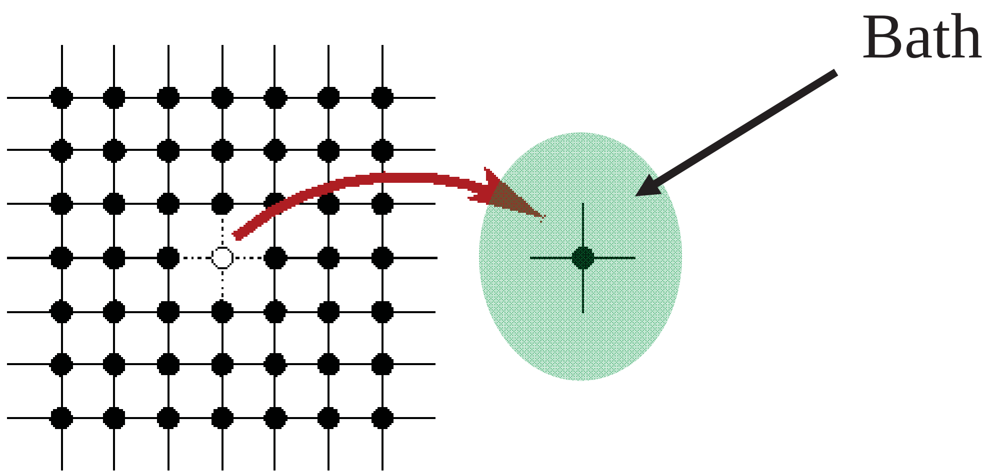
Method

"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* = *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.

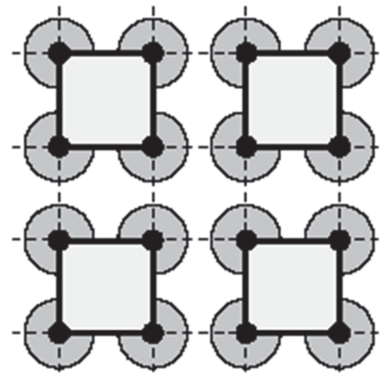


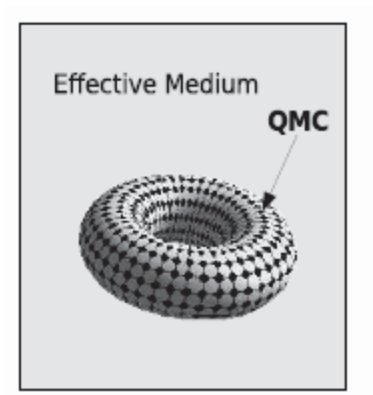
W. Metzner and D. Vollhardt, PRL (1989)
A. Georges and G. Kotliar, PRB (1992)
M. Jarrell PRB (1992)
A. Georges et al. RMP (1996)

DMFT, (*d* = *3*)

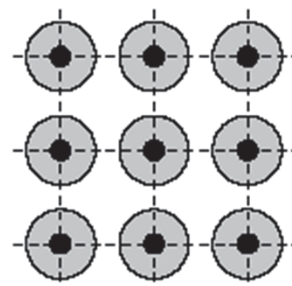
2d Hubbard: Quantum cluster method

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

Details on method in Lecture 4

Many active groups

- Paris: A. Georges, M. Ferrero, O. Parcollet
- Rutgers: K. Haule, G. Kotliar,
- Bâton Rouge: M. Jarrell
- Columbia: A. Millis
- Michigan: E. Gull
- Oakridge: Th. Maier, S.Okamoto
- Tokyo: M. Imada, Motome, Sakai
- Julich: A. Liebsch
- Graz: M. Aichhorn
- Hamburg: Potthoff
- LPS: M. Civelli
- ESRF: L. de Medici
- Trieste: M. Capone
- Vienna: Held
- Royal Holloway: G. Sordi
- Sherbrooke: D. Sénéchal, B. Kyung, P. Sémon, A.-M.S. Tremblay

Bio break

A.-M.S. Tremblay
"Strongly correlated superconductivity"
Chapt. 10 : *Emergent Phenomena in Correlated Matter Modeling and Simulation*, *Vol. 3*, E. Pavarini, E. Koch, and U. Schollwöck (eds.)
Verlag des Forschungszentrum Jülich, 2013