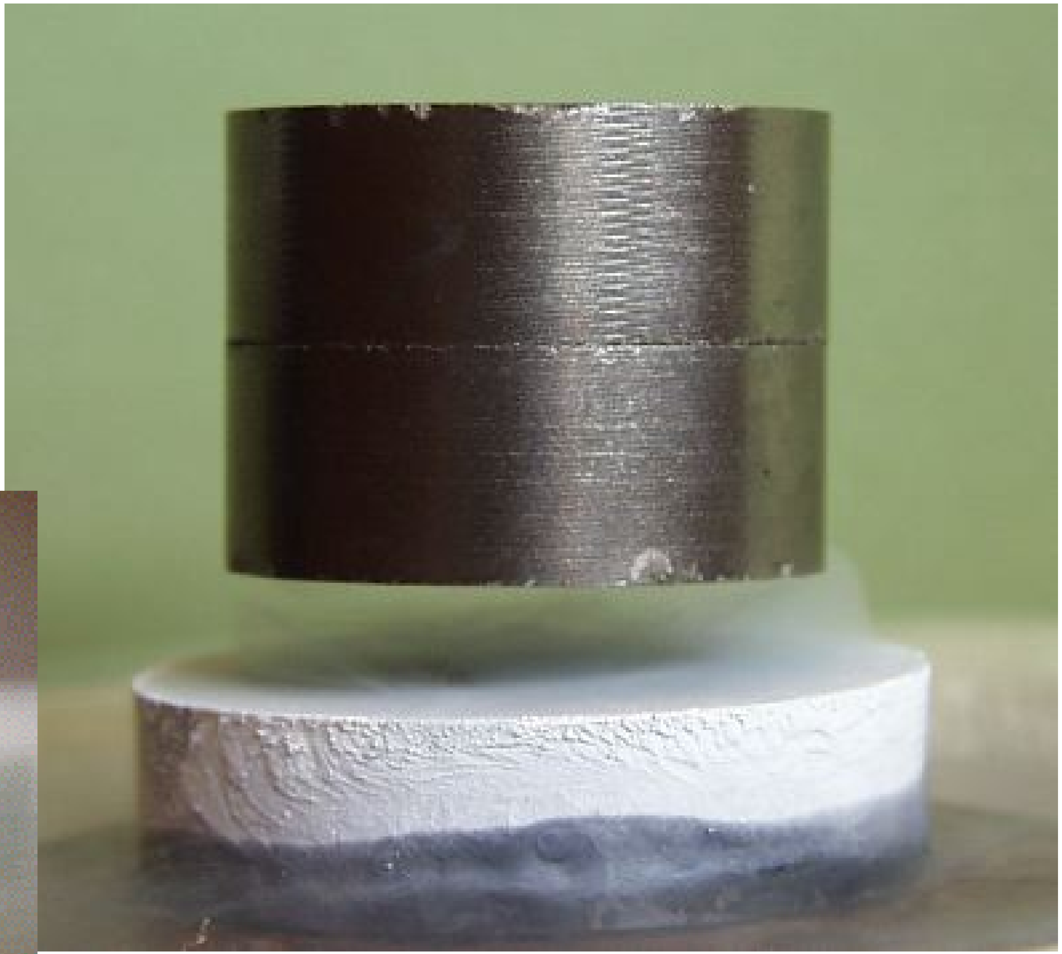
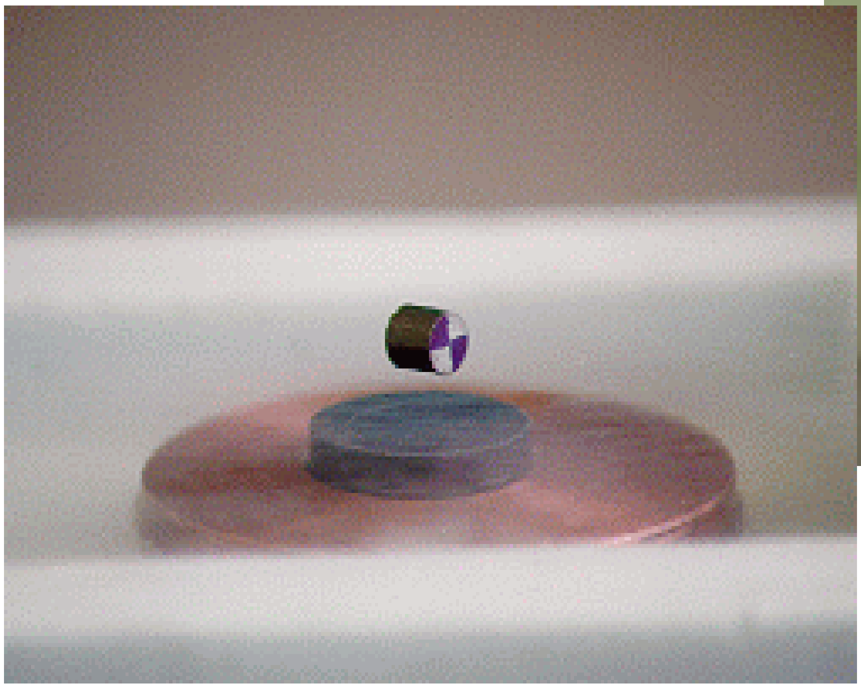
# What does this have to do with quantum magnetism?

Perfect diamagnetism (Shielding of magnetic field)

(Meissner effect)







André-Marie Tremblay

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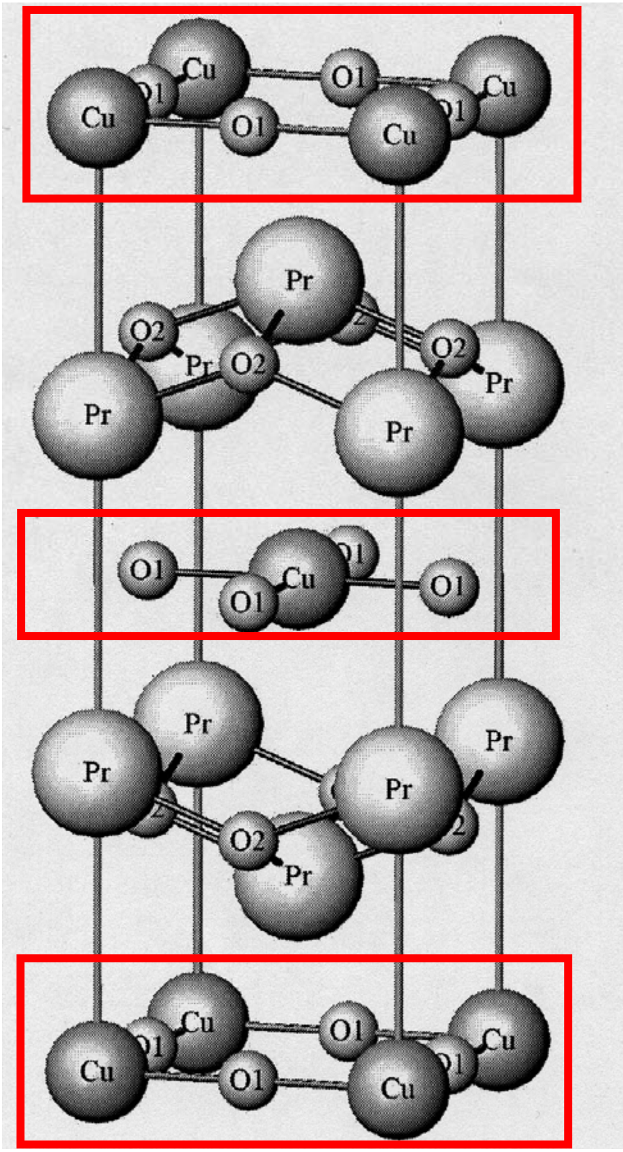
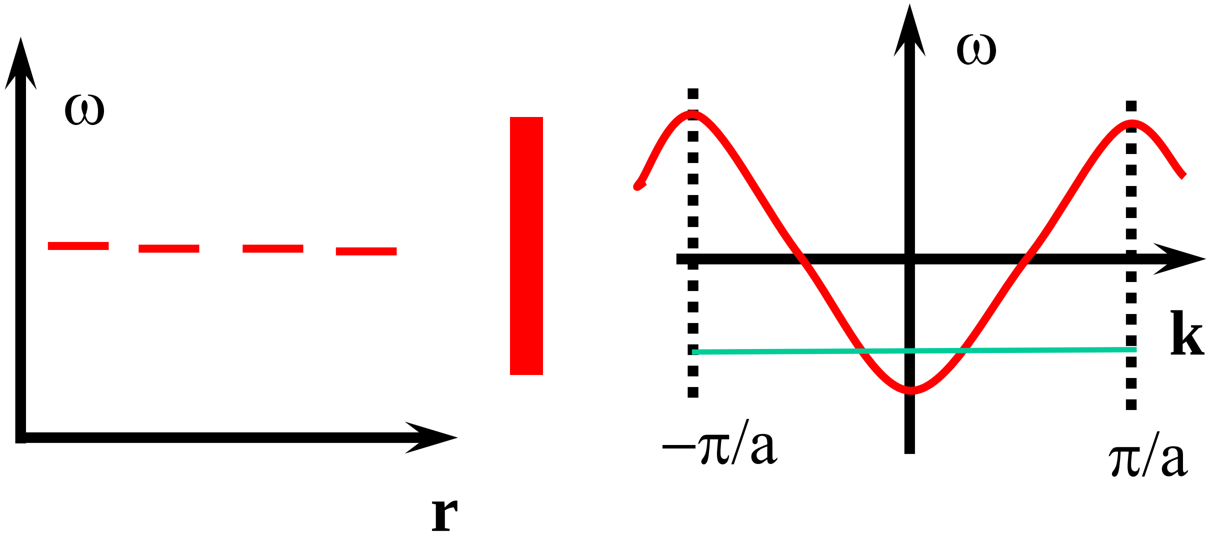
# $CuO_2$ planes





$YBa_2Cu_3O_{7-\delta}$

# Recall some basic Solid State Physics

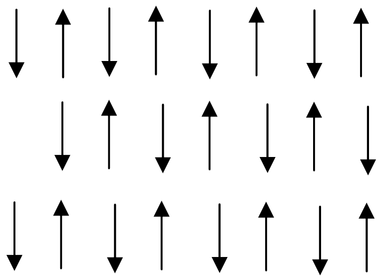


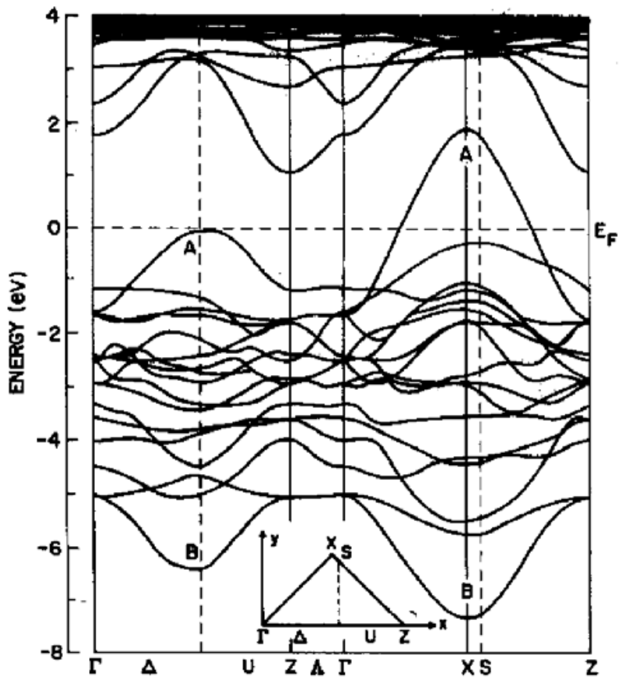
# Failure of the « Fermi liquid approach » in High Tc

*n = 1*,

Metal according to band theory

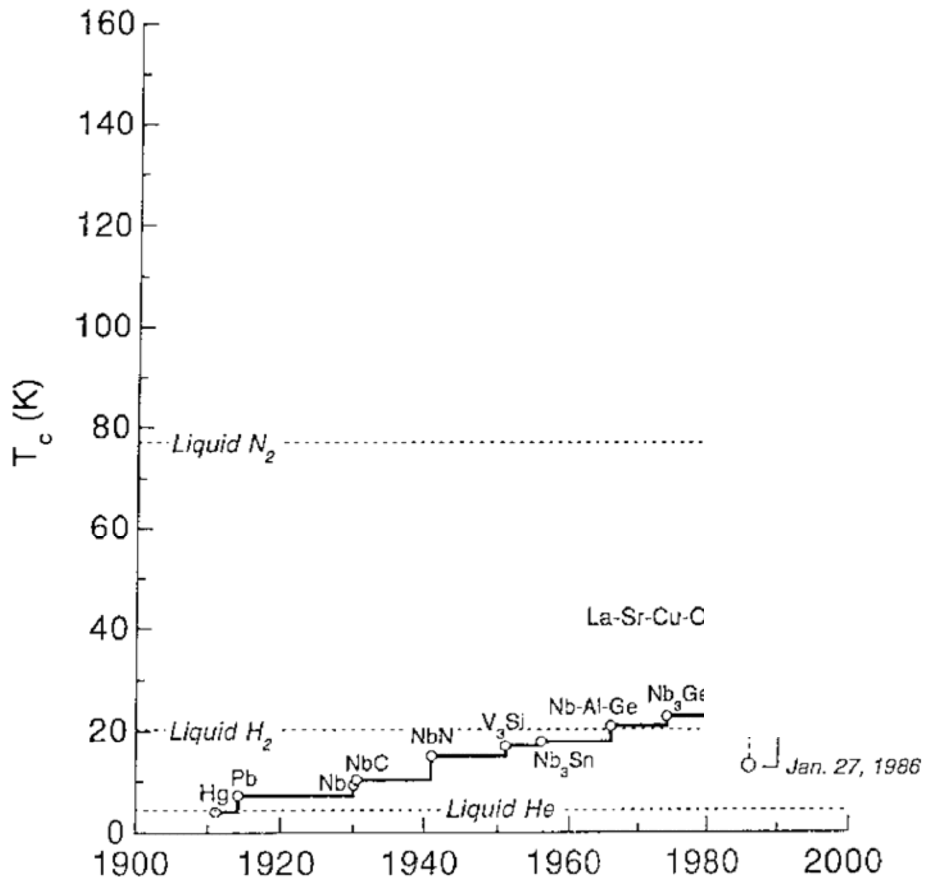
Antiferromagnetic insulator in reality





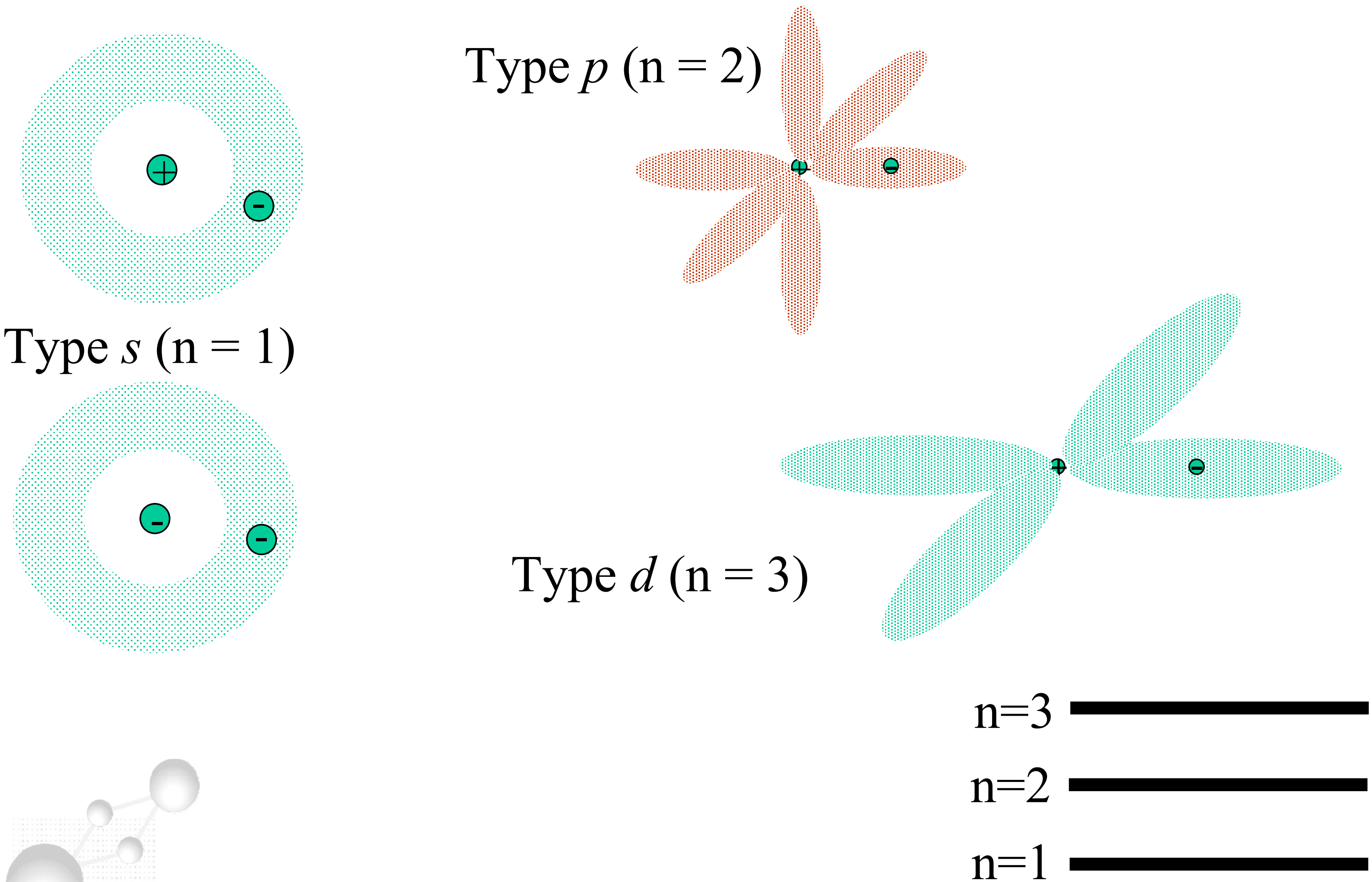
# High-temperature superconductivity

Away from half-filling



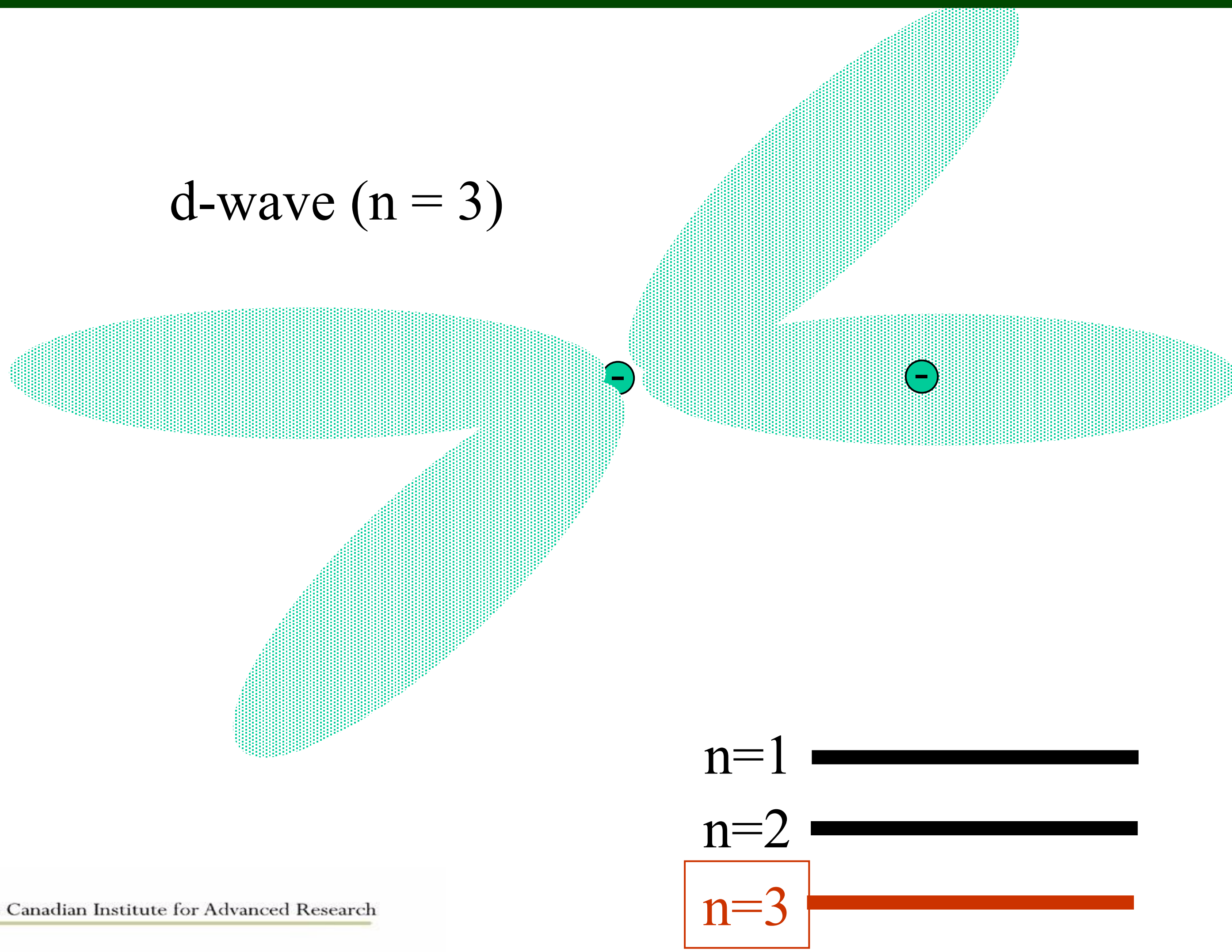
160
140
120
100
80
60
40
20
0
$T_c$ (K)
Liquid $N_2$
Liquid $H_2$
Liquid He
La-Sr-Cu-C
Hg
Pb
Nb
NbC
NbN
$V_3Si$
$Nb_3Sn$
Nb-Al-Ge
$Nb_3Ge$
Jan. 27, 1986
1900
1920
1940
1960
1980
2000

# Unusual experimental facts about HTSC: several possibilities for Cooper pairs



# Superconductivity is d-wave

d-wave (n = 3)




CIAR The Canadian Institute for Advanced Research

UBC : Bonn, Hardy, Liang



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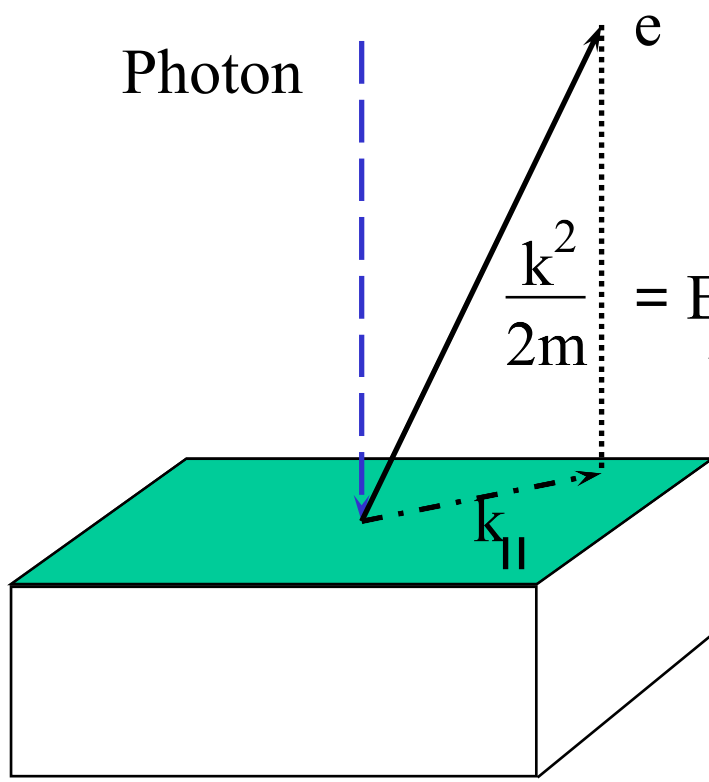
# An « anomalous » normal state

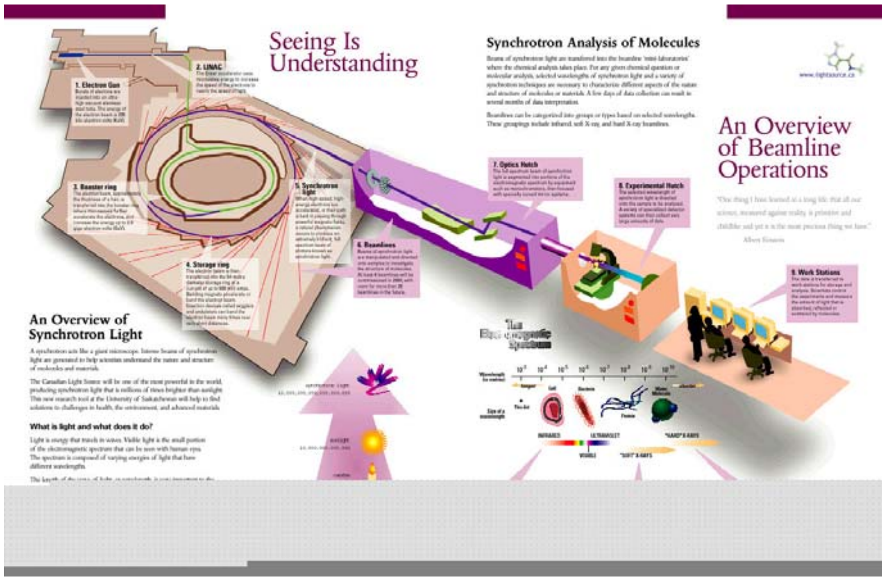
# Observing electronic states in *d = 2*

## Angle Resolved Photoemission Spectroscopy (ARPES)




$$\frac{k^2}{2m} = E_{ph} + \omega + \mu - W$$

# Synchrotron radiation



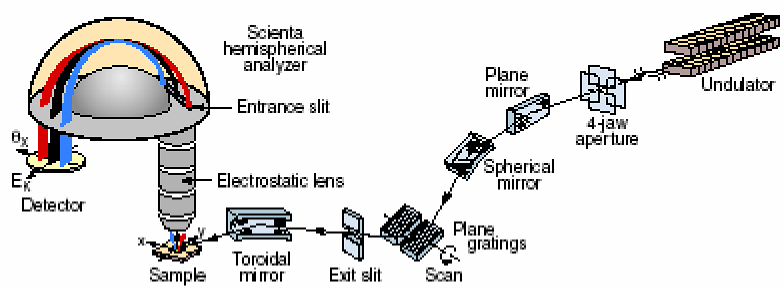
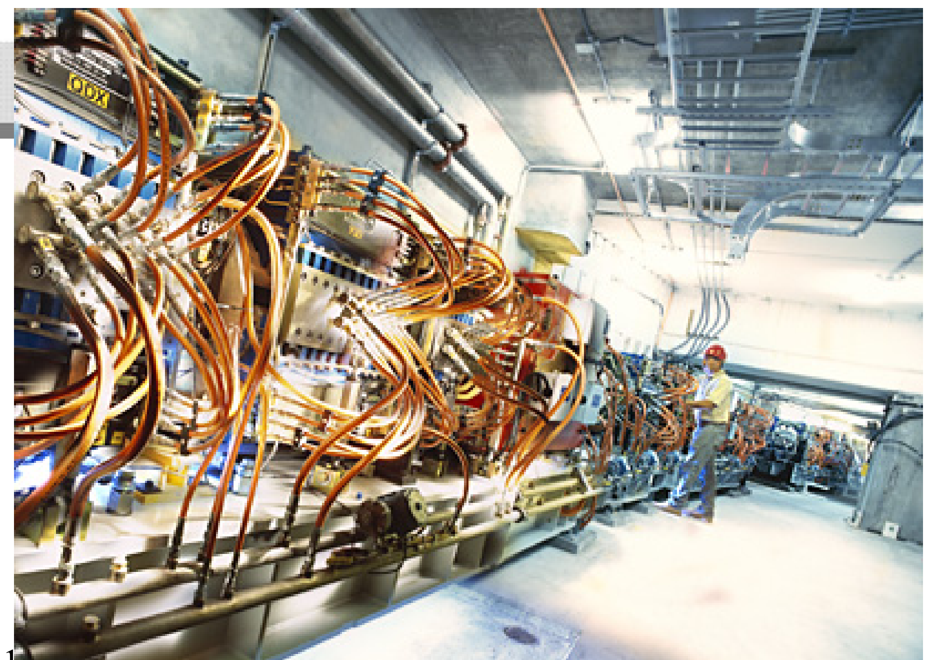
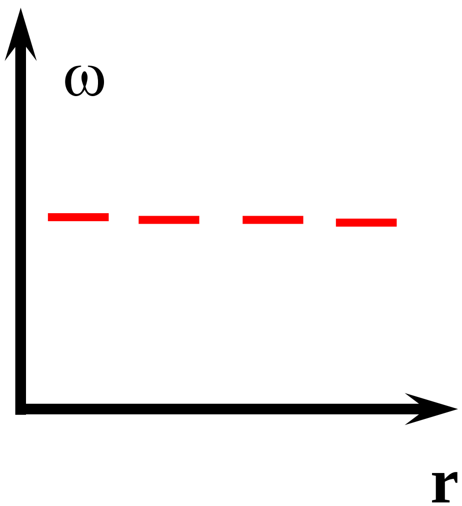



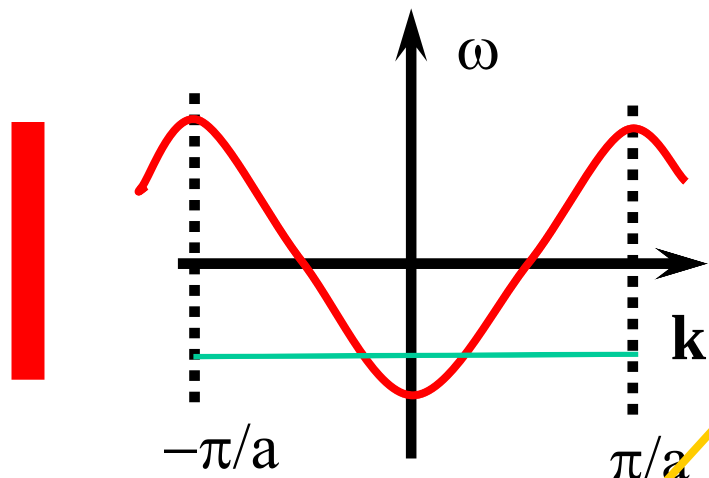

FIG. 6 Generic beamline equipped with a plane grating monochromator and a Scienta spectrometer [Color].

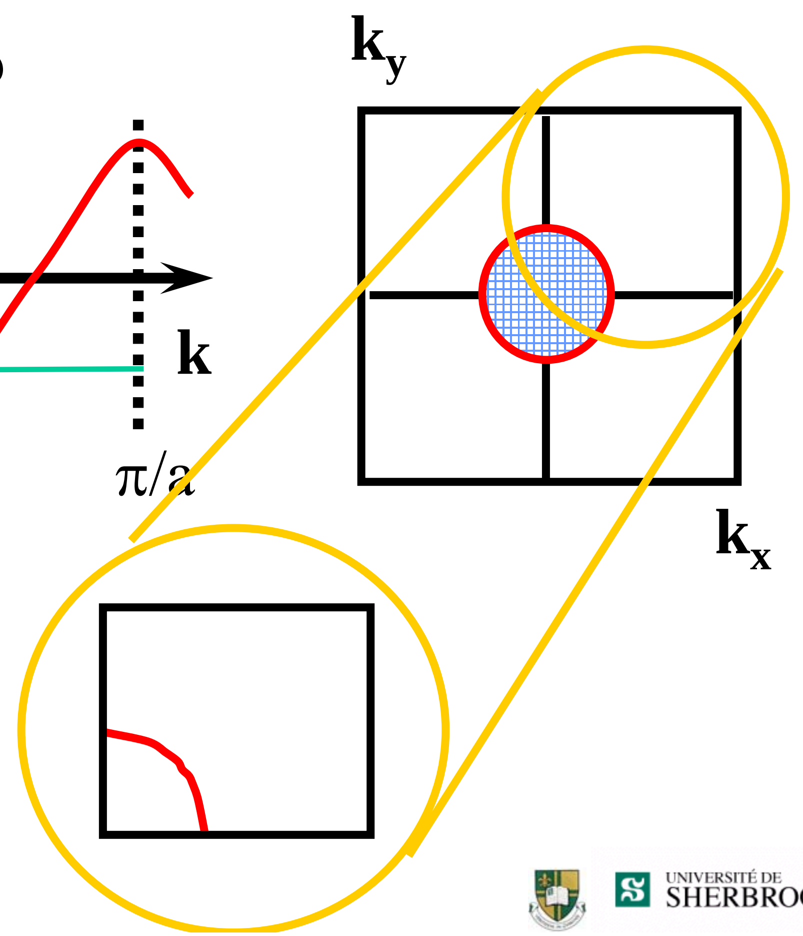
Damascelli, Shen, Hussain, 2002.



# Recall some basic Solid State Physics

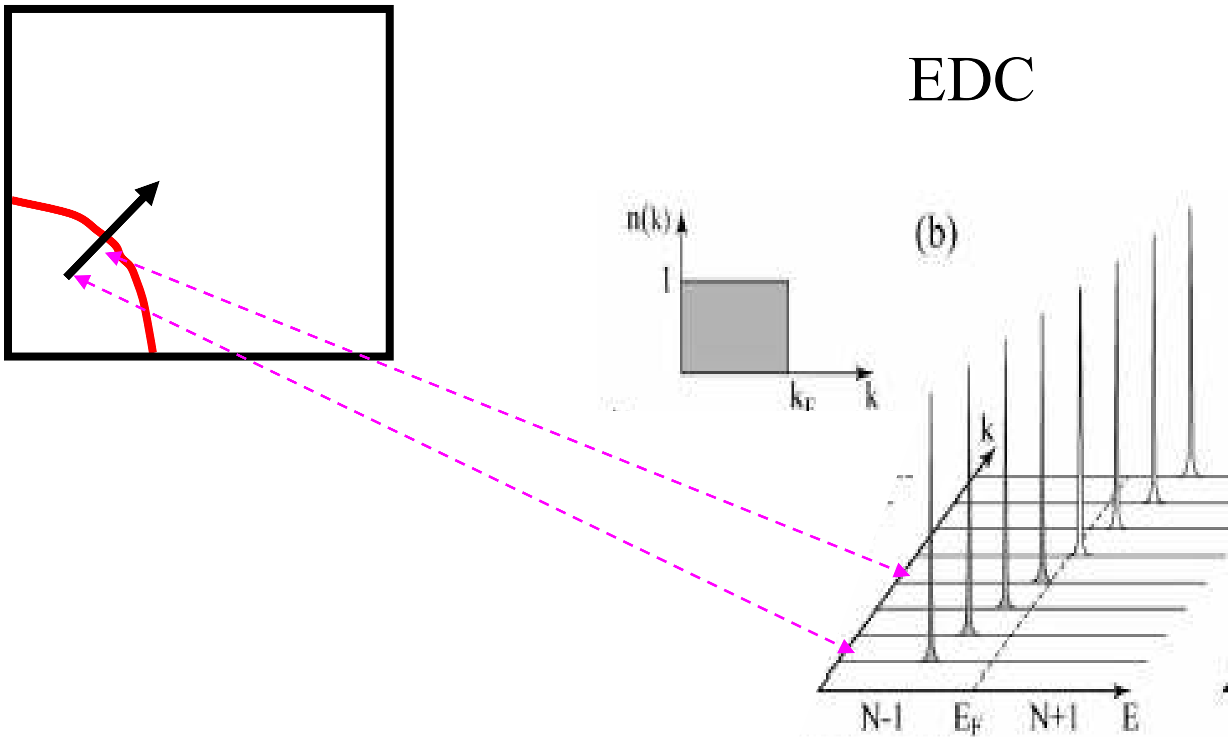


# Non-interacting case

EDC




Damascelli, Shen, Hussain, RMP 75, 473 (2003)



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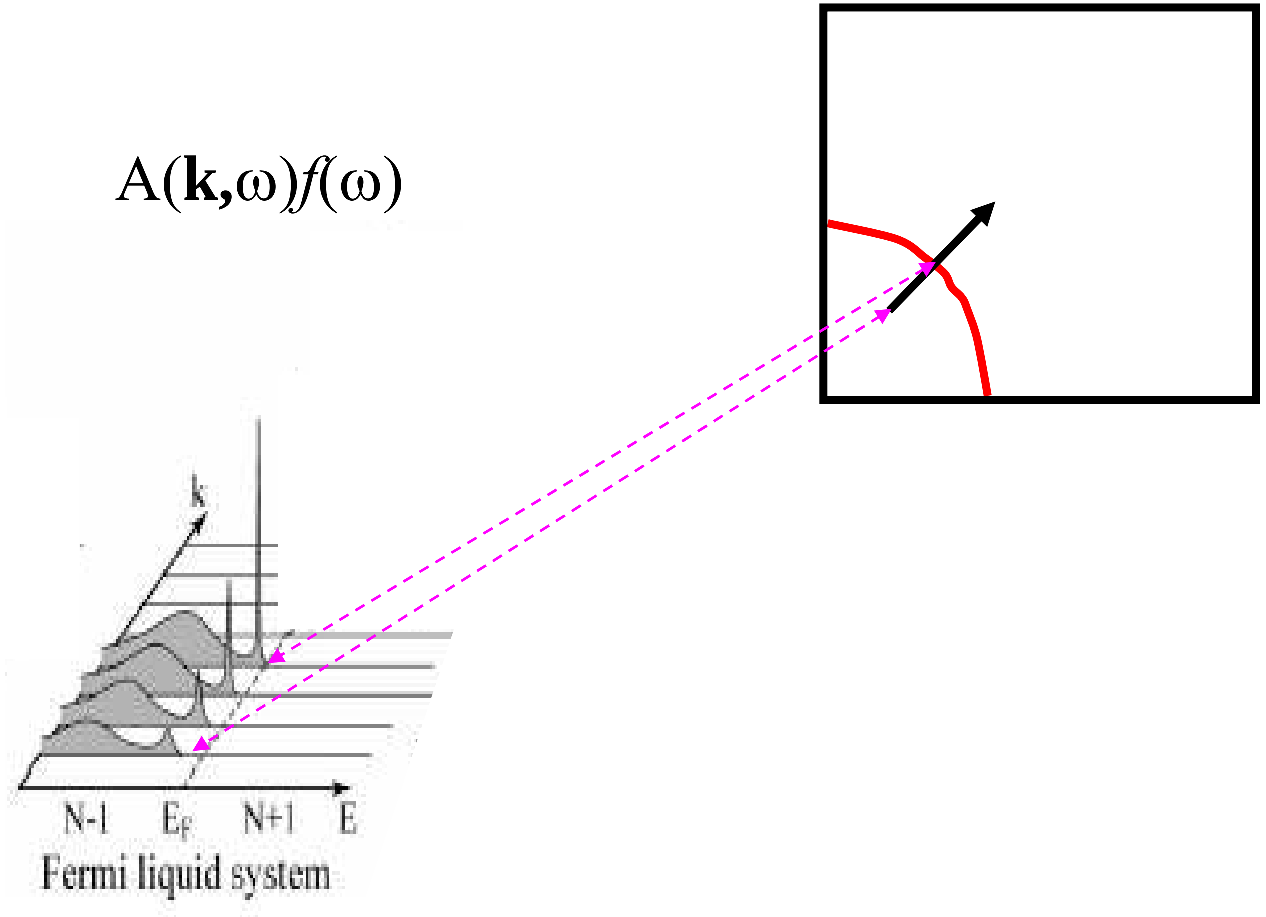
# With interactions : the Fermi liquid

$A(\mathbf{k},\omega)f(\omega)$






Damascelli, Shen, Hussain, RMP 75, 473 (2003)

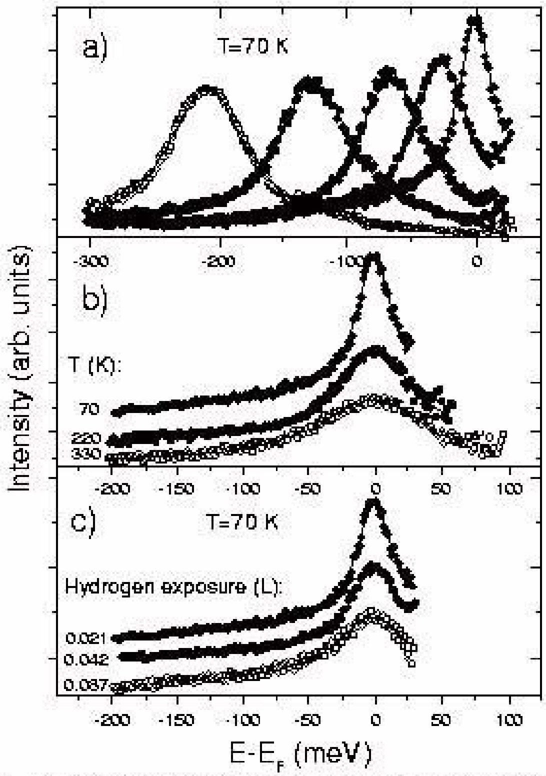



FIG. 2. Spectral intensity as a function of binding energy for constant emission angle, normalized to the experimentally determined Fermi cut-off. Data are symbols, while lines are fits to the Lorentzian peaks with a linear background. The dependence on the binding energy (a), temperature (b), and hydrogen exposure (c) is shown.

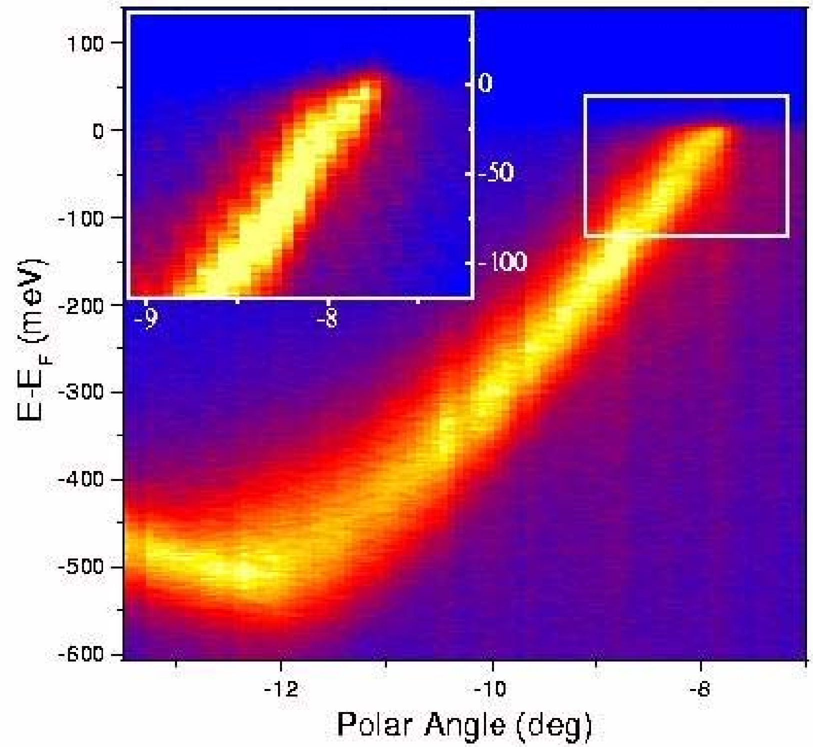
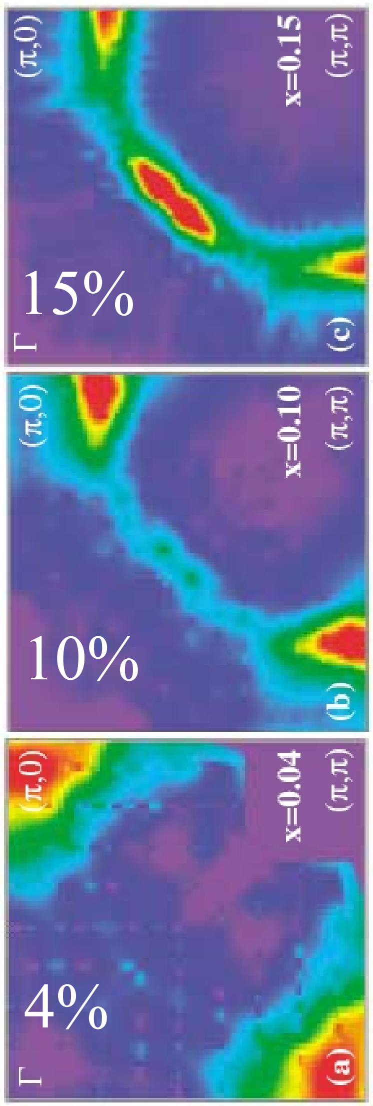
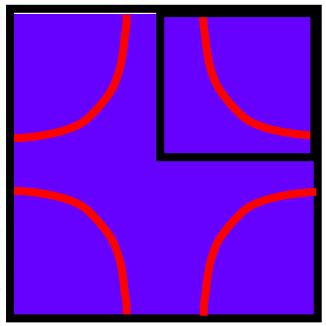



FIG. 1. ARPES intensity plot of the Mo(110) surface recorded along the $\overline{\Gamma}-\overline{\mathrm{N}}$ line of the SBZ at 70 K Shown in the inset is the spectrum of the region around $k_F$ taken with special attention to the surface cleanliness.

T. Valla, A. V. Fedorov, P. D. Johnson, and S. L. Hulbert
P.R.L. **83**, 2085 (1999).

# Pseudogap: Fermi surface of an e-doped high $T_c$



Armitage *et al.* PRL **87**, 147003; **88**, 257001

# Experimental phase diagram

Mott Insulator

Electron doping

Hole doping

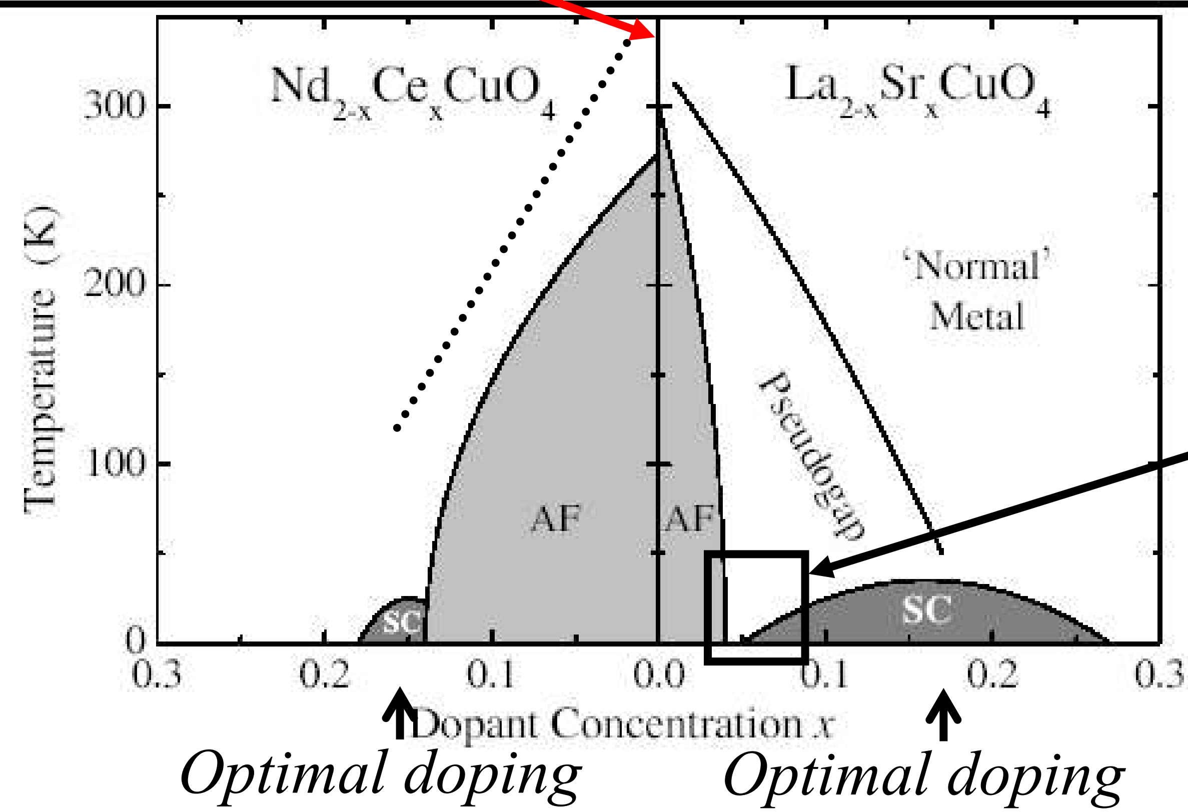



FIG. 1 Phase diagram of n and p-type superconductors.

Stripes

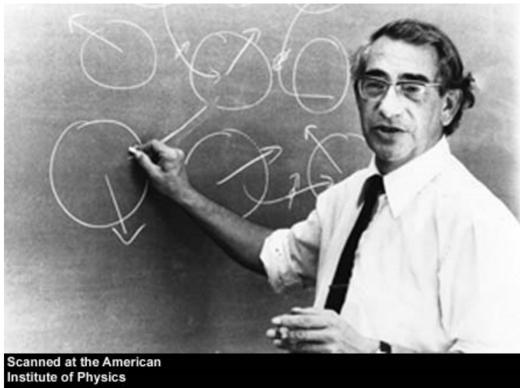
$n$, electron density

Damascelli, Shen, Hussain, RMP 75, 473 (2003)

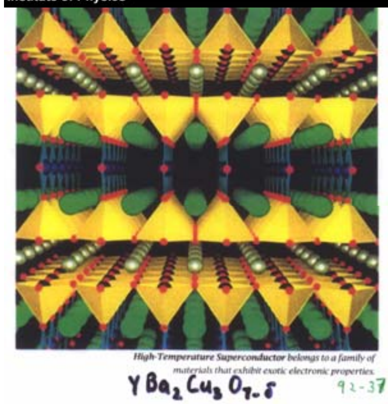
# Outline of all three hours

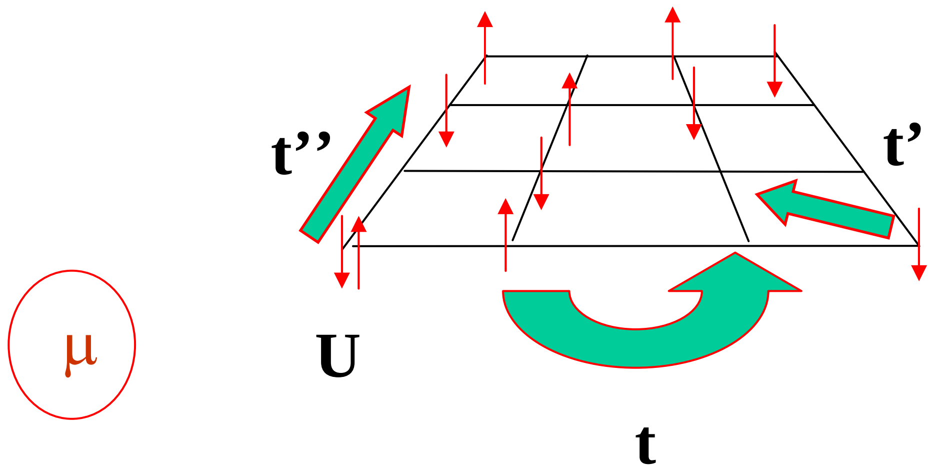
- The Hubbard model : itinerant *vs* localized behavior
- Methodology (non-perturbative)
- Results and concordance between methods.
- Comparisons with experiment

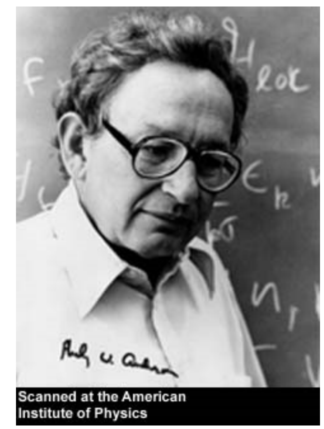
# The Hubbard model



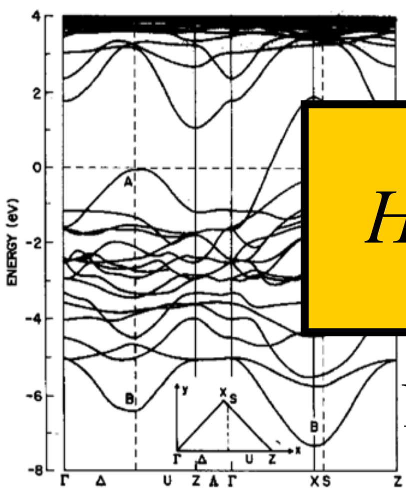

Simplest microscopic model for $Cu\ O_2$ planes.




LSCO

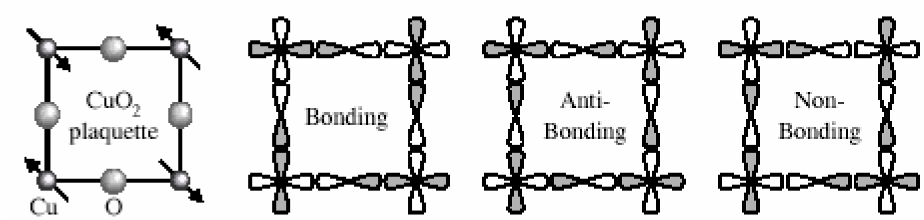


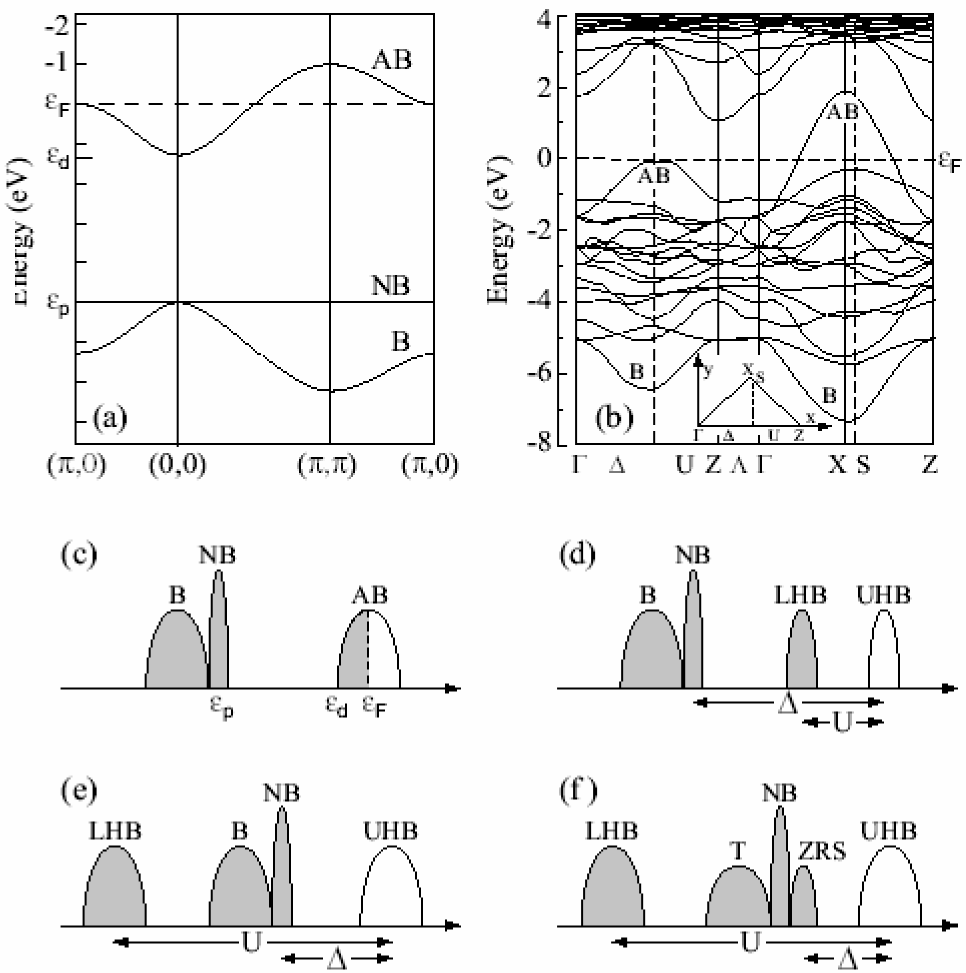

$$H = -\sum_{<ij>\sigma} t_{i,j}\left(c_{i\sigma}^{\dagger}c_{j\sigma} + c_{j\sigma}^{\dagger}c_{i\sigma}\right) + U\sum_{i} n_{i\uparrow}n_{i\downarrow}$$

No mean-field factorization for d-wave superconductivity

# An effective model

A. Macridin *et al.*, cond-mat/0411092






Damascelli, Shen, Hussain, RMP 75, 473 (20 )

# One band Hubbard model

$$H = \sum_{\sigma} \int \mathrm{d}^3 r \; \psi_\sigma^\dagger(\mathbf{r}) \left( -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) \right) \psi_\sigma(\mathbf{r})$$
$$+ \sum_{\sigma,\sigma'} \int \frac{\mathrm{d}^3 r \mathrm{d}^3 r'}{2} U(\mathbf{r}-\mathbf{r}') \psi_\sigma^\dagger(\mathbf{r}) \psi_{\sigma'}^\dagger(\mathbf{r}') \psi_{\sigma'}(\mathbf{r}') \psi_\sigma(\mathbf{r})$$

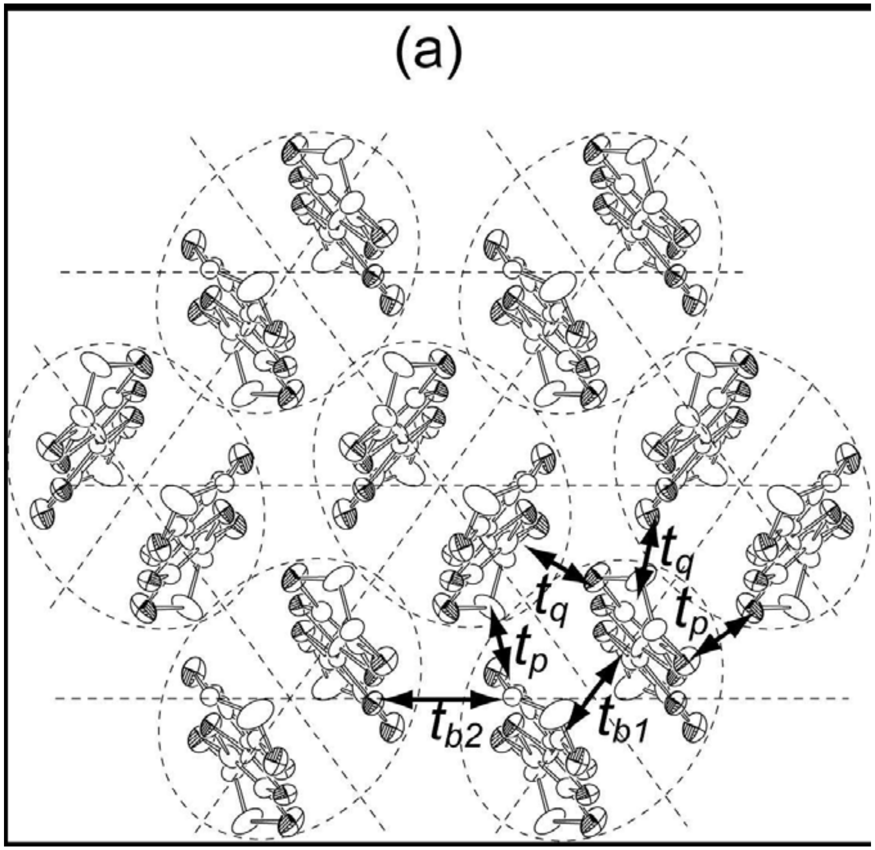
$$\psi(\mathbf{r}) = \sum_{\mathbf{n} \in \Gamma} c_{\mathbf{n}} w(\mathbf{r} - \mathbf{n})$$

$$H_2 = \frac{1}{4} \sum_{\substack{ijkl \\ \sigma_i \sigma_j \sigma_k \sigma_l}} \langle i\sigma_i, j\sigma_j | U | k\sigma_k, l\sigma_l \rangle c_{i\sigma_i}^\dagger c_{j\sigma_j}^\dagger c_{l\sigma_l} c_{k\sigma_k}$$

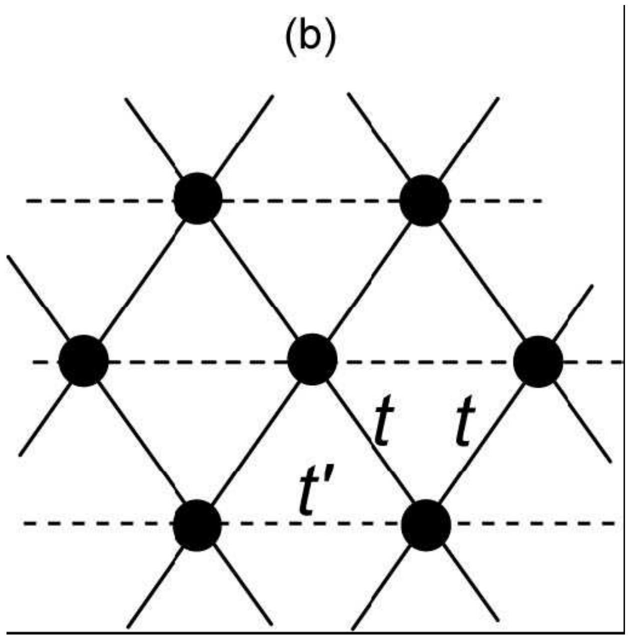
Direct exchange is ferromagnetic !

# One-band Hubbard model for organics

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




Y. Shimizu, et al. Phys. Rev. Lett. **91**, 107001(2003)

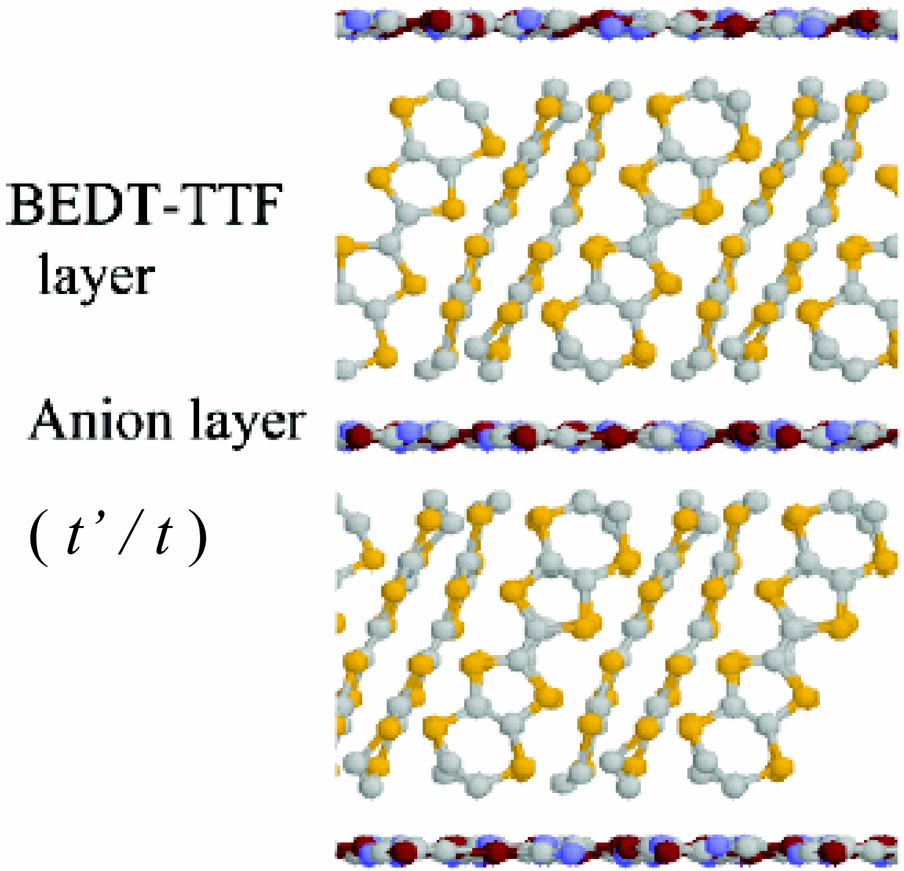


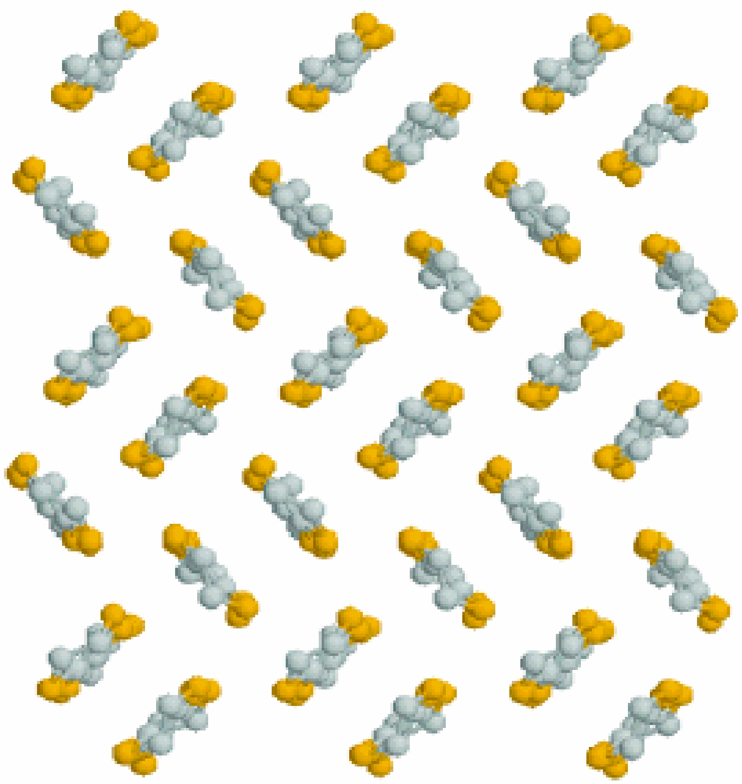

$t \approx 50\ \text{meV}$

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

$t'/t \sim 0.6 - 1.1$

# Layered organics (κ–BEDT-X family)



*n = 1*



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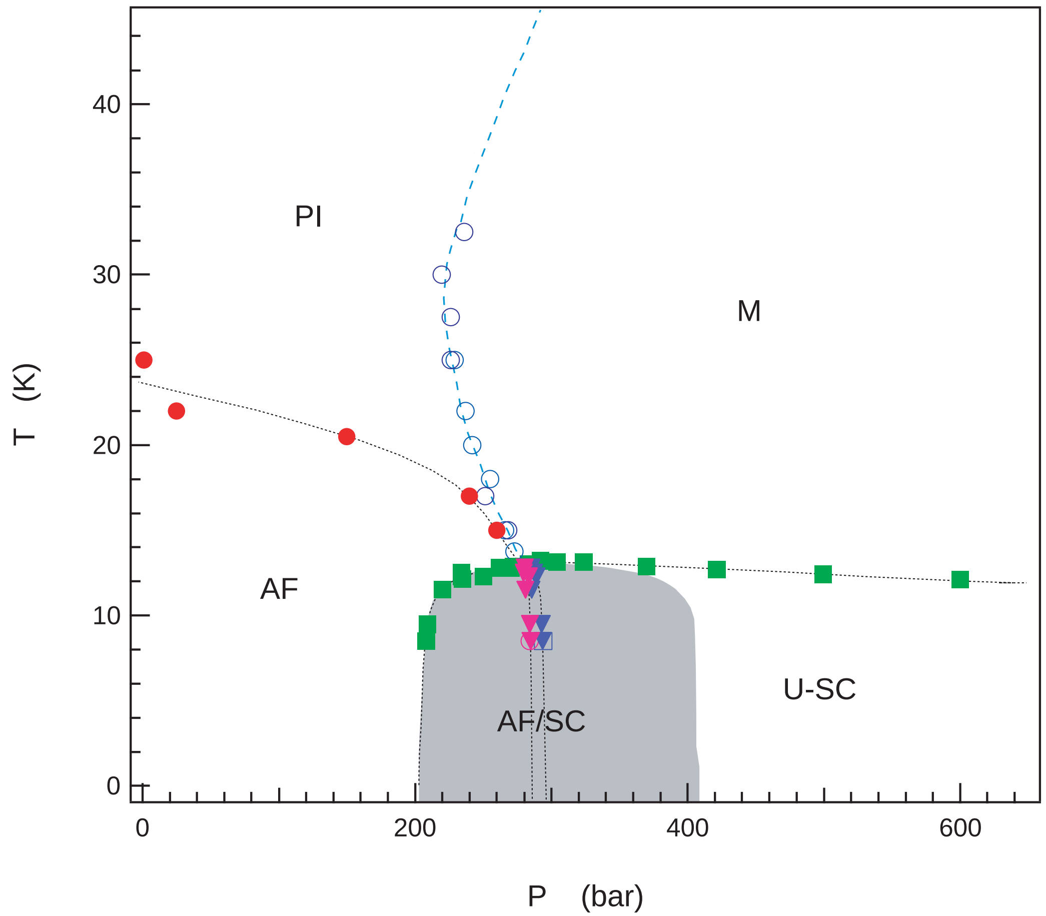
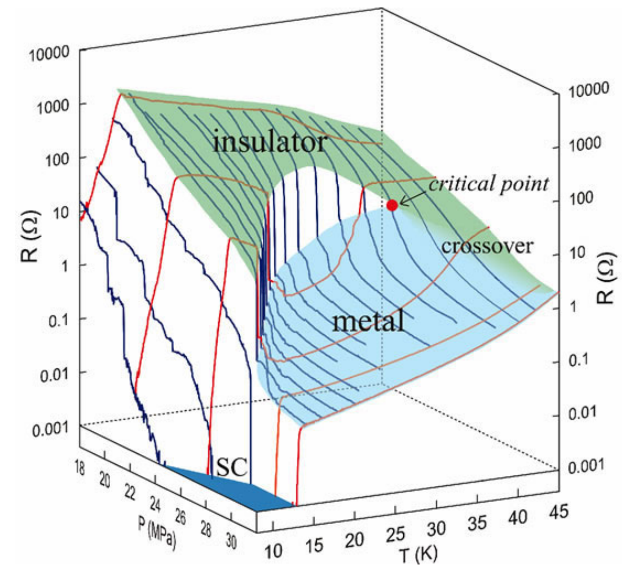
# Experimental phase diagram for Cl



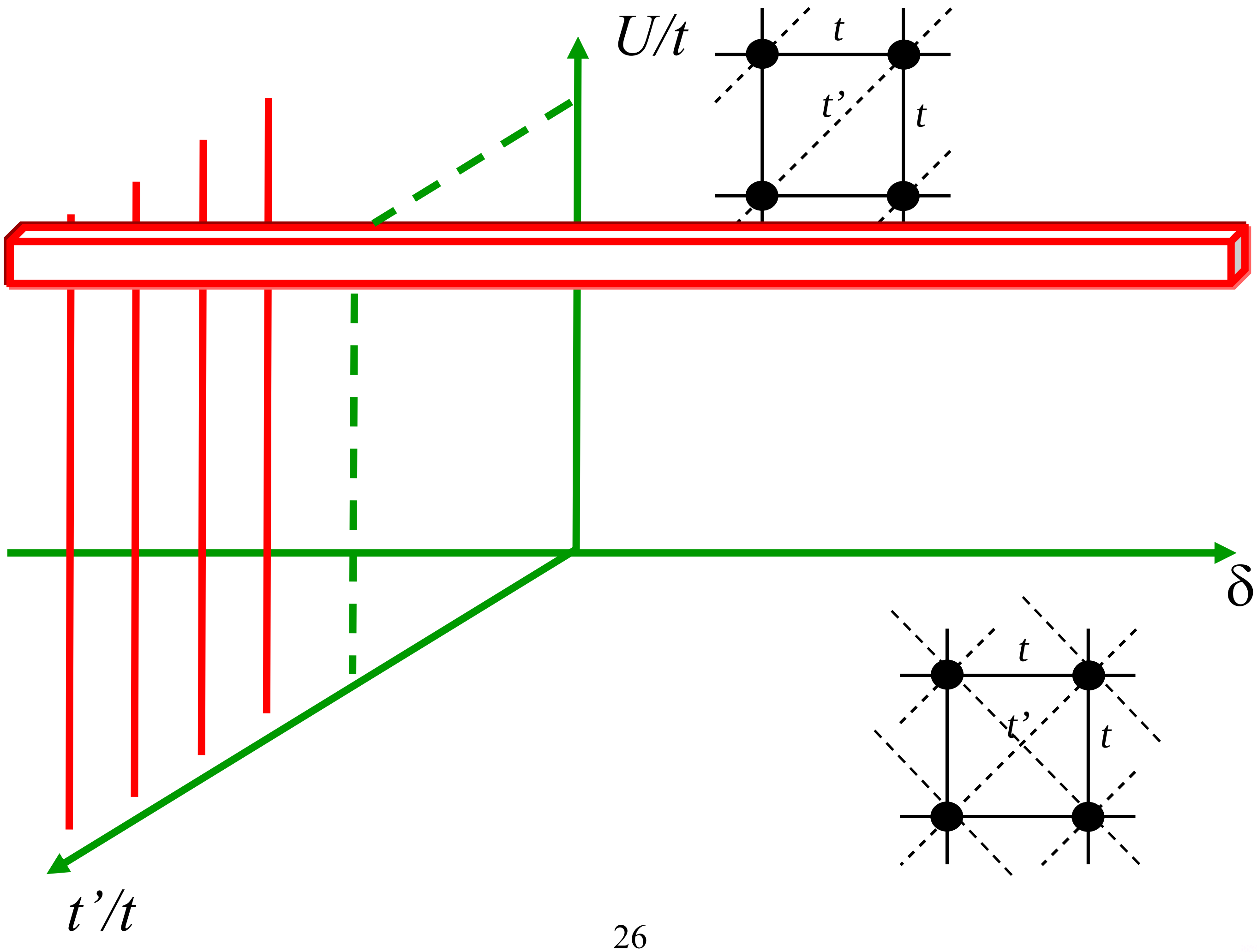




F. Kagawa, K. Miyagawa, + K. Kanoda
PRB **69** (2004) +Nature **436** (2005)

## Diagramme de phase (X=Cu[N$(CN)_2$]Cl)

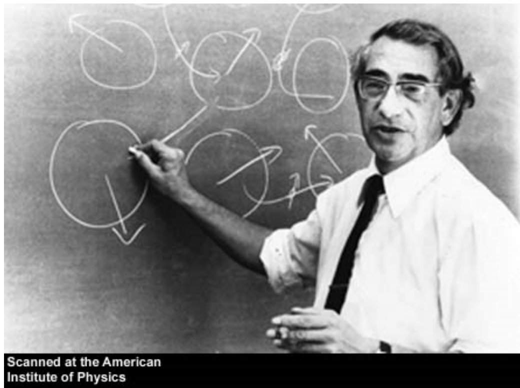
S. Lefebvre et al. PRL **85**, 5420 (2000), P. Limelette, et al. PRL 91 (2003)

# Perspective



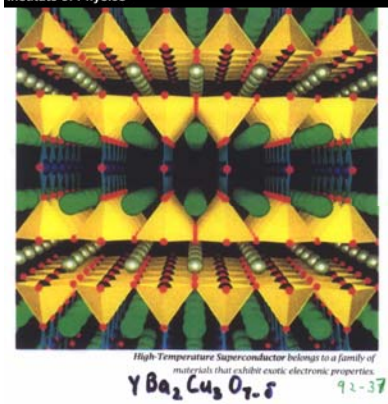
# « Solutions » of the Hubbard model

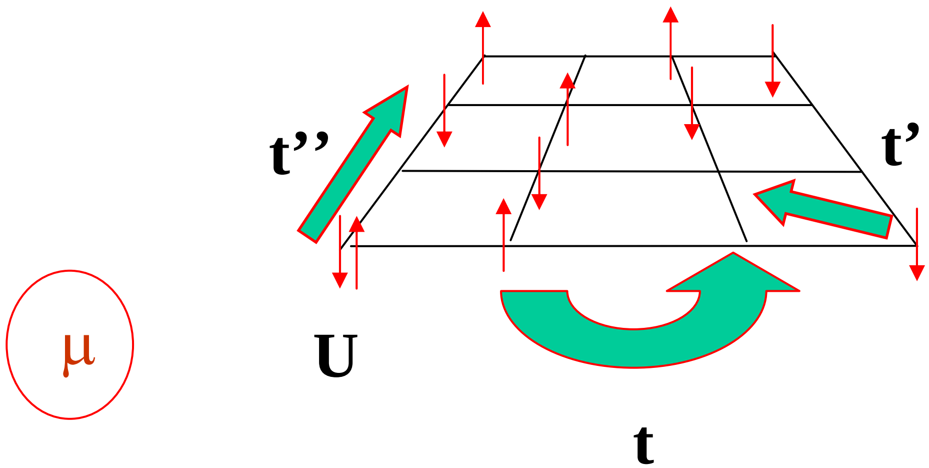
- Bethe *ansatz* in one dimension (correlation functions?).
- Renormalization group in one dimension or quasi-one dimension (spin-charge separation, Luttinger liquid)
  - *Solyom, Bourbonnais*
- Nagaoka theorem
- In two or three dimension :
  - Gutzwiller approximation
  - Various forms of slave bosons (+ gauge fields) mean-field theory.
- Infinite dimension (Dynamical Mean-Field Theory)
- ……

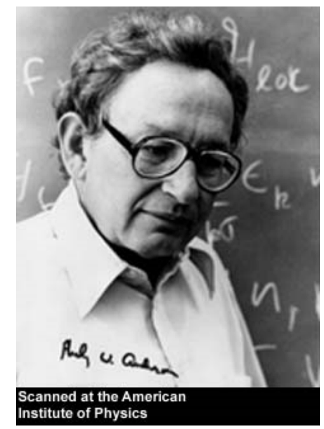



# The Hubbard model

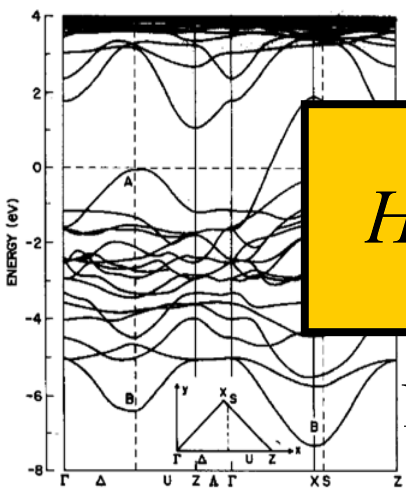
Simplest microscopic model for $Cu\ O_2$ planes.



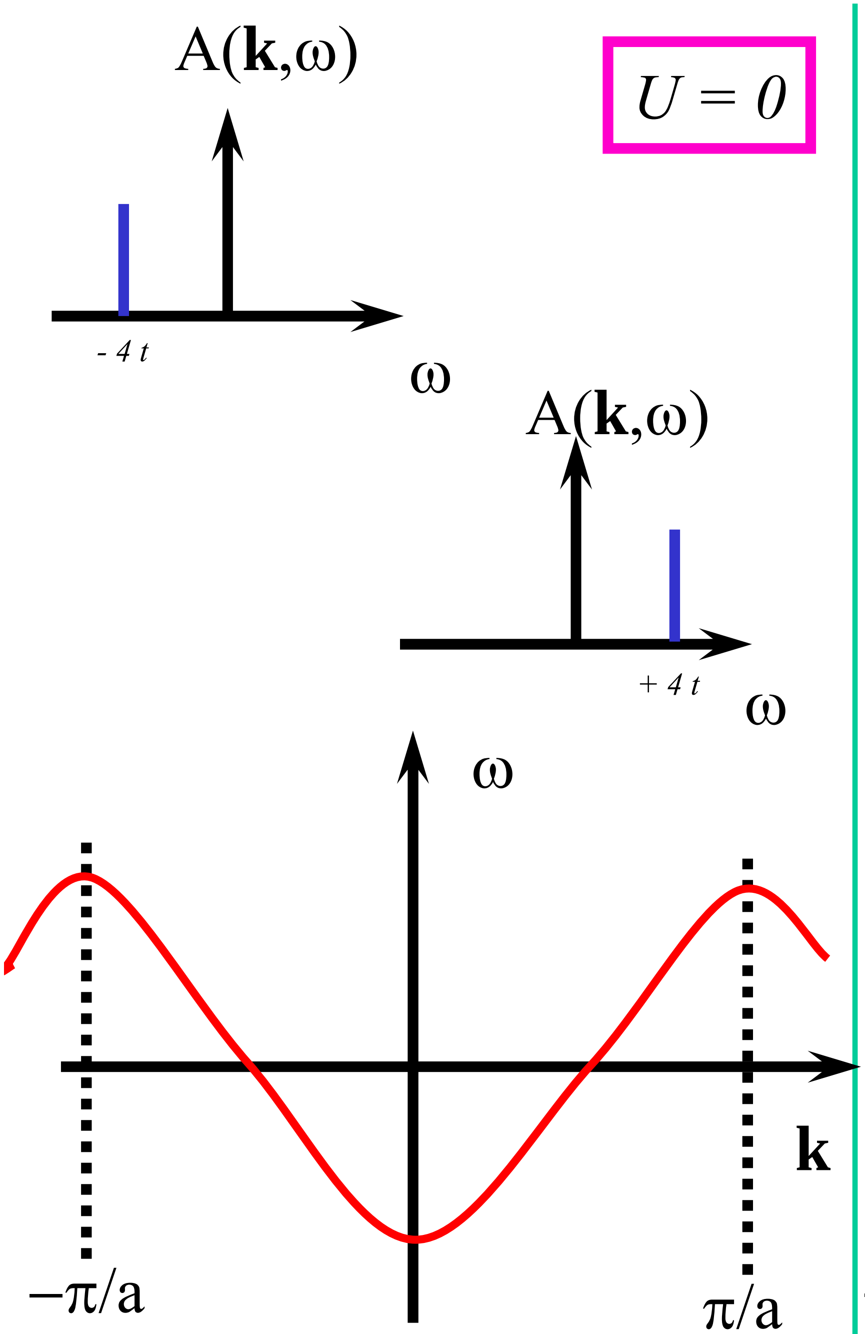



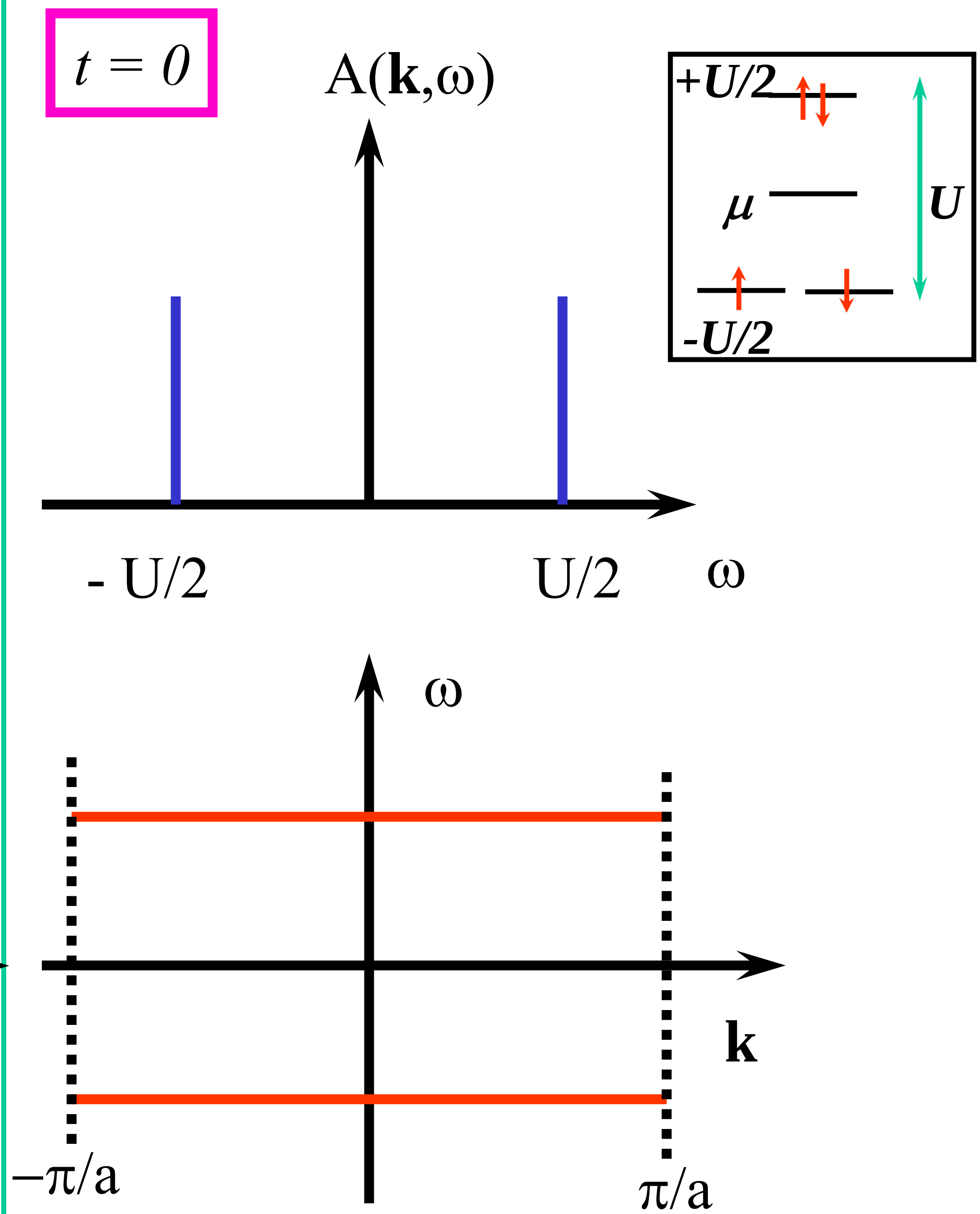

LSCO



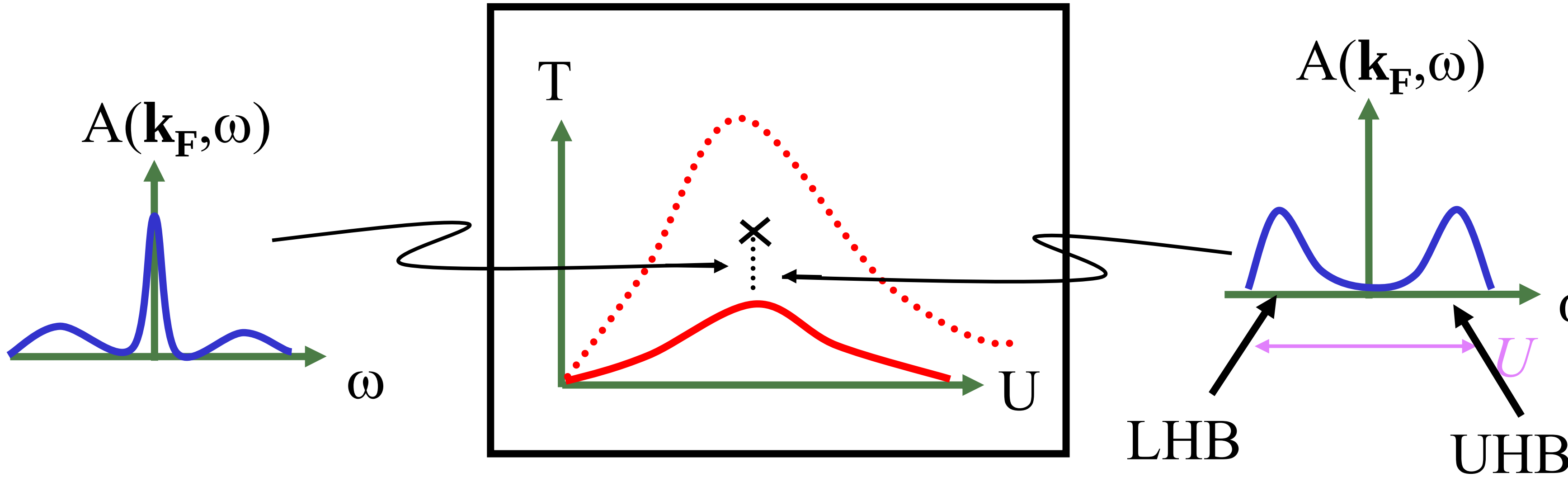

$$H = -\sum_{<ij>\sigma} t_{i,j}\left(c^\dagger_{i\sigma}c_{j\sigma} + c^\dagger_{j\sigma}c_{i\sigma}\right) + U\sum_i n_{i\uparrow}n_{i\downarrow}$$

No mean-field factorization for d-wave superconductivity


A(k,ω)
U = 0
- 4 t
ω
A(k,ω)
+ 4 t
ω
ω
k
−π/a
π/a

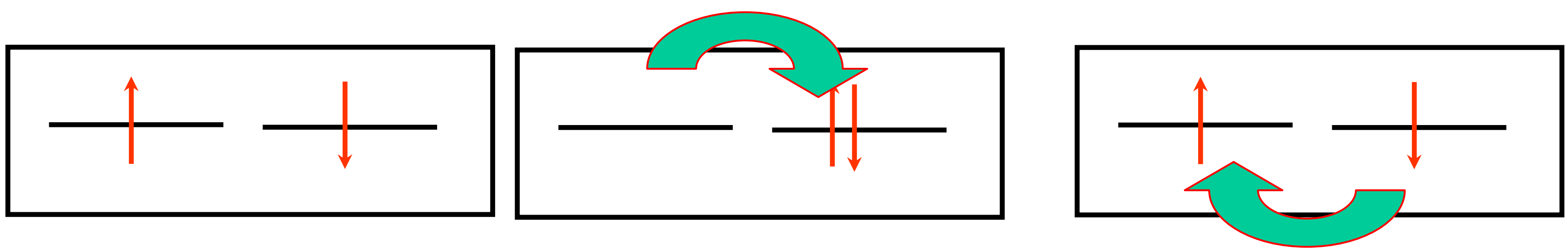

t = 0
A(k,ω)
+U/2
μ
U
-U/2
- U/2
U/2
ω
ω
k
−π/a
π/a

# *Weak* vs *strong* coupling, *n=1*




$U \sim 1.5W \quad (W = 8t)$

Mott transition




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

# A hierarchy of effective models (see Schrödinger *vs* Dirac)

- $t - J$ model : applying second order degenerate perturbation theory

$$|\psi_\alpha\rangle = |\alpha\rangle + \sum_{E_m>0} \frac{\langle m|H_1|\alpha\rangle}{E_\alpha - E_m}|m\rangle$$

$$= |\alpha\rangle - \frac{1}{U}\sum_\beta \langle\beta|H_1|\alpha\rangle|\beta\rangle$$

$$= |\alpha\rangle - \frac{1}{U}\sum_m |m\rangle\langle m|H_1|\alpha\rangle$$

$$= |\alpha\rangle - \frac{1}{U}H_1|\alpha\rangle$$

# $n = 1$ the Heisenberg model

$$\langle\psi_{\alpha'}|(H_0+H_1)|\psi_\alpha\rangle = \left(\langle\alpha'| - \frac{1}{U}\langle\alpha'|H_1\right)(H_0+H_1)\left(|\alpha\rangle - \frac{1}{U}H_1|\alpha\rangle\right)$$
$$= -\frac{1}{U}\langle\alpha'|H_1^2|\alpha\rangle + \mathcal{O}(1/U^2)$$

$$H_1 = -t\sum_{\langle ij\rangle,\sigma}(c_{i,\sigma}^\dagger c_{j,\sigma} + c_{j,\sigma}^\dagger c_{i,\sigma})$$

$$H_1^2 = t^2\sum_{\langle ij\rangle,\sigma}\sum_{\langle kl\rangle,\sigma'}(c_{i,\sigma}^\dagger c_{j,\sigma} + c_{j,\sigma}^\dagger c_{i,\sigma})(c_{k,\sigma'}^\dagger c_{l,\sigma'} + c_{l,\sigma'}^\dagger c_{k,\sigma'})$$

# $n$ = *1* the Heisenberg model

$$H_{\mathrm{eff.}} = \frac{4t^2}{U} \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

Worthwhile decrease in size of Hilbert space !

# Is this model enough for the AFM at *n = 1?*

Coldea *et al.* PRL (2001)

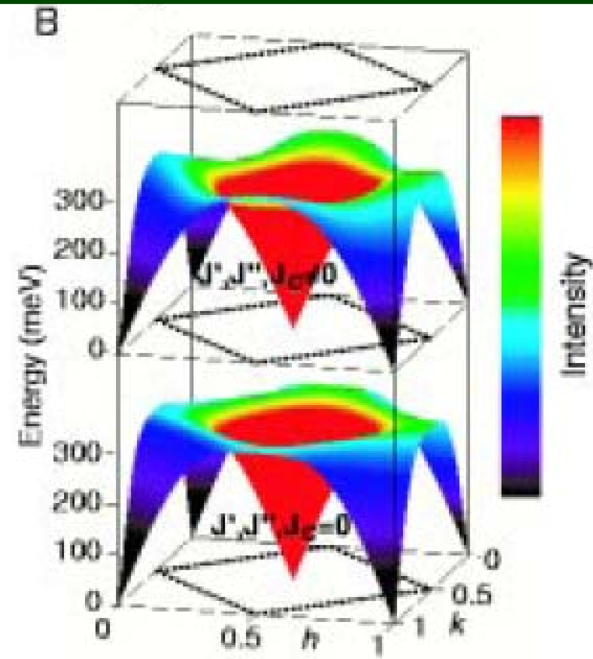
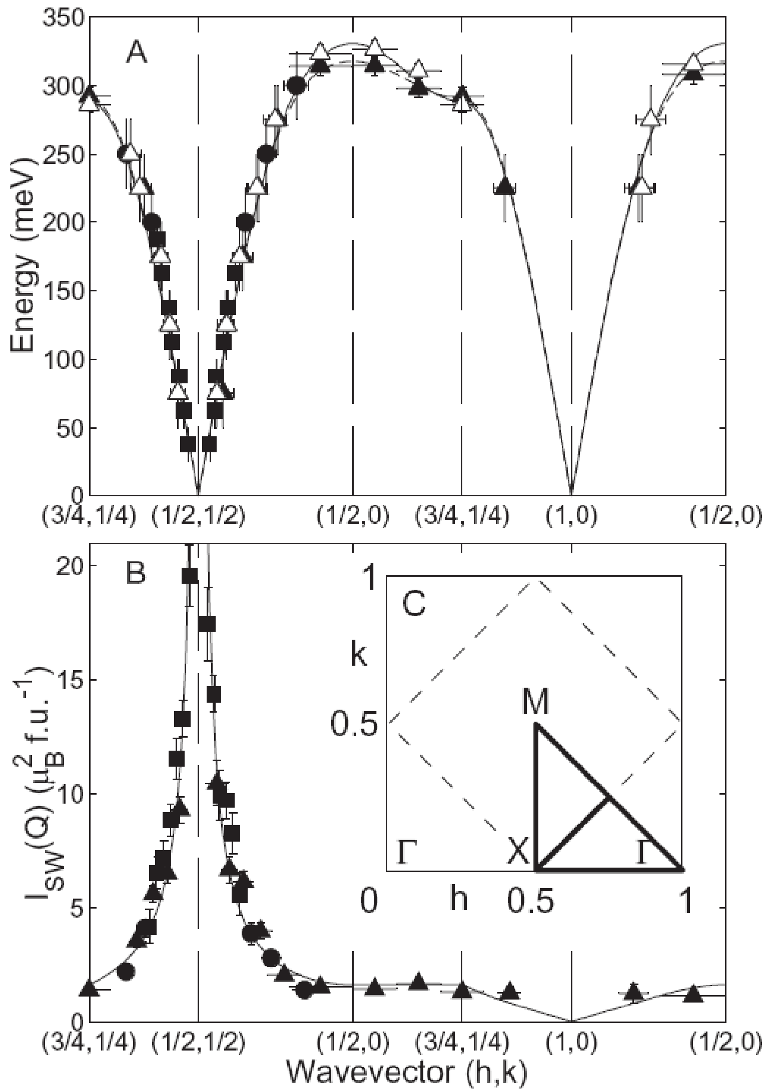



FIG. 1. (color) **A** The $CuO_2$ plane showing the atomic orbitals (Cu $3d_{x^2-y^2}$ and O $2p_{x,y}$) involved in the magnetic interactions. $J$, $J'$ and $J''$ are the first-, second- and third-nearest-neighbor exchanges and $J_c$ is the cyclic interaction which couples spins at the corners of a square plaquette. Arrows indicate the spins of the valence electrons involved in the exchange. **B** Lower surface is the dispersion relation for $J$=136 meV and no higher-order magnetic couplings or quantum corrections. The upper surface shows the effect of the higher-order magnetic interactions determined by the present experiment. Color is spin-wave intensity.

# Including $t(t/U)^3$ terms




$$S_i \cdot S_{i'} + J'' \sum_{\langle i,i'' \rangle} S_i \cdot S_{i''}$$

$$_k \cdot S_l) + (S_i \cdot S_l)(S_k \cdot S_j) \qquad (1)$$

$$J = 4t^2/U - 24t^4/U^3, \; J_c = 80t^4/U^3$$

$$J' = J'' = 4t^4/U^3$$

$$U/t \sim 7 - 9$$

Delannoy *et al.* + the



## APPENDIX A: SPIN HAMILTONIAN WITH $t$, $t'$ AND $t''$

The introduction of $t'$ and $t''$ will to first order renormalized the coupling constants already present in the spin Hamiltonian.

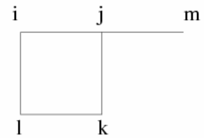
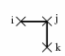



FIG. 6: Label of the different sites

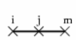
Some terms are added to the one obtained when $t'$ and $t''$ are not taken into account, but some new terms will be included with new topologies. In order to simplify the notations, we are introducing some notations :

$$\begin{aligned}
\mathrm{P}_1^{i,j,k,l} &= \Big\{(\vec{S_i}\cdot\vec{S_j})\,(\vec{S_k}\cdot\vec{S_l}) \\
&\quad +(\vec{S_i}\cdot\vec{S_l})\,(\vec{S_k}\cdot\vec{S_j}) - (\vec{S_i}\cdot\vec{S_k})\,(\vec{S_j}\cdot\vec{S_l})\Big\} \\
\mathrm{P}_2^{i,j,k,l} &= \Big\{\vec{S_i}\cdot\vec{S_j} + \vec{S_i}\cdot\vec{S_k} + \vec{S_i}\cdot\vec{S_l} \\
&\quad + \vec{S_j}\cdot\vec{S_k} + \vec{S_j}\cdot\vec{S_l} + \vec{S_k}\cdot\vec{S_l}\Big\}
\end{aligned} \tag{A1}$$

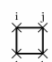
The $\mathrm{P}_1$ and $\mathrm{P}_2$ terms are developed below. On the figures, the symbol —×— means that the corresponding sites takes a role in the expression of the coupling interaction, whereas the symbol —○— means that the corresponding site is transparent in the electronic process (i.e. the electron 'hops over' that site). Because of the current interest in diluted Mott-Hubbard systems, such as in the $La_2Cu_xZn_{1-x}O_4$? ? ? , we keep track in the derivation of the spin Hamiltonian of the occupation of the sites visited by the electrons. $\epsilon_i = 1$ if a site $i$ is occupied by a spin, $\epsilon_i = 0$ if the site is not occupied.



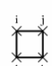
$4\,\frac{t'^2}{U}\,\vec{S_i}\cdot\vec{S_k}\,\{\epsilon_i\epsilon_k\}$



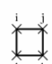
$4\,\frac{t''^2}{U}\,\vec{S_i}\cdot\vec{S_m}\,\{\epsilon_i\epsilon_m\}$



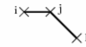
$-8\,\frac{t'^2t^2}{U^3}\,\{\epsilon_i\epsilon_j\epsilon_k\epsilon_l\}\,P_2^{i,j,k,l}$



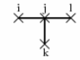
$4\,\frac{t'^2t^2}{U^3}\,\{\epsilon_i\epsilon_j\epsilon_k\}\,(\vec{S_i}\cdot\vec{S_j} + \vec{S_j}\cdot\vec{S_k})$



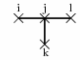
$160\,\frac{t'^2t^2}{U^3}\,(\vec{S_i}\cdot\vec{S_k})(\vec{S_j}\cdot\vec{S_l})\,\{\epsilon_i\epsilon_j\epsilon_k\epsilon_l\}$



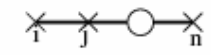
$4\,\frac{t'^2t^2}{U^3}\,\vec{S_i}\cdot\vec{S_k}\,\{\epsilon_i\epsilon_j\epsilon_k\}$



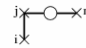
$80\,\frac{t'^2t^2}{U^3}\,\epsilon_i\epsilon_j\epsilon_k\epsilon_l\;\mathrm{P}_1^{i,j,k,l}$



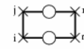
$4\,\frac{t'^2t^2}{U^3}\,\epsilon_i\epsilon_j\epsilon_k\epsilon_l\,(-1)\;\mathrm{P}_2^{i,j,k,l}$



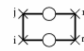
$4\,\frac{t''^2t^2}{U^3}\,\vec{S_i}\cdot\vec{S_n}\,\{\epsilon_i\epsilon_j\epsilon_n\}$



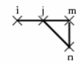
$4\,\frac{t''^2t^2}{U^3}\,\vec{S_i}\cdot\vec{S_n}\,\{\epsilon_i\epsilon_j\epsilon_n\}$



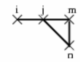
$80\,\frac{t''^2t^2}{U^3}\,\epsilon_i\epsilon_j\epsilon_m\epsilon_n\,\mathrm{P}_1^{i,j,m,n}$



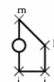
$4\,\frac{t''^2t^2}{U^3}\,\epsilon_i\epsilon_j\epsilon_m\epsilon_n\,(-1)\;\mathrm{P}_2^{i,j,m,n}$



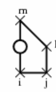
$80\,\frac{t^2}{U^3}t't''\,\epsilon_i\epsilon_j\epsilon_m\epsilon_n\;\mathrm{P}_1^{i,j,n,m}$



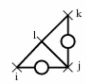
$4\,\frac{t^2}{U^3}t't''\,\epsilon_i\epsilon_j\epsilon_m\epsilon_n\,(-1)\;\mathrm{P}_2^{i,j,n,m}$



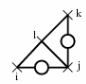
$80\,\frac{t^2t't''}{U^3}\,\epsilon_i\epsilon_j\epsilon_m\epsilon_k\;\mathrm{P}_1^{i,j,k,m}$



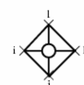
$4\,\frac{t^2t't''}{U^3}\,\epsilon_i\epsilon_j\epsilon_m\epsilon_k\,(-1)\;\mathrm{P}_2^{i,j,k,m}$



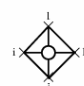
$80\,\frac{t'^2t''^2}{U^3}\,\epsilon_i\epsilon_j\epsilon_l\epsilon_k\;\mathrm{P}_1^{i,j,k,l}$



$4\,\frac{t'^2t''^2}{U^3}\,\epsilon_i\epsilon_j\epsilon_l\epsilon_k\,(-1)\;\mathrm{P}_2^{i,j,k,l}$



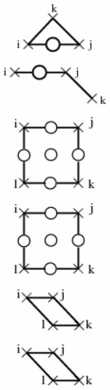
$160\,\frac{t'^2t''^2}{U^3}\,\epsilon_i\epsilon_j\epsilon_l\epsilon_k\,\Big\{(\vec{S_i}\cdot\vec{S_k})(\vec{S_j}\cdot\vec{S_l})\Big\}$
$+80\,\frac{t'^4}{U^3}\,\epsilon_i\epsilon_j\epsilon_l\epsilon_k\;\mathrm{P}_1^{i,j,k,l}$



$4\,\frac{t'^2t''^2}{U^3}\,\epsilon_i\epsilon_j\epsilon_l\epsilon_k\,(-1)\,\mathrm{P}_2^{i,j,k,l}$

# Delannoy *et al.* + thesis 2006






$$4\frac{t'^2t''^2}{U^3}\,\epsilon_i\epsilon_j\epsilon_k\left\{\vec{S_i}\cdot\vec{S_k}+\vec{S_j}\cdot\vec{S_l}\right\}$$

$$4\frac{t'^2t''^2}{U^3}\,\epsilon_i\epsilon_j\epsilon_k\left\{\vec{S_i}\cdot\vec{S_k}\right\}$$

$$80\frac{t''^4}{U^3}\,\epsilon_i\epsilon_j\epsilon_k\epsilon_l\ \mathrm{P}_1^{i,j,k,l}$$

$$4\frac{t''^4}{U^3}\,\epsilon_i\epsilon_j\epsilon_k\epsilon_l\ \mathrm{P}_2^{i,j,k,l}$$

$$80\frac{t^2t'^2}{U^3}\,\epsilon_i\epsilon_j\epsilon_k\epsilon_l\ \mathrm{P}_1^{i,j,k,l}$$

$$4\frac{t^2t'^4}{U^3}\,\epsilon_i\epsilon_j\epsilon_k\epsilon_l\ \mathrm{P}_2^{i,j,k,l}$$

## APPENDIX B: CALCULATION OF THE CHARGE RENORMALIZATION FACTOR

We start with the $t$, $t'$, $t''$, $U$ Hubbard model and use a method explained in Ref. **?** .

$$H_{\rm H} = T + T' + T'' + V \qquad \text{(B1)}$$

$$= -t\sum_{i,j_1;\sigma} c^\dagger_{i,\sigma}c_{j_1,\sigma} - t'\sum_{i,j_2;\sigma} c^\dagger_{i,\sigma}c_{j_2,\sigma} - t'\sum_{i,j_3;\sigma} c^\dagger_{i,\sigma}c_{j_2,\sigma} + U\sum_i n_{i,\uparrow}n_{i,\downarrow}, \qquad \text{(B2)}$$

$j_1$, $j_2$ and $j_3$ are respectively the first, second and third nearest neighbors of $i$. Fourier transforming this expression leads to:

$$H_{\rm H} = \sum_{k,\sigma}(\epsilon_k+\epsilon'_k+\epsilon''_k)c^\dagger_{k,\sigma}c_{k,\sigma} + \frac{U}{2N}\sum_{k,k',q}\sum_{\sigma,\sigma',\beta,\beta'}\delta_{\sigma,\sigma'}\delta_{\beta,\beta'}c^\dagger_{k',\sigma}c^\dagger_{-k'+q,\beta'}c_{-k+q,\beta}c_{k,\sigma}, \qquad \text{(B3)}$$

where :

$$\begin{cases} \epsilon_k = -2t(\cos(k_x)+\cos(k_y)), \\ \epsilon'_k = -2t'(\cos(k_x+k_y)+\cos(k_x-k_y)), \\ \epsilon''_k = -2t''(\cos(2k_x)+\cos(2k_y)). \end{cases} \qquad \text{(B4)}$$

Our goal here is to obtain the sublattice magnetization defined by :

$$M = \langle\Omega|S^z_{\mathbf{Q}}|\Omega\rangle, \qquad \text{(B5)}$$

(here we will consider the case where the magnetization is polarized around the $\hat{z}$ direction). $|\Omega\rangle$ is the spin density wave groundstate and $\mathbf{Q}$ a nesting wave vector. The charge density operator $S^i_{\mathbf{q}}$ is defined by :

$$S^i_{\mathbf{q}} = \frac{1}{N}\sum_{k,\alpha,\beta} c^\dagger_{k+q,\alpha}\hat{\sigma}^i_{\alpha,\beta}c_{k,\beta}, \qquad \text{(B6)}$$

$N$ being the number of sites.

In order to diagonalize this hamiltonian, we introduce the bogoliubov transformation :

$$\begin{cases} \gamma^c_{k,\alpha} = u_k c_{k,\alpha} + v_k\sum_\beta \hat{\sigma}^3_{\alpha,\beta}c_{k+Q,\beta}, \\ \gamma^v_{k,\alpha} = v_k c_{k,\alpha} - u_k\sum_\beta \hat{\sigma}^3_{\alpha,\beta}c_{k+Q,\beta}. \end{cases} \qquad \text{(B7)}$$

Our goal is to diagonalize the system through the relations :

$$\begin{cases} \left[H_{\rm H},\gamma^c_{k,\sigma}\right] = E_k\gamma^c_{k,\sigma}, \\ \left[H_{\rm H},\gamma^v_{k,\sigma}\right] = -E_k\gamma^v_{k,\sigma}. \end{cases} \qquad \text{(B8)}$$

Injecting (B7) in the Hamiltonian (B3), we get :

$$E_k = \epsilon'_k + \epsilon''_k \pm \sqrt{\Delta^2+\epsilon_k^2}, \qquad \text{(B9)}$$

where the density wave gap $\Delta$ is defined by :

$$\Delta = -\frac{UM}{2}. \qquad \text{(B10)}$$

The Bogoliubov coefficients $u_k$ and $v_k$ are obtained using :

$$\begin{cases} u_k^2 = \frac{1}{2}\left(1+\frac{\epsilon_k}{E_k-\epsilon'_k-\epsilon''_k}\right), \\ v_k^2 = \frac{1}{2}\left(1-\frac{\epsilon_k}{E_k-\epsilon'_k-\epsilon''_k}\right), \end{cases} \qquad \text{(B11)}$$

from that we can infer that

$$M = \langle\Omega|S^z_{\mathbf{Q}}|\Omega\rangle = \frac{1}{N}\sum_k u_k v_k\ ; \qquad \text{(B12)}$$

hence :

$$M = \frac{1}{N}\sum_k \frac{1}{2}\frac{\Delta}{E_k-\epsilon'_k-\epsilon''_k}. \qquad \text{(B13)}$$

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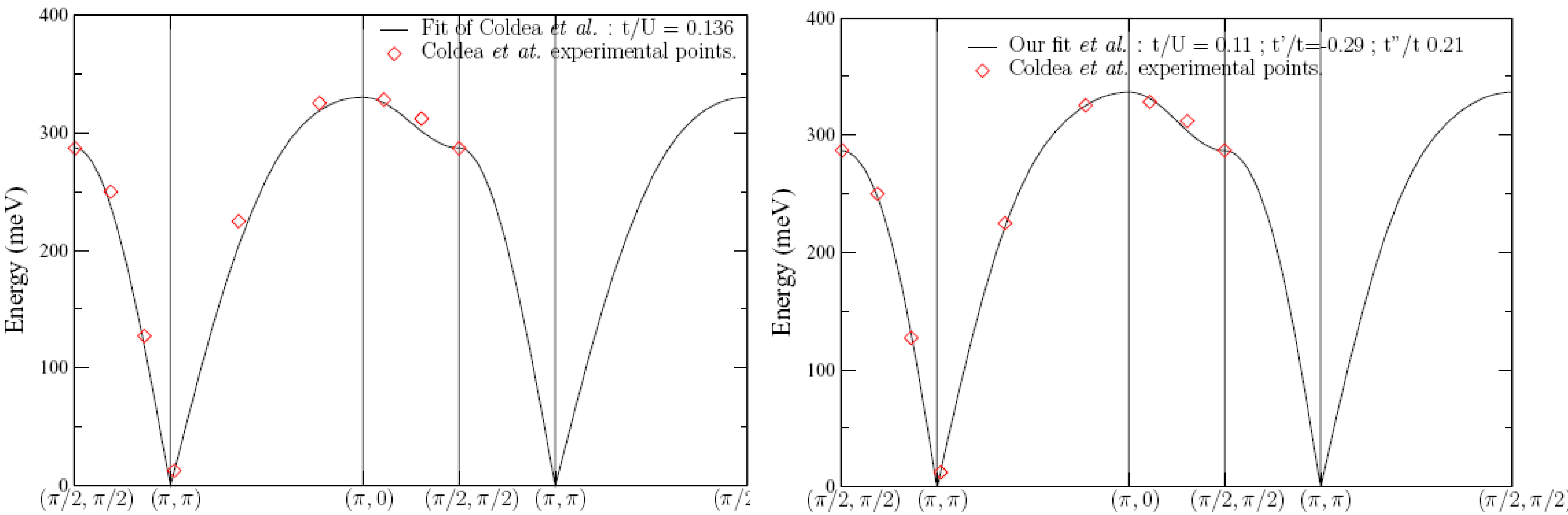
# Alternate set of parameters




$$\begin{cases} t/U &= 0.1 & \pm 0.05\ , \\ t'/t &= -0.35 & \pm 0.05\ , \\ t''/t &= 0.22 & \pm 0.05\ , \\ t &= 0.35 & \text{eV} \\ U &= 3.5 & \text{eV} \end{cases}$$

Delannoy *et al.* + thesis 2006

# General methods for the derivation of effective spin Hamiltonians : all canonically equivalent

Chernyshev *et al.* PRB 2004

- Brillouin-Wigner degenerate perturbation theory
  - Expansion of denominators
- Resolvent operator (for Hamiltonian)
- Canonical transformation

# Canonical transformation

$$\langle\psi'|H|\psi\rangle = \langle\alpha'|e^{iS}He^{-iS}|\alpha\rangle$$

$$e^{iS}Ae^{-iS} = A + [iS,A] + \tfrac{1}{2}[iS,[iS,A]] + \ldots$$

$$H = H_0 + V_D + V_X$$

$$S_X = S_1 + S_2 + \ldots$$

$$S = S_D + S_X$$

$$S_D = 0$$

$$\begin{aligned} e^{iS}(H_0 + V_D + V_X)e^{-iS} &= H_0 + V_D \\ &+ V_X + [iS_1, H_0] \\ &+ [iS_2, H_0] + [iS_1, V_D] \\ &+ [iS_1, V_X] + \frac{1}{2}[iS_1,[iS_1,H_0]] \end{aligned}$$

$$V_D = T_0$$

$$V_X = T_1 + T_{-1}$$

$$[H_0, T_m] = mUT_m$$

# Beware ! When spin is not spin…

- A paradox

$$\widetilde{M}_s^\dagger = \frac{1}{N}\sum_i S_i^z(-1)^i.$$

$$|0\rangle_H = e^{-iS}|0\rangle_s$$

$$\langle O\rangle = \frac{{}_H\langle 0|O_H|0\rangle_H}{{}_H\langle 0|0\rangle_H}$$

$$O_s = e^{iS}O_H e^{-iS}$$

$$\frac{{}_H\langle 0|O_H|0\rangle_H}{{}_H\langle 0|0\rangle_H} = \frac{{}_s\langle 0|O_s|0\rangle_s}{{}_s\langle 0|0\rangle_s}$$

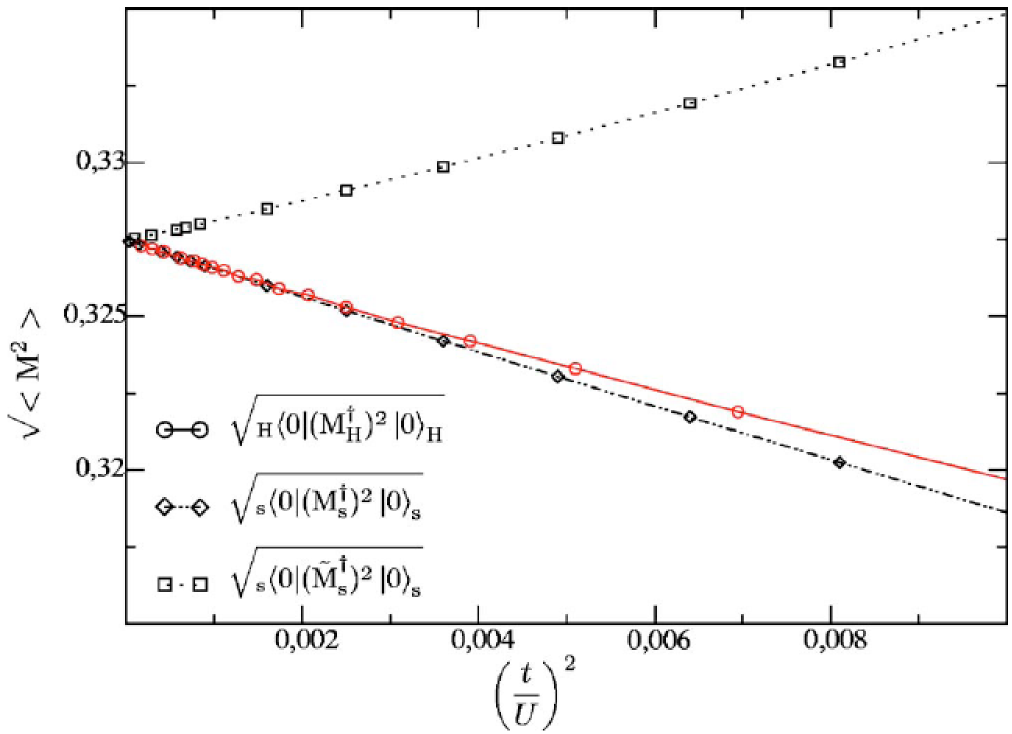



FIG. 2. (Color online) $t/U$ dependence of the staggered magnetization $M_{2,s}^\dagger$, $M_{2,H}^\dagger$ and $\widetilde{M}_{2,s}$ for a $2\times 4$ lattice.

$$M_s^\dagger = \frac{1}{N}\left(\sum_i S_i^z(-1)^i - 2\frac{t^2}{U^2}\sum_{\langle i,j\rangle}(S_i^z - S_j^z)(-1)^i\right)$$

$$M_s^\dagger = \left(1 - 2z\frac{t^2}{U^2}\right)\widetilde{M}_s^\dagger$$

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# Back to the general problem: Theoretical difficulties

- Low dimension
  - (quantum and thermal fluctuations)

- Large residual interactions
  - (Potential ~ Kinetic)
  - Expansion parameter?
  - Particle-wave?

- By now we should be as quantitative as possible!

# Theory without small parameter: How should we proceed?

- Identify important physical principles and laws to constrain non-perturbative approximation schemes
  - From weak coupling (kinetic)
  - From strong coupling (potential)
- Benchmark against "exact" (numerical) results.
- Check that weak and strong coupling approaches agree at intermediate coupling.
- Compare with experiment

# Question

- Is the Hubbard model rich enough to contain the essential physics of the cuprates and the organics? (e- and h-doped and layered?)
- Yes (in part):
  - New theoretical approaches
  - Increase in computing power
  - Theoretical approaches (numerical, analytical) give consistent results even if the starting points are very different.

# Mounting evidence for d-wave in Hubbard

- **Weak coupling (U << W)**
  - AF spin fluctuations mediated pairing with d-wave symmetry
    - (Bickers et al., PRL 1989; Monthoux et al., PRL 1991; Scalapino, JLTP 1999, Kyung et al. (2003))
  - RG → Groundstate d-wave superconducting
    - (Bourbonnais (86), Halboth, PRB 2000; Zanchi, PRB 2000, Berker 2005)
- **Strong coupling (U >> W)**
  - Early mean-field
    - (Kotliar, Liu 1988, Inui et al. 1988)
  - Finite size simulations of t-J model
    - Groundstate superconducting
    - (Sorella et al., PRL 2002; Poilblanc, Scalapnio, PRB 2002)

# Numerical methods that show Tc at strong coupling

## DCA

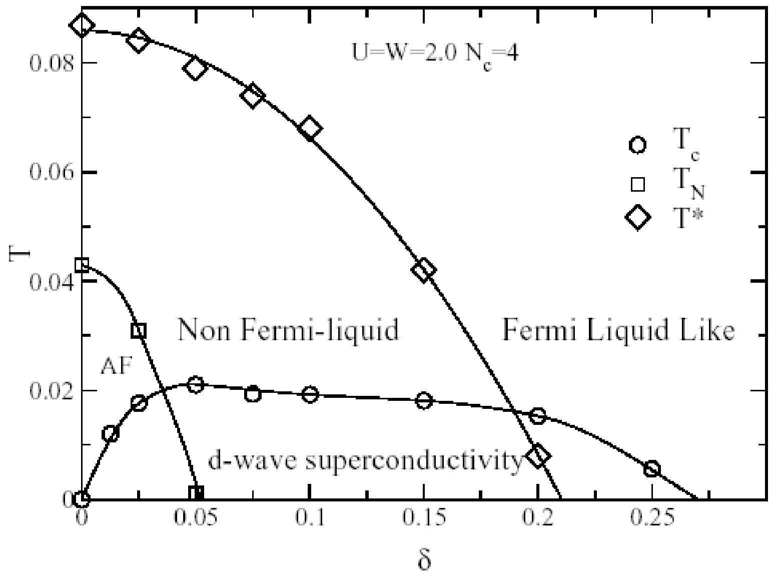


FIG. 5. The temperature-doping phase diagram of the 2D Hubbard model calculated with QMC and DCA for $N_c = 4$, $U = 2$. $T_N$ and $T_c$ were calculated from the divergences of the antiferromagnetic and d-wave susceptibilities, respectively. $T^*$ was calculated from the peak of the bulk magnetic susceptibility.

Th. Maier, M. Jarrell, Th. Pruschke, and J. Keller
Phys. Rev. Lett. 85, 1524 (2000)
T.A. Maier et al. PRL (2005)

## Variational

VOLUME 87, NUMBER 21 PHYSICAL REV

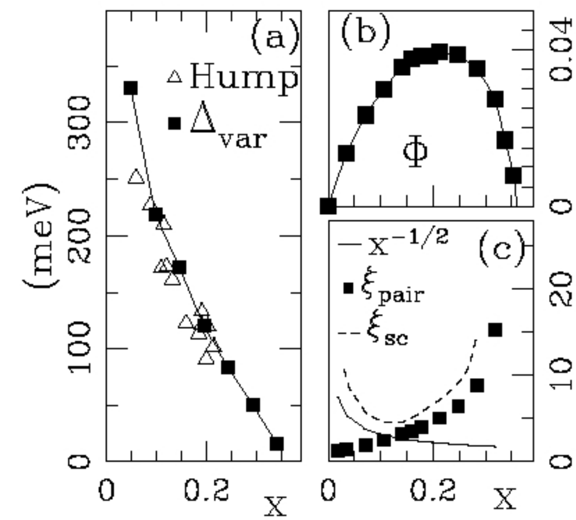


FIG. 1. (a) The variational parameter $\Delta_{\rm var}$ (filled squares) and the $(\pi, 0)$ hump scale (open triangles) in ARPES [10] versus doping. (b) Doping dependence of the $d$-wave SC order parameter $\Phi$. Solid lines in (a) and (b) are guides to the eye. (c) The coherence length $\xi_{\rm sc} \geq \max(\xi_{\rm pair}, 1/\sqrt{x})$.

Paramekanti, M. Randeria, and N. Trivedi
Phys. Rev. Lett. 87, 217002 (2001)



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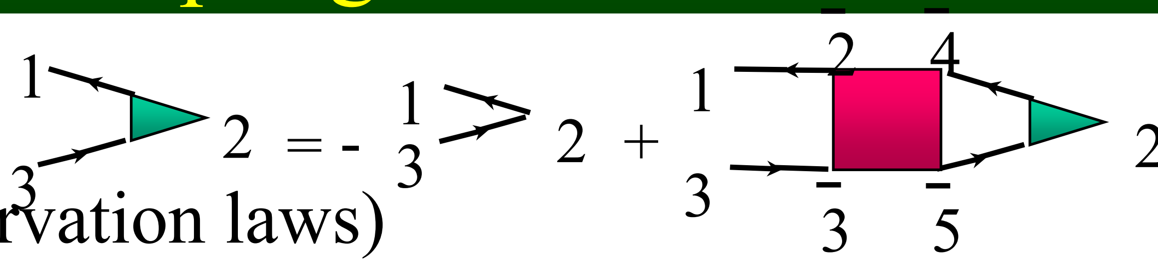
# Methodology

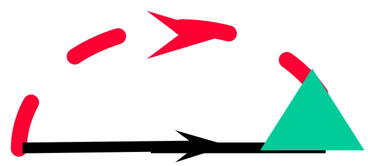
## Weak-coupling approaches

# Theory difficult even at weak to intermediate coupling!




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

$\Sigma$ =



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



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# TPSC

# Two-Particle Self-Consistent Approach (U < 8t)

## - How it works

- 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)

# 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:

$$\begin{aligned}\Sigma_{\sigma}\left(1,\overline{1};\{\phi\}\right)G_{\sigma}\left(\overline{1},2;\{\phi\}\right) &= -U\left\langle c^{\dagger}_{-\sigma}\left(1^{+}\right)c_{-\sigma}\left(1\right)c_{\sigma}\left(1\right)c^{\dagger}_{\sigma}\left(2\right)\right\rangle_{\phi} \\ &\approx A_{\{\phi\}}G^{(1)}_{-\sigma}\left(1,1^{+};\{\phi\}\right)G^{(1)}_{\sigma}\left(1,2;\{\phi\}\right)\end{aligned}$$

2. Factorization

# TPSC…

$$U_{sp} = U\frac{\langle n_\uparrow n_\downarrow\rangle}{\langle n_\uparrow\rangle\langle n_\downarrow\rangle}$$ Kanamori-Brückner screening

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

3. The F.D. theorem and Pauli principle

$$\left\langle (n_\uparrow - n_\downarrow)^2 \right\rangle = \langle n_\uparrow\rangle + \langle n_\downarrow\rangle - 2\langle n_\uparrow n_\downarrow\rangle$$

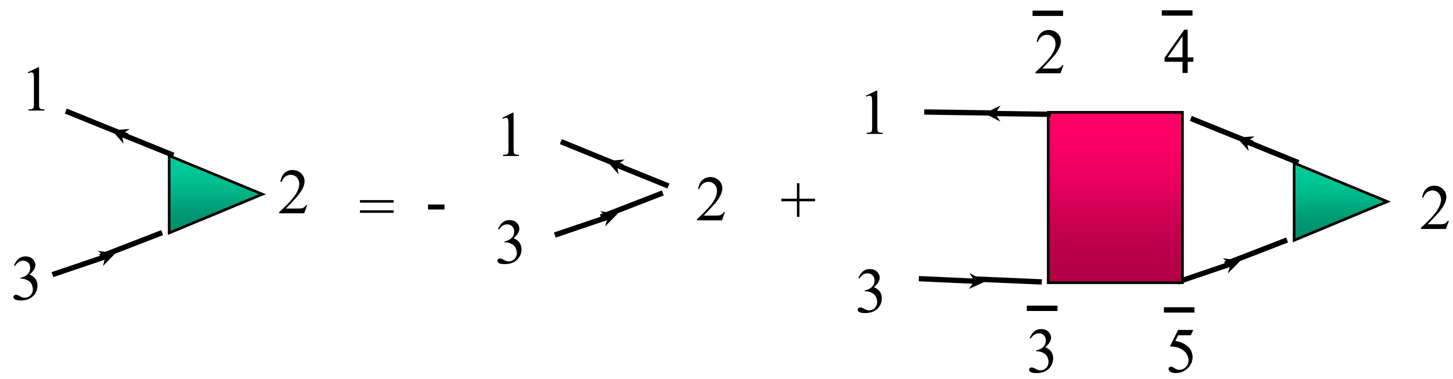
$$\frac{T}{N}\sum_q \chi_{sp}^{(1)}(q) = n - 2\langle n_\uparrow n_\downarrow\rangle$$

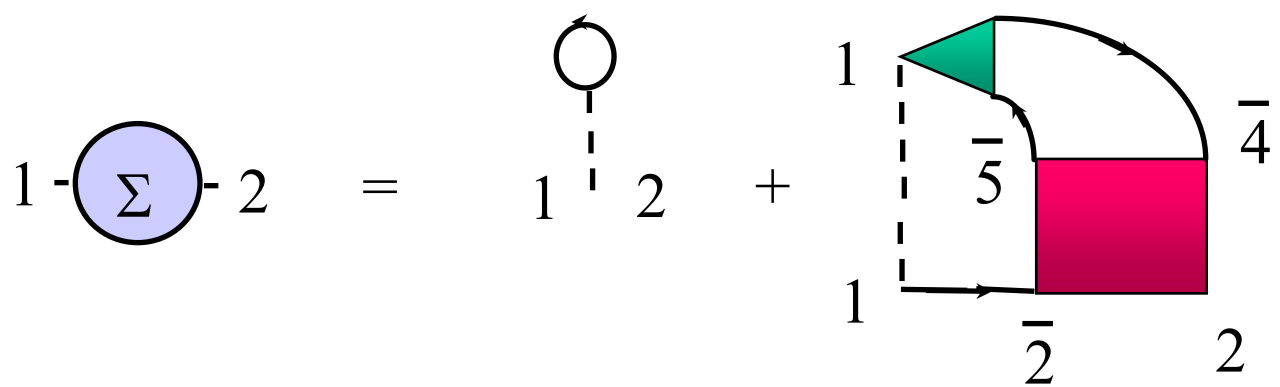
**II: Improved self-energy**

Insert the first step results
into exact equation: $\Sigma_\sigma(1,\bar{1};\{\phi\})\,G_\sigma(\bar{1},2;\{\phi\}) = -U\left\langle c_{-\sigma}^\dagger(1^+)\,c_{-\sigma}(1)\,c_\sigma(1)\,c_\sigma^\dagger(2)\right\rangle_\phi$

$$\Sigma_\sigma^{(2)}(k) = Un_{\bar\sigma} + \frac{U}{8}\frac{T}{N}\sum_q\left[3U_{sp}\chi_{sp}^{(1)}(q) + U_{ch}\chi_{ch}^{(1)}(q)\right]G_\sigma^{(1)}(k+q)$$

## A better approximation for single-particle properties (Ruckenstein)





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

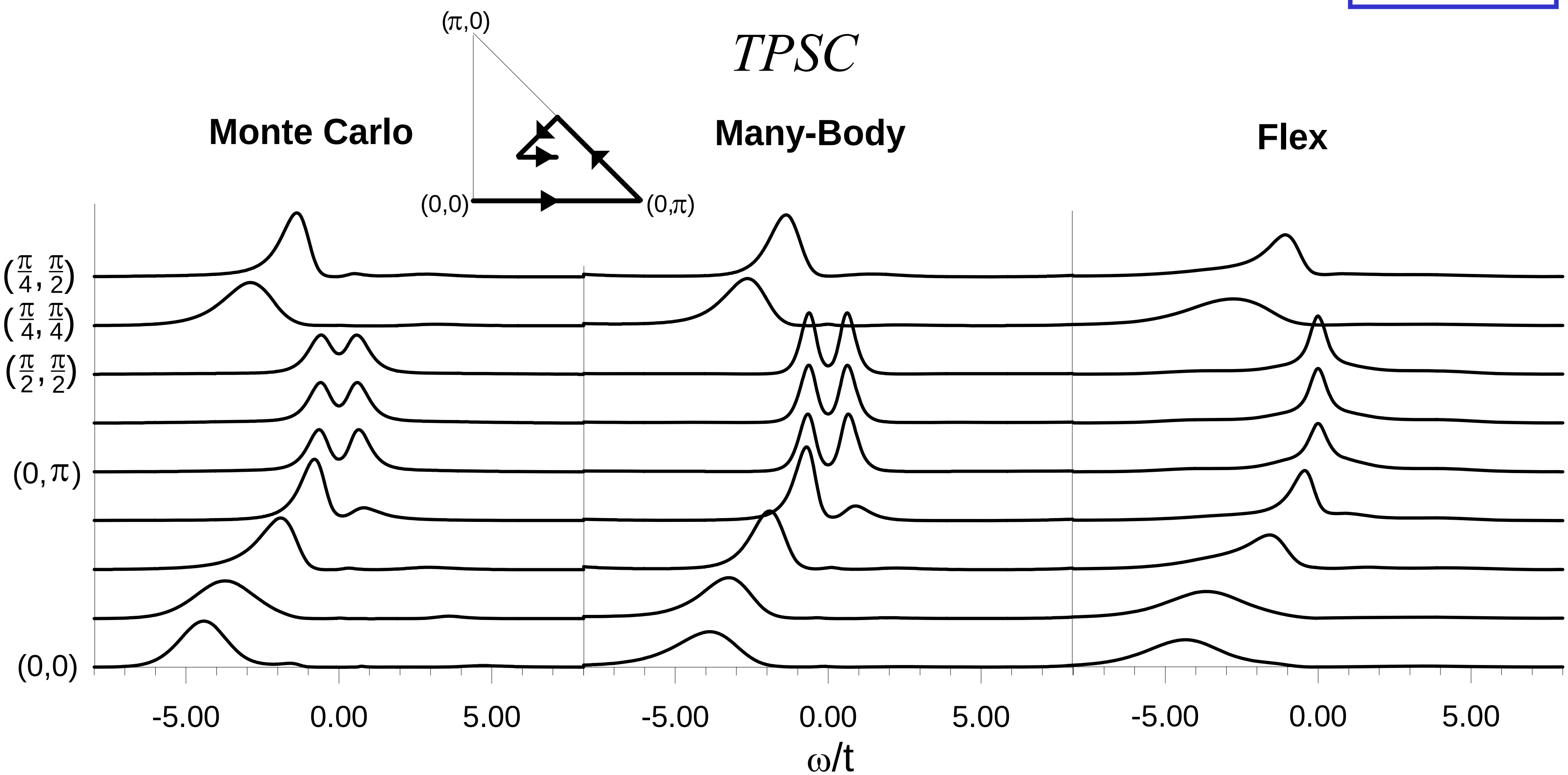
# Benchmarks for TPSC

# **Benchmark for TPSC :** Quantum Monte Carlo

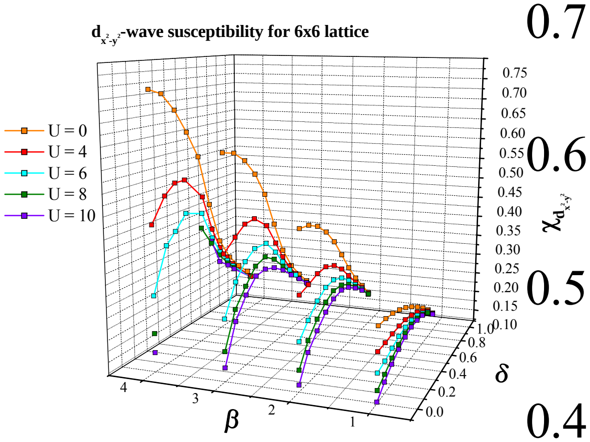
- Advantages of QMC
  – Sizes much larger than exact diagonalizations
  – As accurate as needed
- Disadvantages of QMC
  – Cannot go to very low temperature in certain doping ranges, yet low enough in certain cases to discard existing theories.

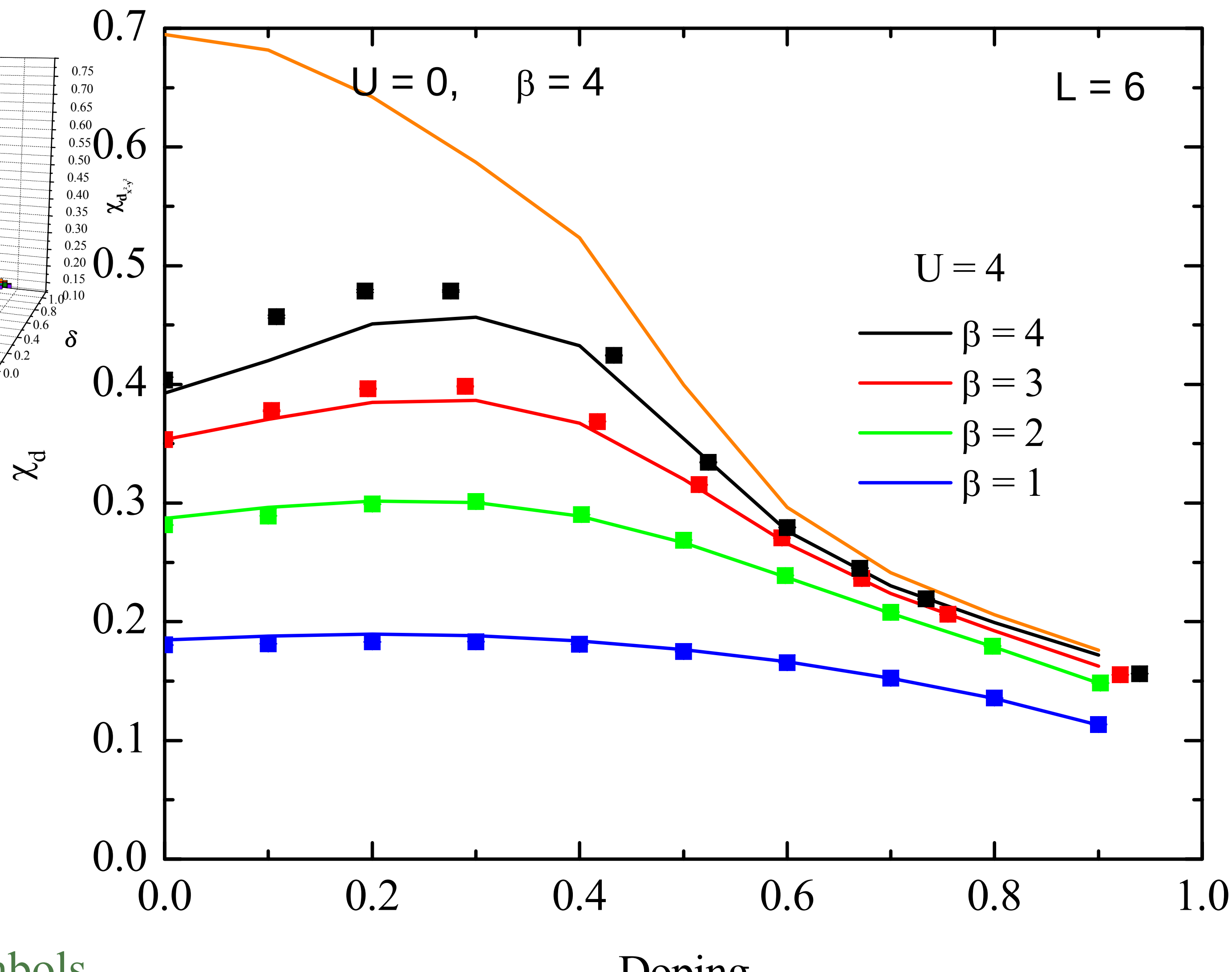
Proofs...

$U = +4$
$\beta = 5$




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




QMC: symbols.
Solid lines analytical.

Kyung, Landry, A.-M.S.T

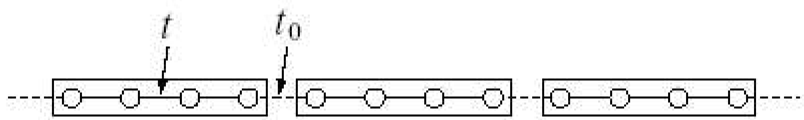
# Methodology

Strong-coupling approaches

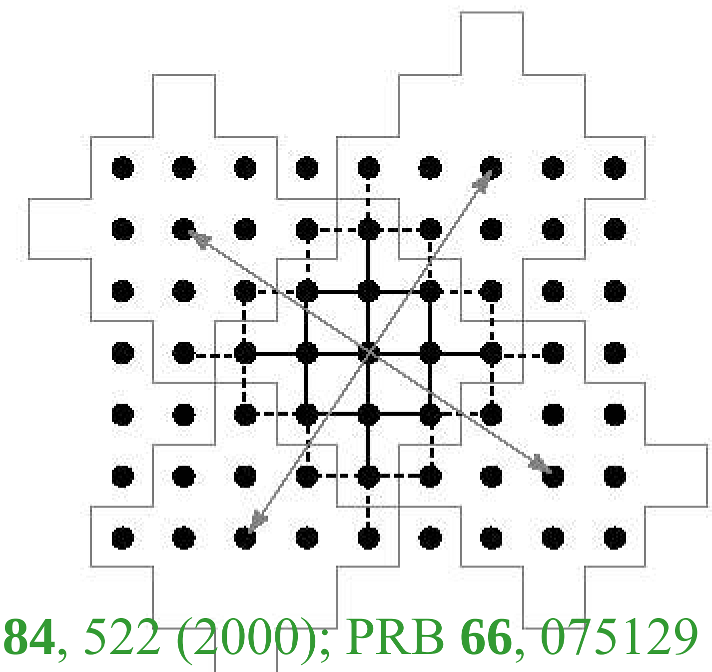
# Cluster perturbation theory

# Cluster perturbation theory (CPT)

- Tile the lattice into identical clusters
- Solve exactly (numerically) within a cluster
- Treat inter-cluster hopping in perturbation theory




Vary cluster shape and size



W. Metzner, PRB **43**, 8549 (1991). Pairault, Sénéchal, AMST, PRL **80**, 5389 (1998).

David Sénéchal

D. Sénéchal *et al.*, PRL. **84**, 522 (2000); PRB **66**, 075129 (2002), Gross, Valenti, PRB **48**, 418 (1993).

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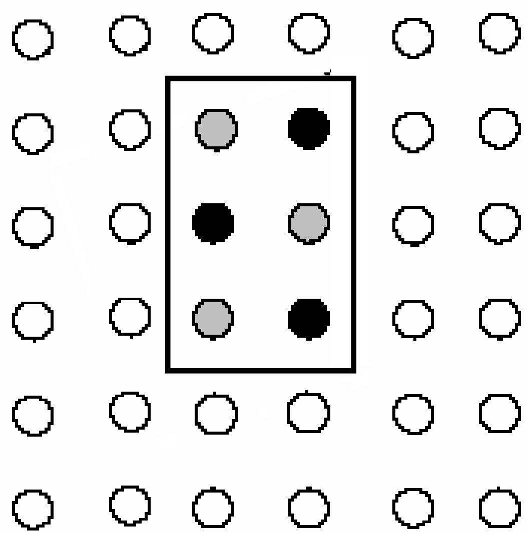
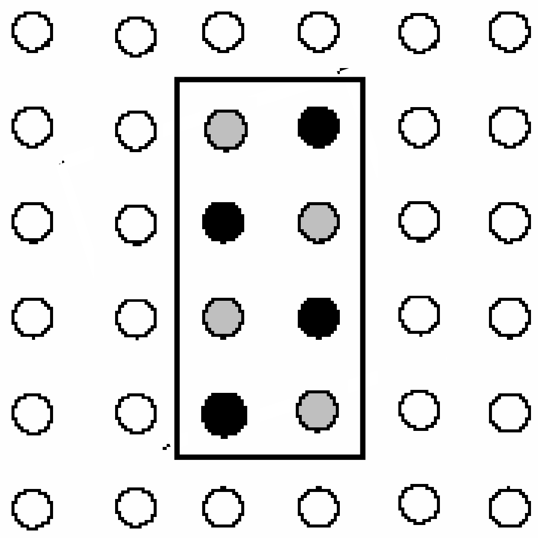
# Different clusters

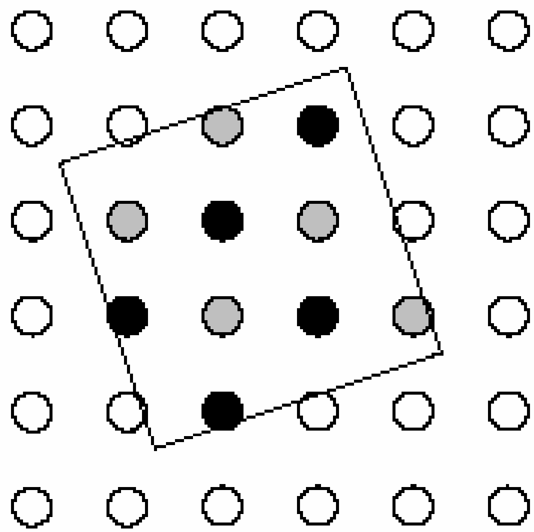
David Sénéchal



*L = 6*



*L = 8*



*L = 10*

inter-cluster hopping

intra-cluster hopping

cluster index

$$t_{ab}^{mn} = t_{ab}^{(c)} \delta_{mn} + V_{ab}^{mn}$$

site index

$$\hat{G}_0^{-1} = \omega - \hat{t} = \omega - \hat{t}^{(c)} - \hat{V}$$

noninteracting Green function

superlattice wavevector

Basic CPT approximation :

$$\hat{G}^{-1}(\mathbf{K},\omega) = \hat{G}^{(c)-1}(\omega) - \hat{V}(\mathbf{K})$$

CPT Green function

Final Fourier transform :

$$G_{\mathrm{CPT}}(\mathbf{k},\omega) = \frac{1}{L}\sum_{a,b=1}^{L} G_{ab}(\mathbf{k},\omega)\mathrm{e}^{-i\mathbf{k}\cdot(\mathbf{r}_a-\mathbf{r}_b)}$$

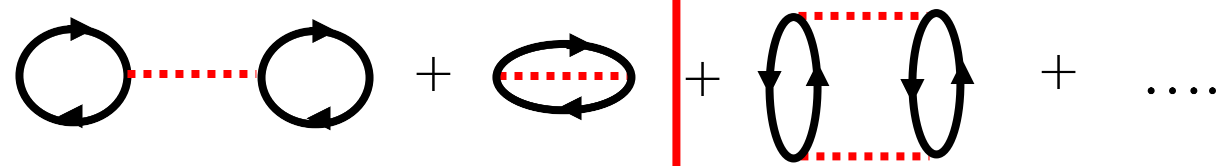
Spectral function :

$$A(\mathbf{k},\omega) = -2 \lim_{\eta\to 0+} \operatorname{Im} G(\mathbf{k},\omega+i\eta)$$

# Self-energy functional approach and special cases

# Dynamical "variational" principle

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

$\Phi[G] =$ 

Universality

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

$$\frac{\delta\Omega_{\mathbf{t}}[G]}{\delta G} = \Sigma - G_{0\mathbf{t}}^{-1} + G^{-1} = 0$$

$$G = \frac{1}{G_{0\mathbf{t}}^{-1} - \Sigma}$$

H.F. if approximate $\Phi$ by first order

FLEX higher order

Then $\Omega$ is grand potential

Related to dynamics (cf. Ritz)

Luttinger and Ward 1960, Baym and Kadanoff (1961)

# Another way to look at this (Potthoff)

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

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

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

Still stationary (chain rule)

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



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

# SFT : Self-energy Functional Theory

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

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

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

For given interaction, $F[\Sigma]$ is a universal functional of $\Sigma$, no explicit dependence on $H_0(\mathbf{t})$. Hence, use solvable cluster $H_0(\mathbf{t'})$ to find $F[\Sigma]$.

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

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).

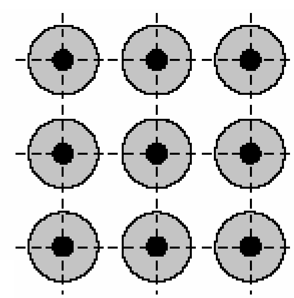
# Variational cluster perturbation theory and DMFT as special cases of SFT

M. Potthoff *et al.* PRL **91,** 206402 (2003).

DCA, Jarrell et al.

Savrasov, Kotliar, PRB (2001)

DMFT



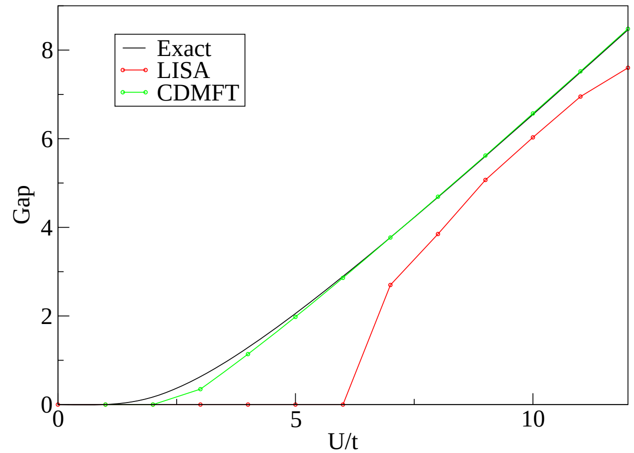
Georges Kotliar, PRB (1992).
M. Jarrell, PRL (1992).
A. Georges, *et al.* RMP (1996).

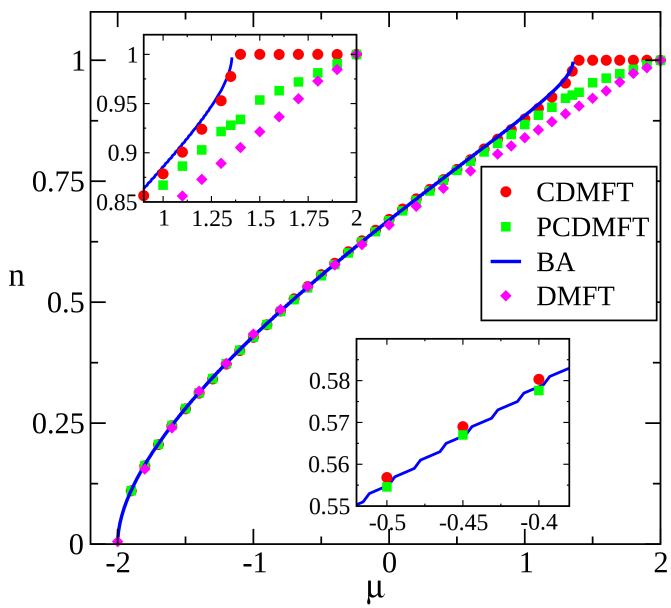
$$T\sum_{\omega_n}\sum_{ij\sigma}\left(\frac{1}{\boldsymbol{G}_{0,\boldsymbol{t}}^{-1}-\boldsymbol{\Sigma}_{\boldsymbol{t}',\boldsymbol{U}}}-\boldsymbol{G}_{\boldsymbol{t}',\boldsymbol{U}}\right)_{ji\sigma}\frac{\partial\Sigma_{ij\sigma}}{\partial\boldsymbol{t}'}=0\,.$$

# Cellular dynamical mean-field theory and Dynamical cluster approximation

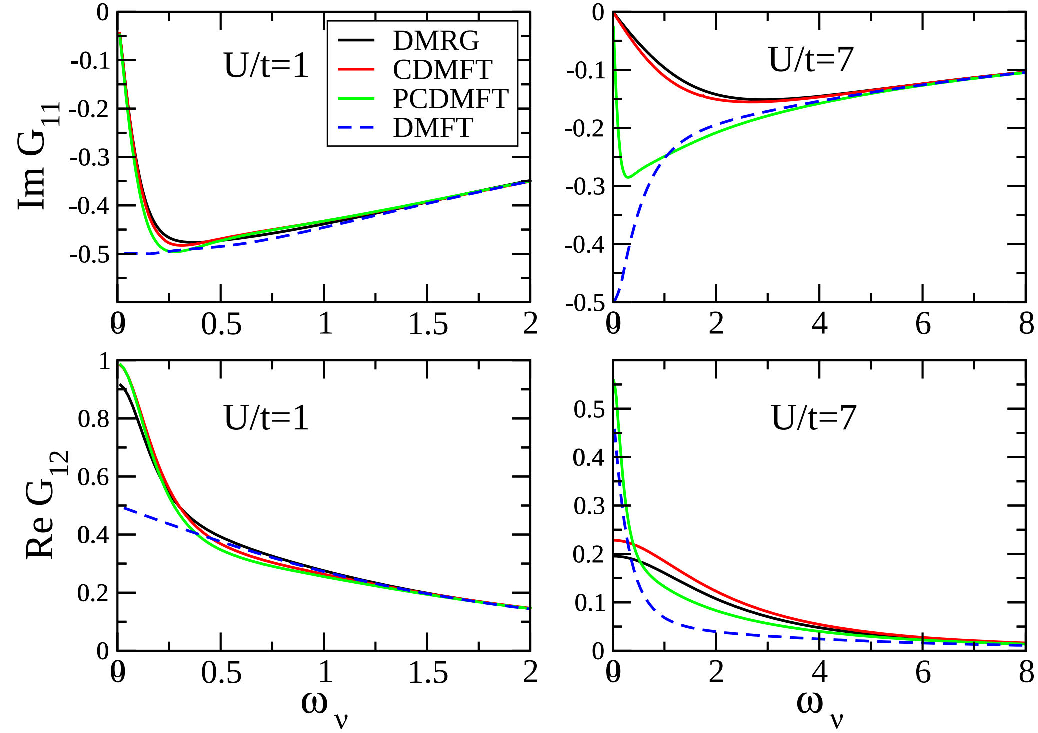
# Benchmarks for quantum cluster approaches

# Quality of approximation made by CDMFT




1D Hubbard model: Worst case scenario




Excellent agreement with exact results in both metallic and insulating limits

Capone, Civelli, SSK, Kotliar, Castellani PRB (2004)

Bolech, SSK, Kotliar PRB (2003)

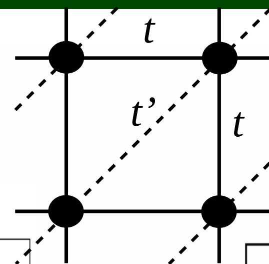
# DCA vs CDMFT

G. Biroli and G. Kotliar, Phys. Rev. B 65, 155112 (2002)
Aryanpour et al. cond-mat/0301460
Maier et al. cond-mat/0205460

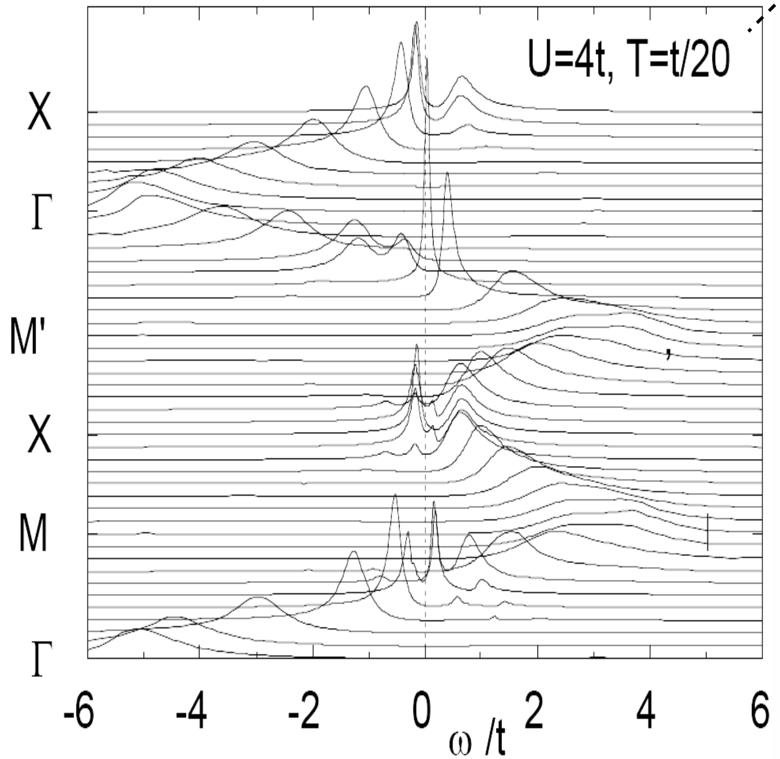
Quantitative aspects of the dynamical impurity approach, Pozgajcic cond-mat/0407172

# Results and concordance between different methods

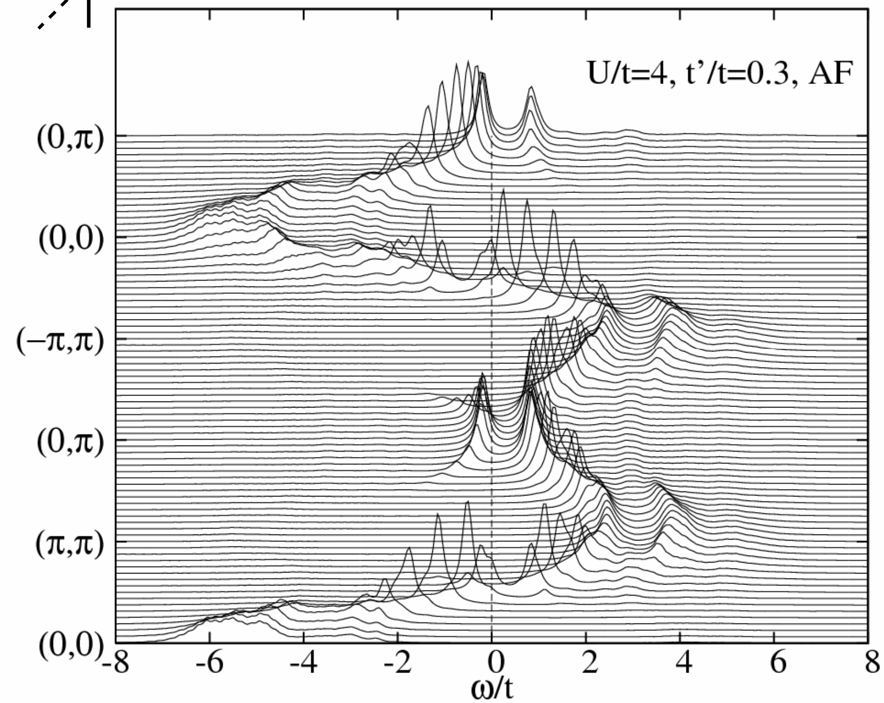
# Comparison, TPSC-CDMFT, *n=1, U=4t*




TPSC



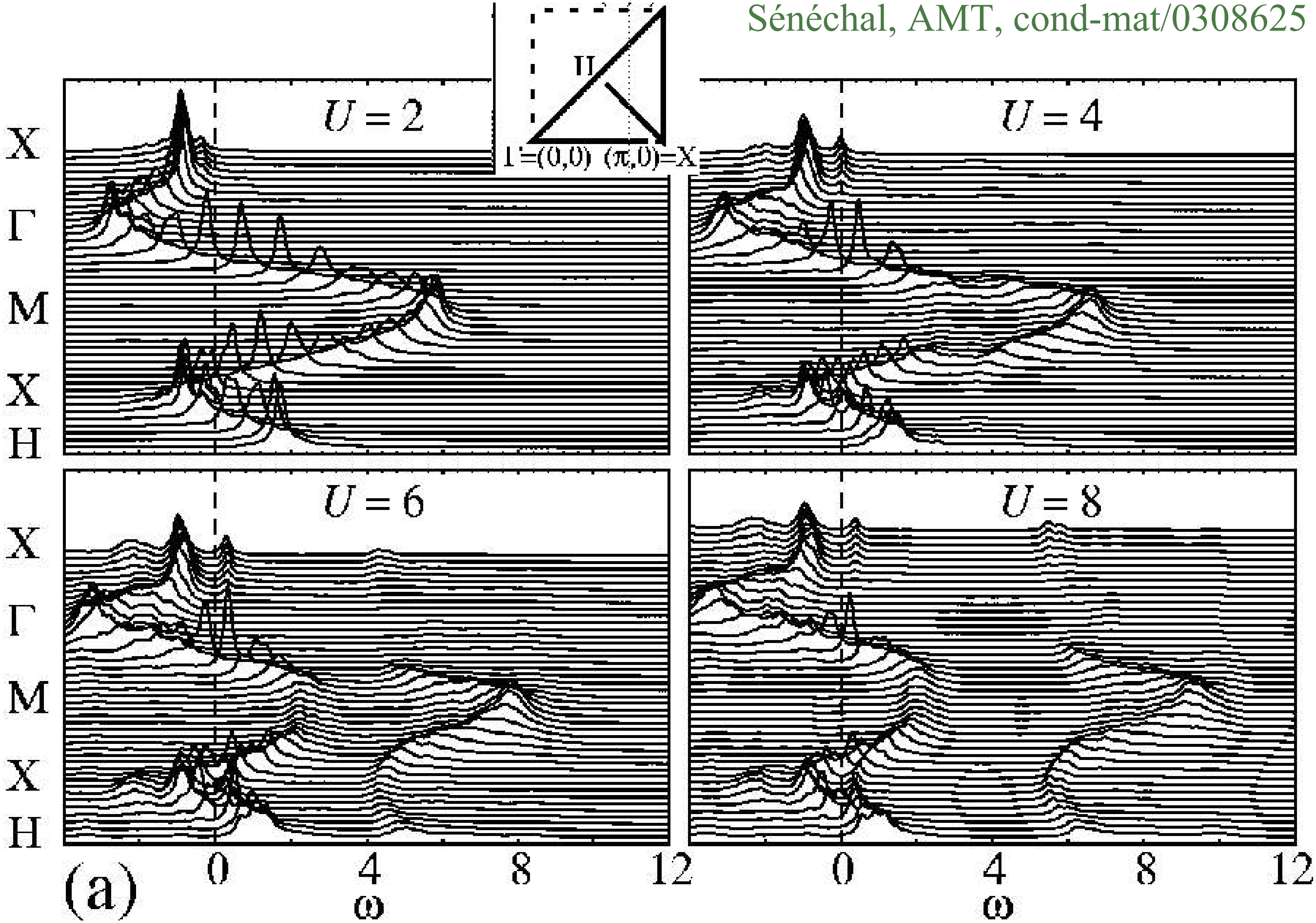

CDMFT



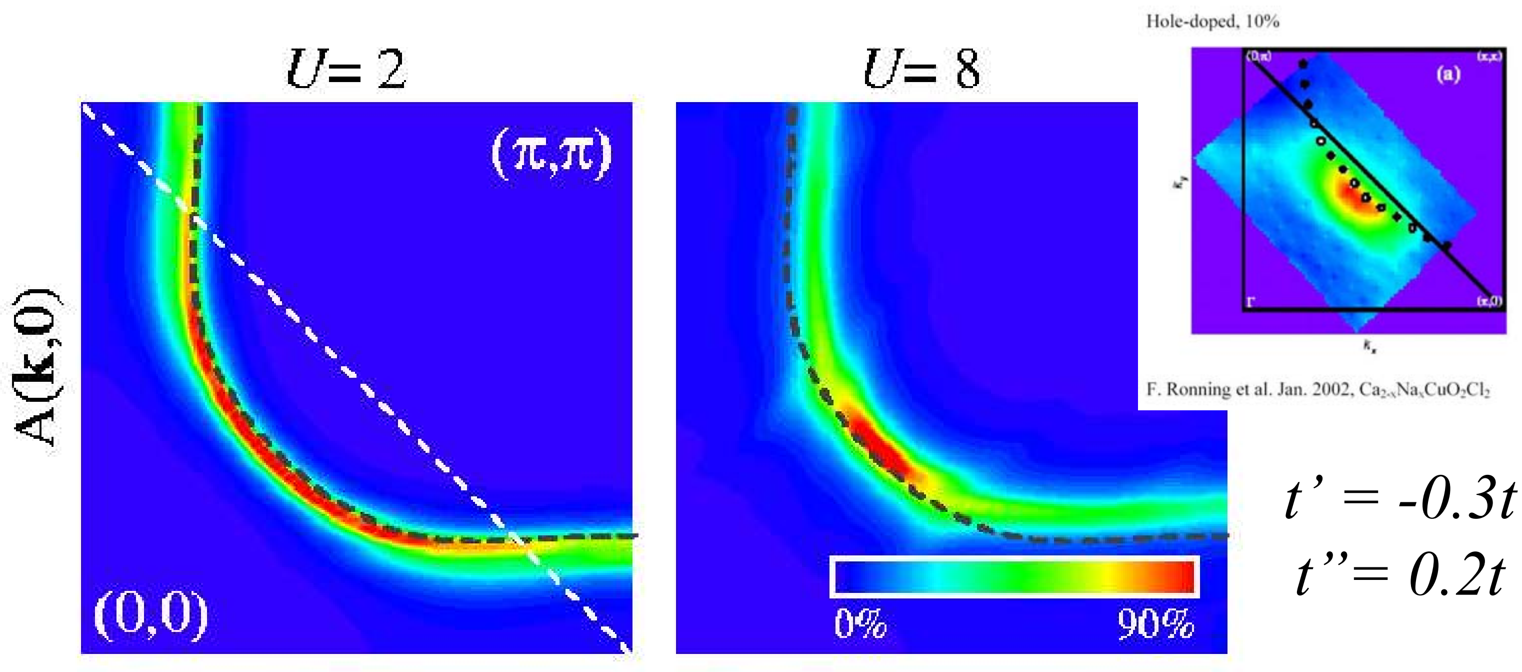
# CPT

# Hole-doped (17%)

Sénéchal, AMT, cond-mat/0308625



# Hole-doped (17%)




$t' = -0.3t$

$t'' = 0.2t$

$\eta = 0.12t$

$\eta = 0.4t$

Sénéchal, AMT, PRL **92**, 126401 (2004).

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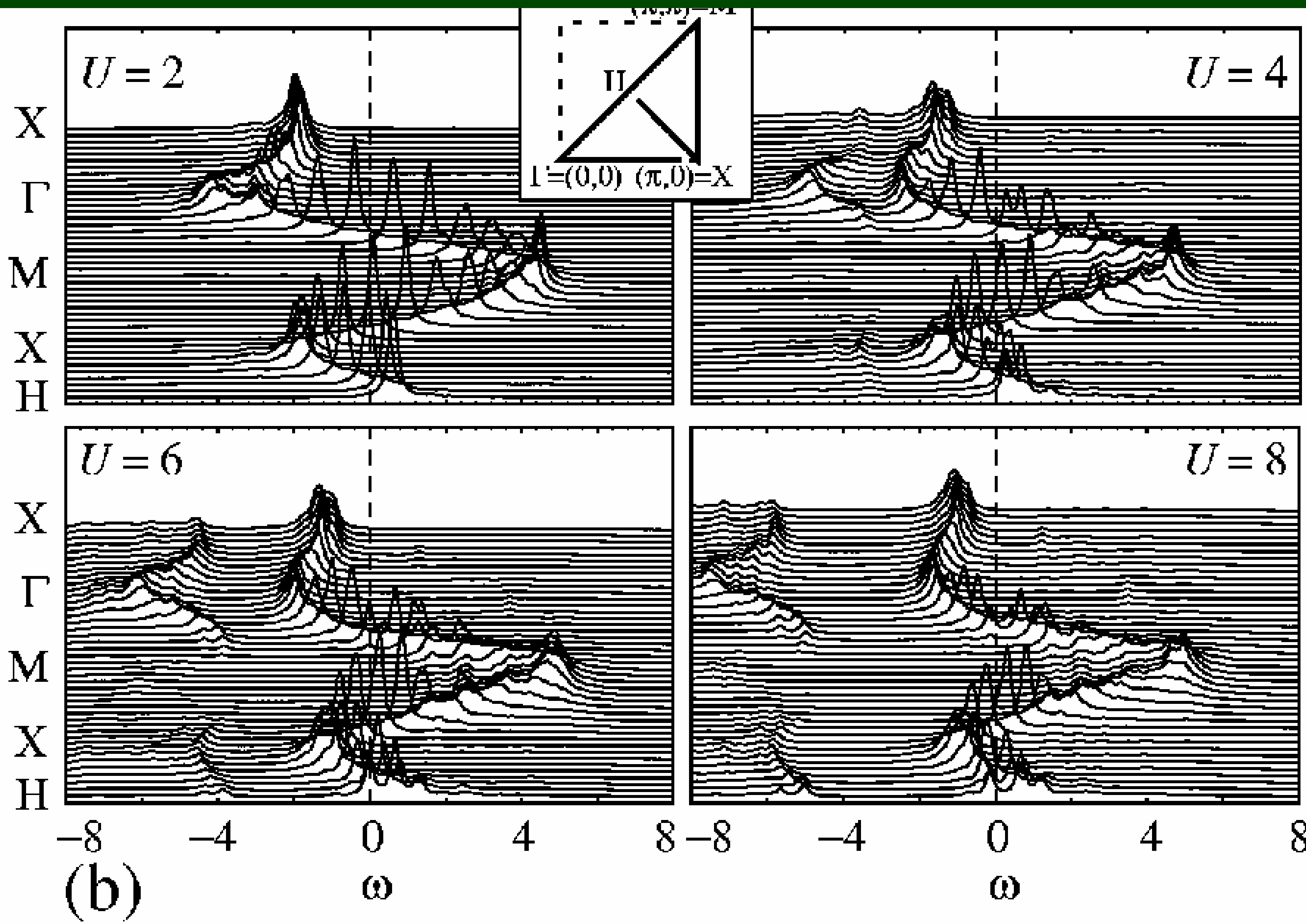
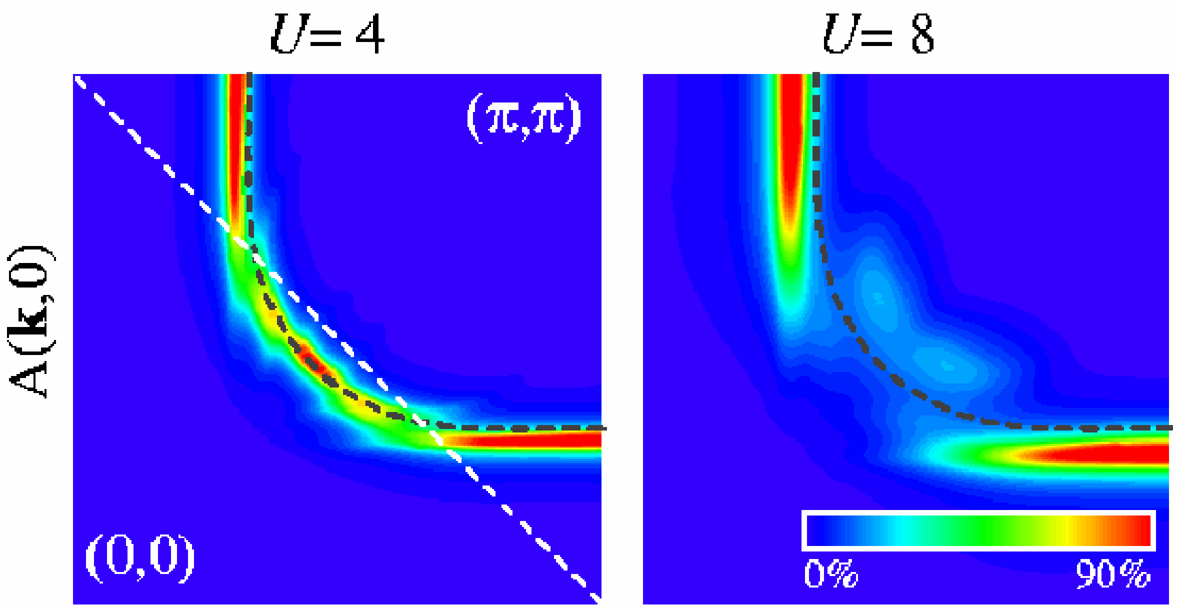
# Electron-doped (17%)



# Electron-doped (17%)



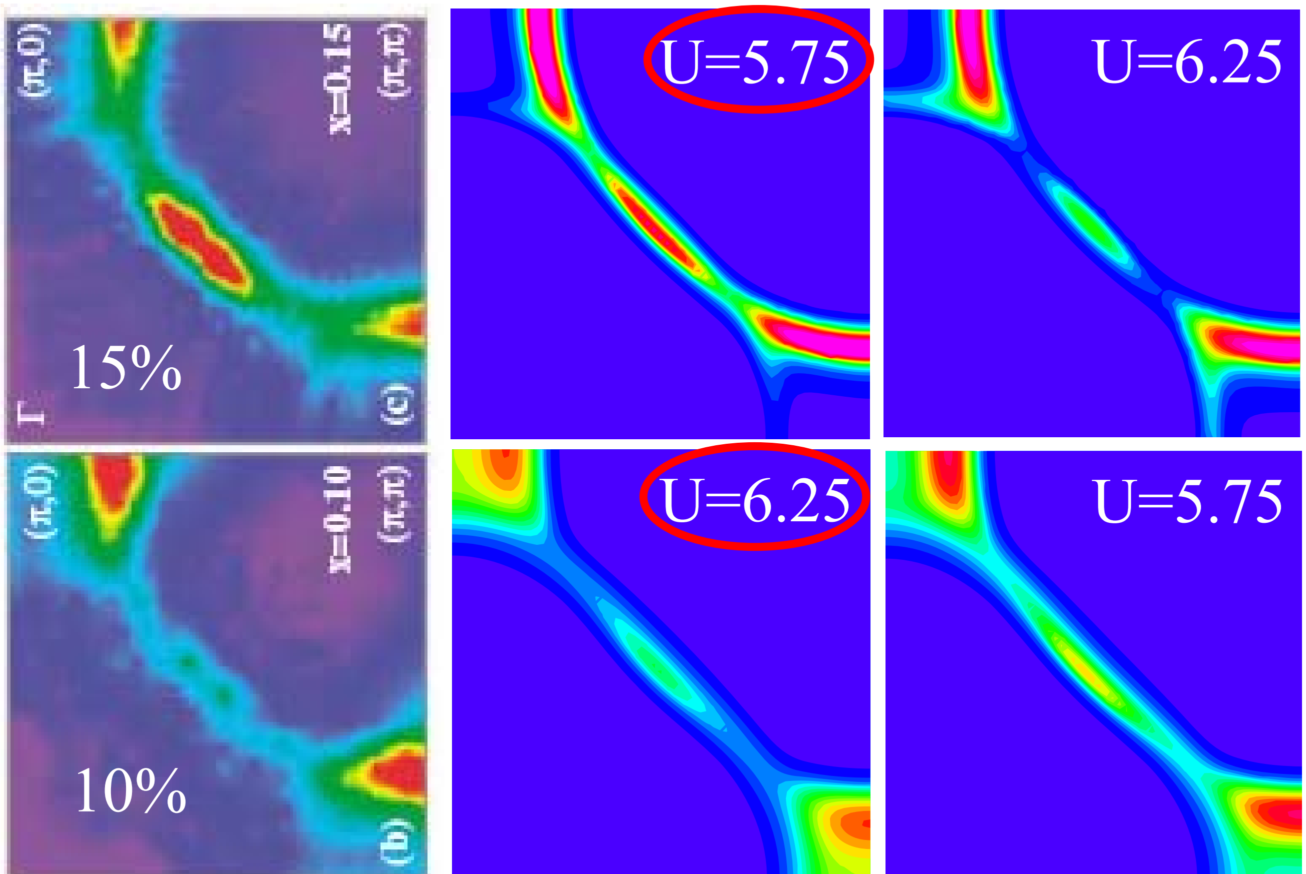

$t' = -0.3t$
$t'' = 0.2t$

$\eta = 0.12t$
$\eta = 0.4t$

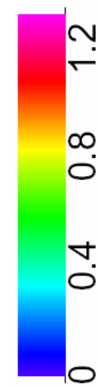
Sénéchal, AMT,
PRL in press

# TPSC : Fermi surface plots

Hubbard repulsion *U* has to…




be not too large

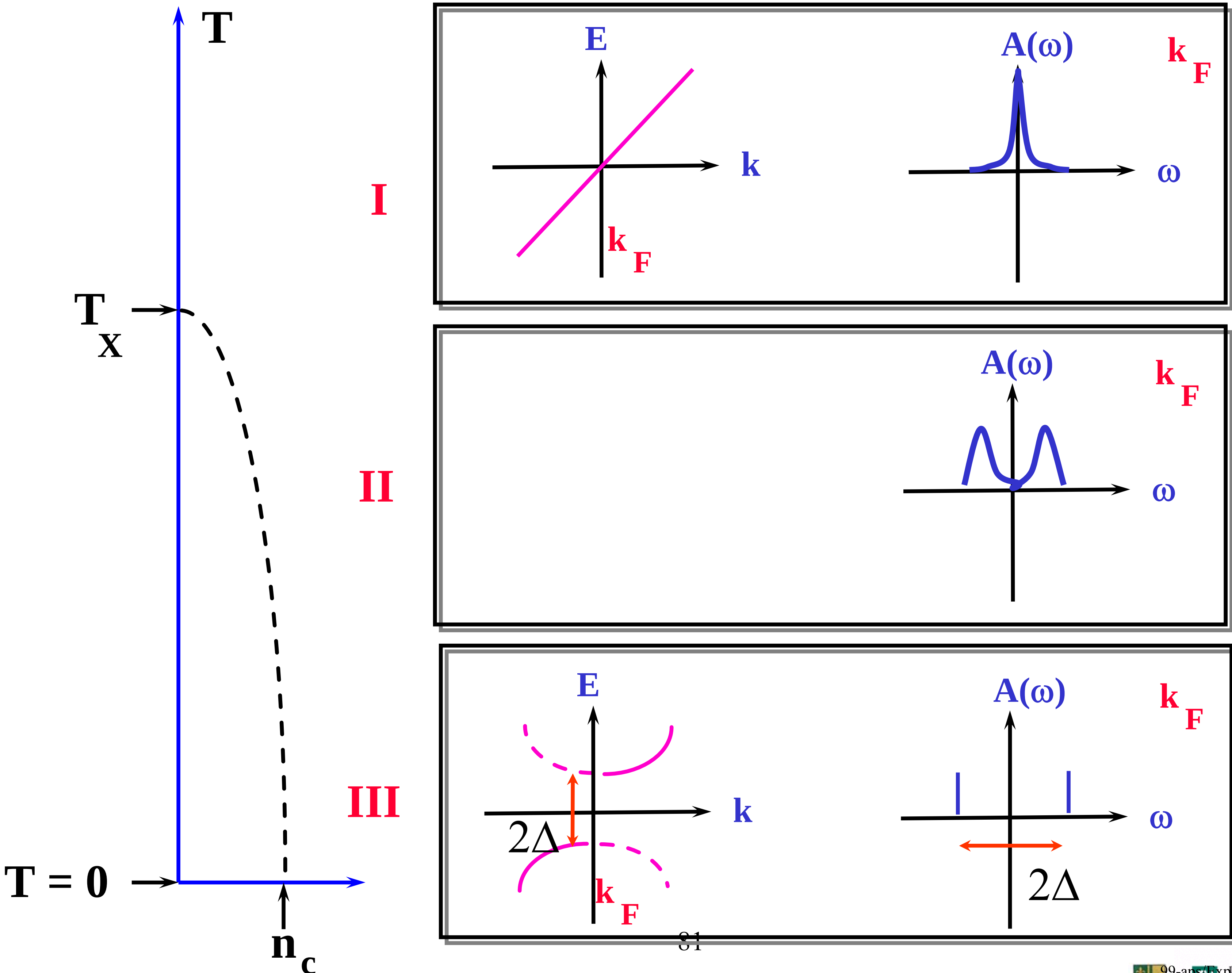



increase for smaller doping



B.Kyung *et al.*,PRB **68**, 174502 (2003)

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


T
T
X
T = 0
n
c
I
II
III
E
k
k
F
A(ω)
ω
2Δ

**Qualitatively new result:**
**effect of critical fluctuations on particles (RC regime)**

$$\hbar\omega_{sf} << k_B T$$

$$\Sigma(\mathbf{k}_F, ik_n) \propto T\int d^d q \frac{1}{q_\perp^{\;2} + q_\parallel^{\;2} + \xi^{-2}} \frac{1}{ik_n + \varepsilon_{-\mathbf{k}+\mathbf{q}}}$$

$$\mathrm{Im}\,\Sigma^R(\mathbf{k}_F, 0) \propto -\frac{T}{v_F}\xi^{3-d}$$

**in 2D:** $\xi > \xi_{th}$ $(\xi_{th} \equiv \hbar v_F / \pi k_B T)$

$$\Delta\varepsilon \approx \nabla\varepsilon_k \cdot \Delta k \approx v_F \hbar \Delta k = k_B T$$

$$\mathrm{Im}\Sigma^R(\mathbf{k}_F, 0) \propto -U\xi / (\xi_{th}\xi_0^2) > 1$$

**in 3D:** marginal case

**in 4D:** quasiparticle survives up to $T_c$

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);

**Analytically :**
**effect of critical fluctuations on particles (RC regime)**

$$\hbar\omega_{sf} << k_B T$$

Imaginary part: compare Fermi liquid, $\lim_{T\to 0} \Sigma''_R(\mathbf{k}_F,0) = 0$

$$\Sigma''_R(\mathbf{k}_F,0) \propto \frac{T}{v_F}\int d^{d-1}q_\perp \frac{1}{q_\perp^2+\xi^{-2}} \propto \frac{T}{v_f}\xi^{3-d} \underset{d=2}{\propto} \frac{\xi}{\xi_{th}}$$

$$\mathrm{Im}\Sigma^R(\mathbf{k}_F,0) \propto -U\xi/\left(\xi_{th}\xi_0^2\right) > 1$$

Why leads to pseudogap

$$A(\mathbf{k},\omega) = \frac{-2\Sigma''_R}{(\omega-\varepsilon_{\mathbf{k}}-\Sigma'_R)^2+\Sigma''^2_R}$$

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);

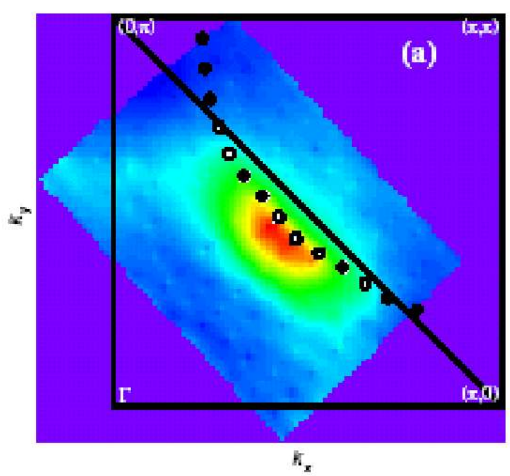
# Comparisons with experiment

# ARPES spectrum, an overview

# Strong coupling pseudogap (U > 8t)
# *t'= -0.3t , t'' = 0.2t*

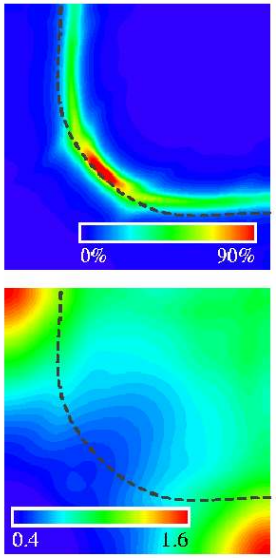
- Different from Mott gap that is local (all k) not tied to ω=0.
- Pseudogap tied to ω=0 and only in regions nearly connected by (π,π). (e and h),
- Pseudogap is independent of cluster shape (and size) in CPT.
- Not caused by AFM LRO
  - No LRO, few lattice spacings.
  - Not very sensitive to *t'*
  - Scales like *t*.

Hole-doped, 10%




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

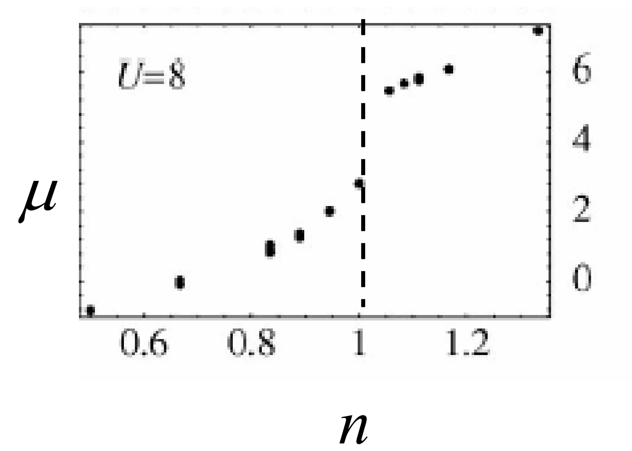
U= 8

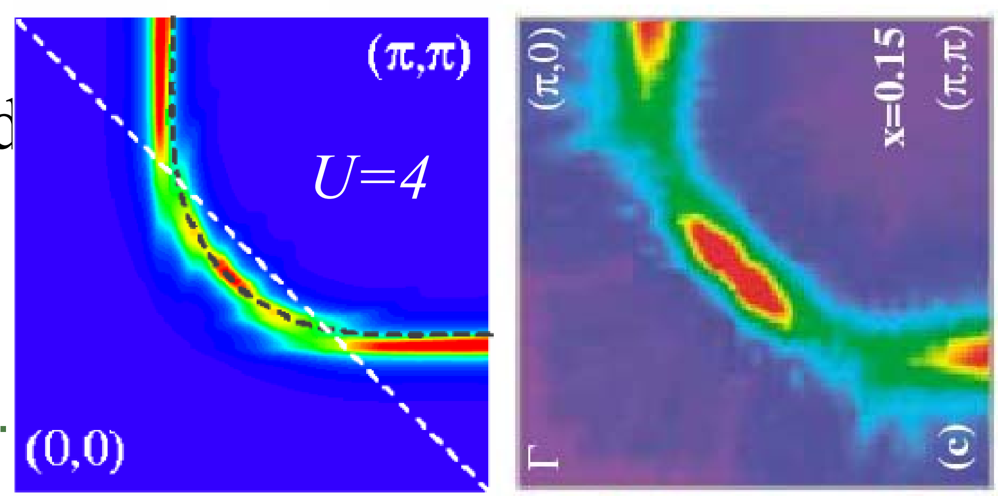



Sénéchal, AMT, PRL **92**, 126401 (2004).

# Weak-coupling pseudogap

- In CPT
  - is mostly a depression in weight
  - depends on system size and shape.
  - located precisely at intersection with AFM Brillouin zone
- Coupling weaker because better screened $U(n) \sim d\mu/dn$

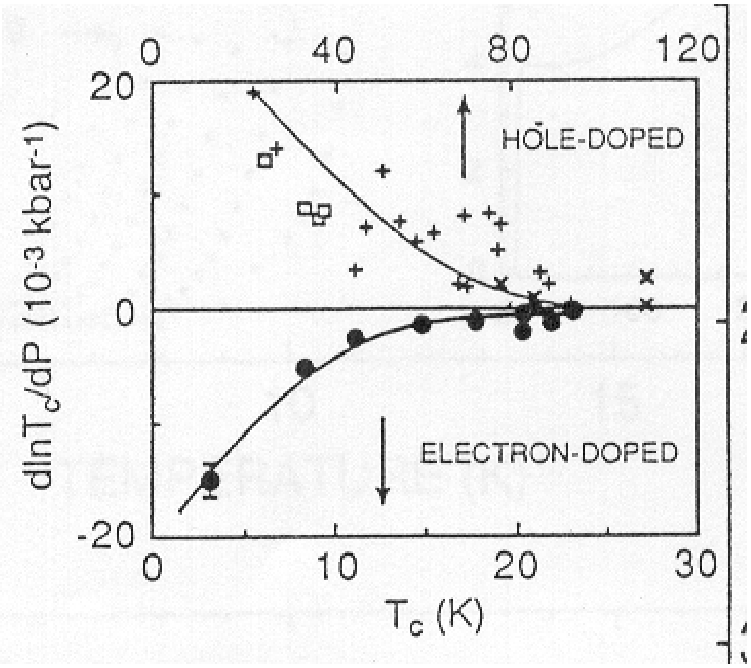



Sénéchal, AMT, PRL **92**, 126401 (2004).

# The pseudogap in electron-doped cuprates

- Near optimal doping $U \sim 6t$
  - Optical gap $1.3eV$ vs $2eV$
  - Weight near the diagonal
    - CPT, Slave-bosons, *t-J*
  - $dT_c/dp$ negative.
  - Simple screening



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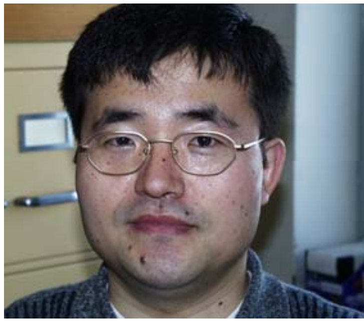
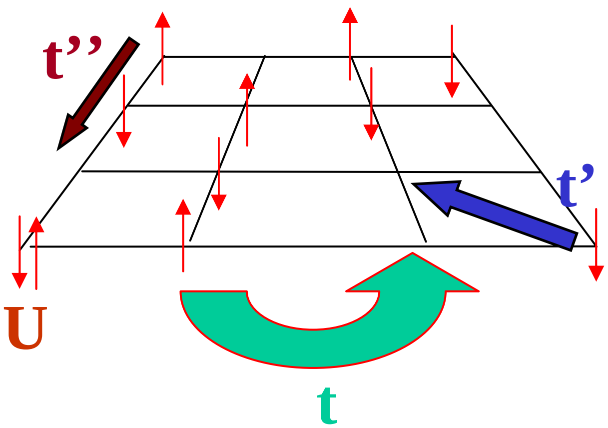


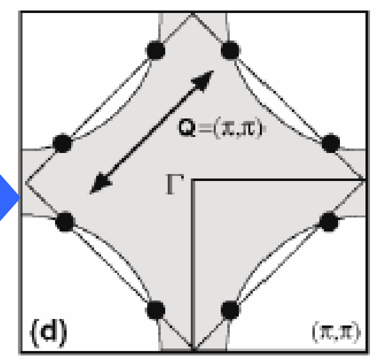
# TPSC

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




fixed

$t' = -0.175t$, $t'' = 0.05t$
$t = 350$ meV, $T = 200$ K

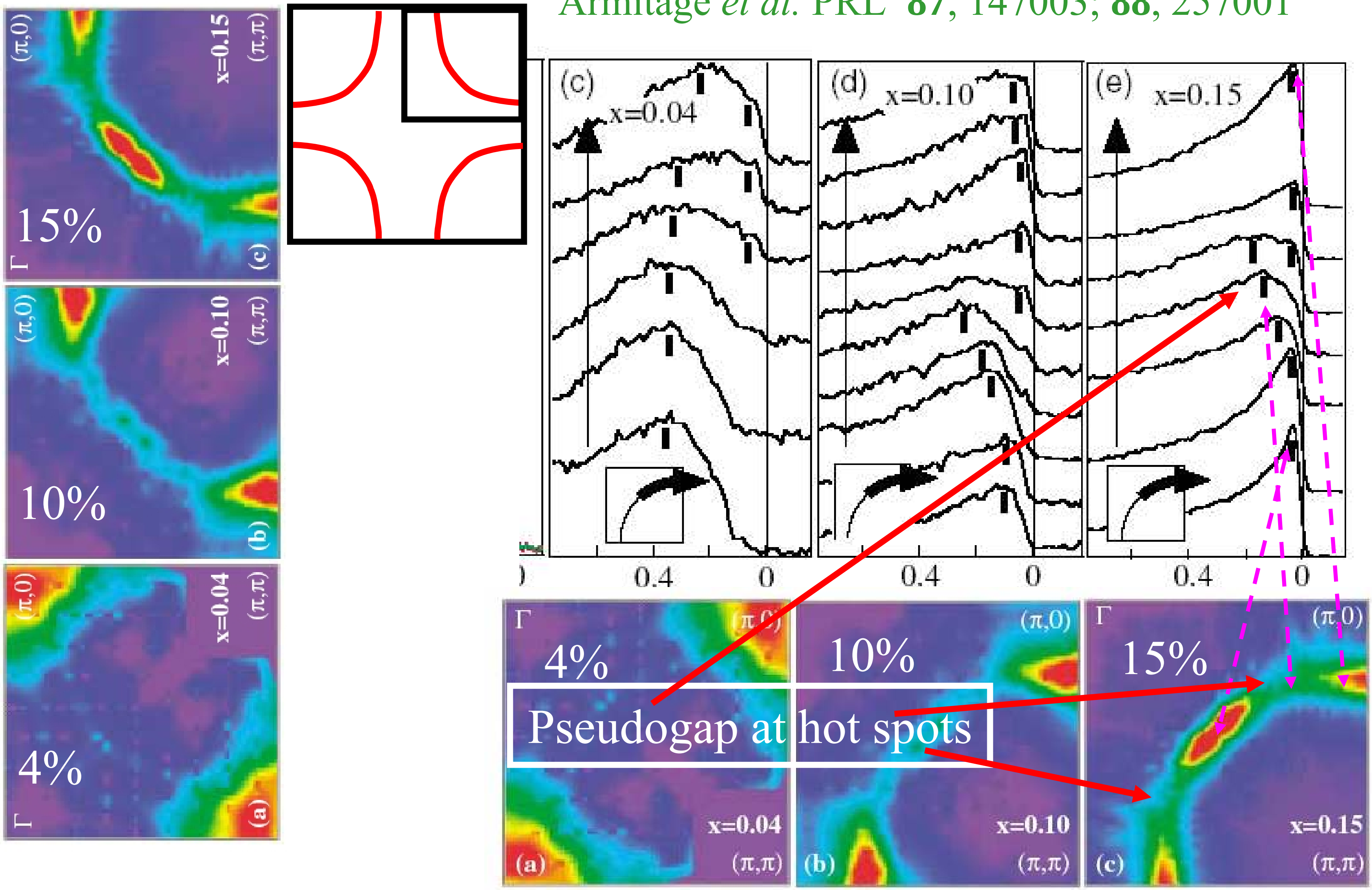



Weak coupling $U<8t$

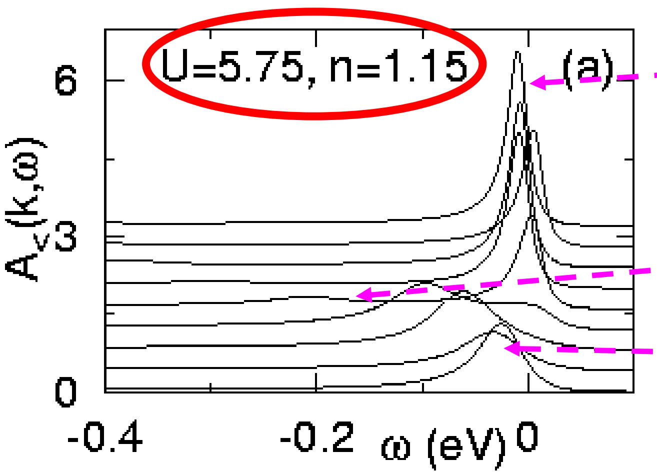
$n=1+x$ – electron filling

# Fermi surface, electron-doped case

Armitage *et al.* PRL **87**, 147003; **88**, 257001

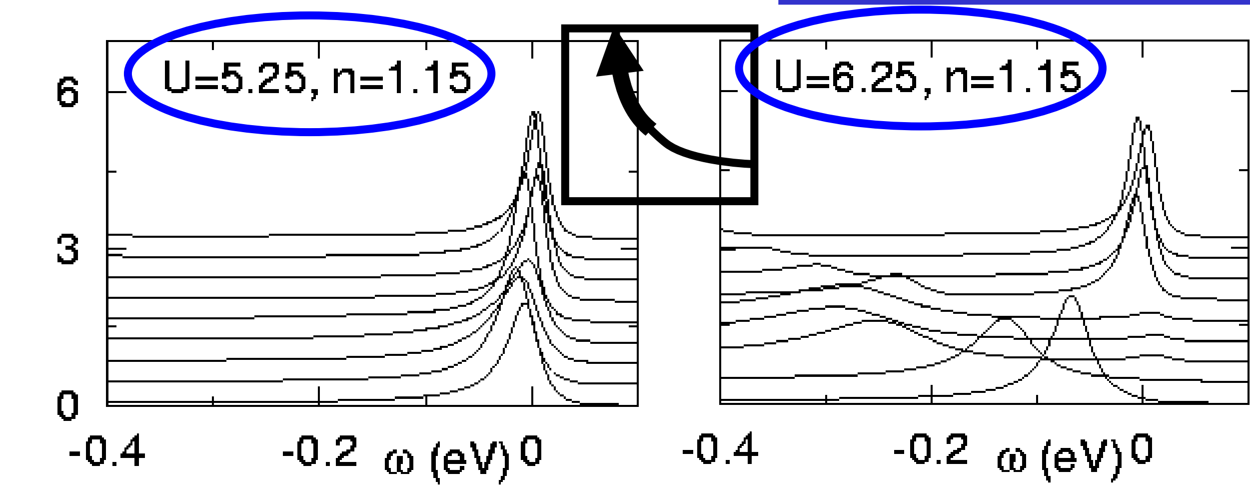


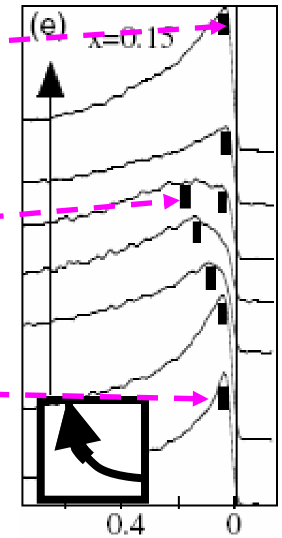
# 15% doping: EDCs along the Fermi surface TPSC



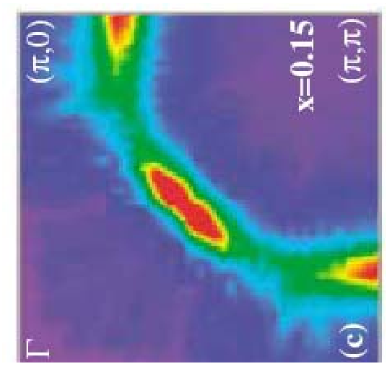

$U_{min} < U < U_{max}$

$U_{max}$ also from CPT



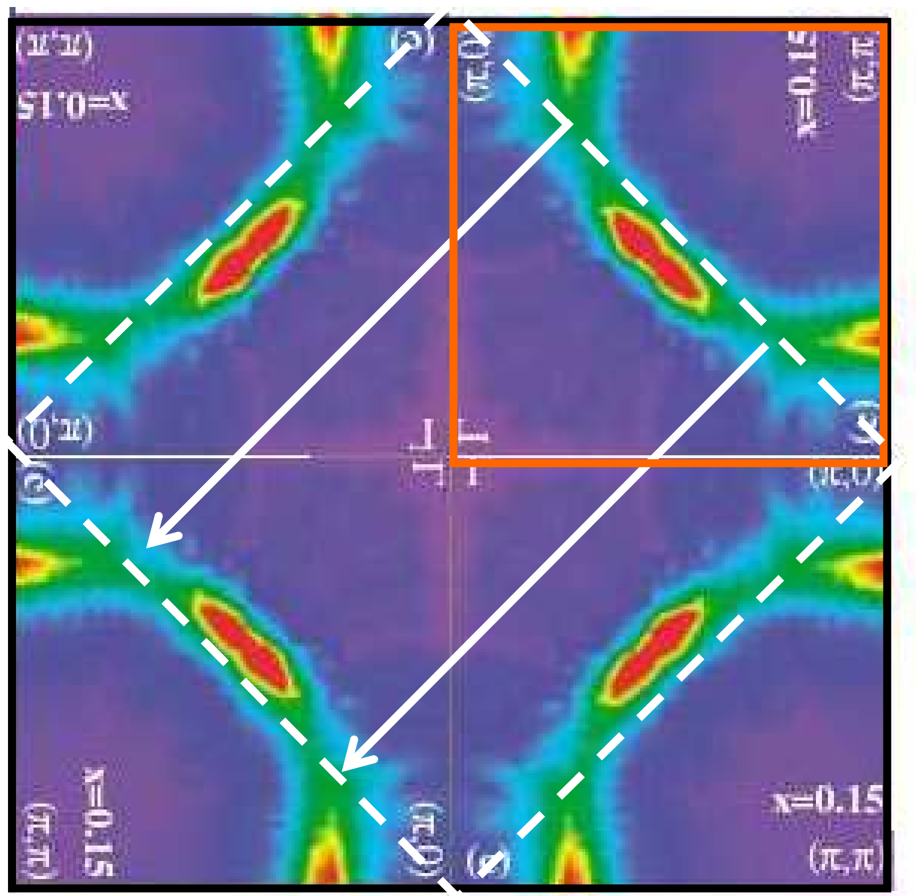




Exp

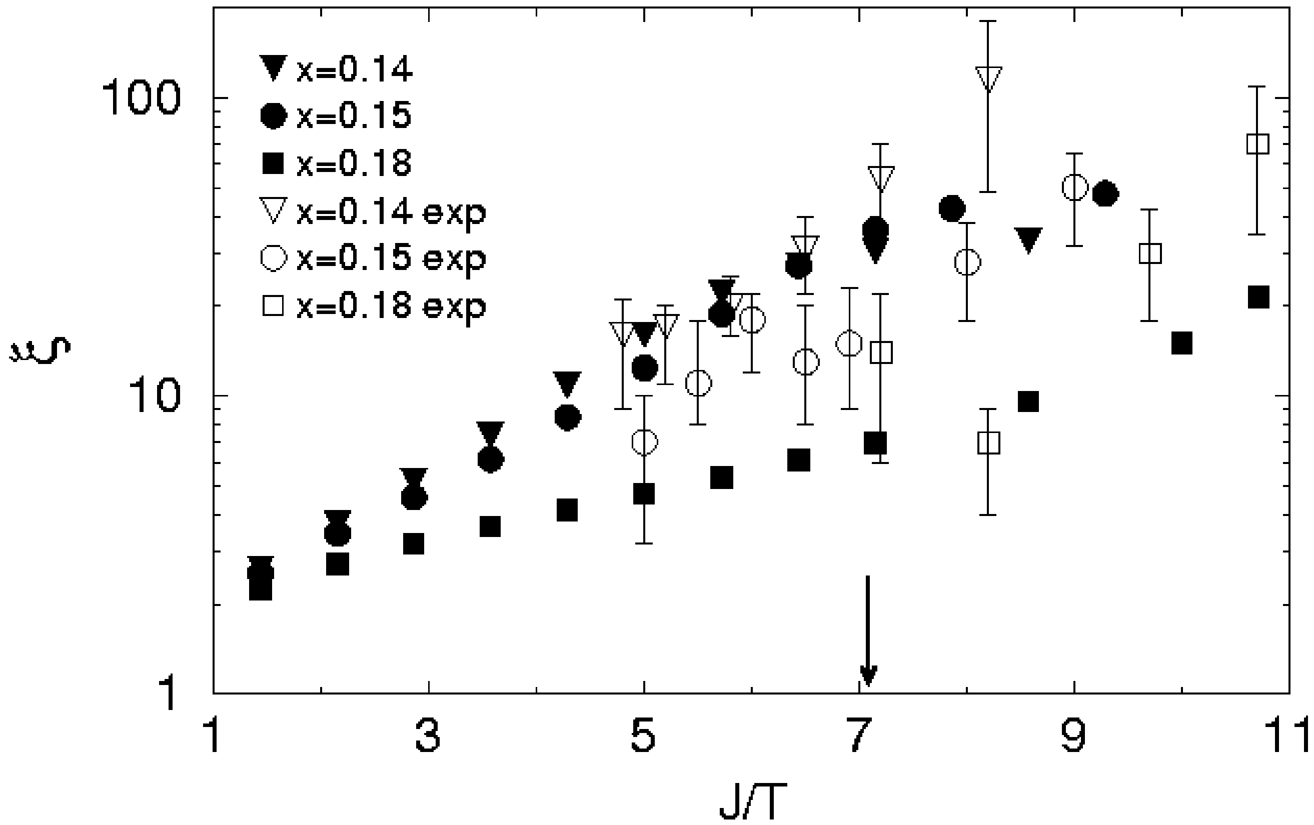



Hankevych, Kyung, A.-M.S.T., PRL, sept. 2004

# Hot spots from AFM quasi-static scattering

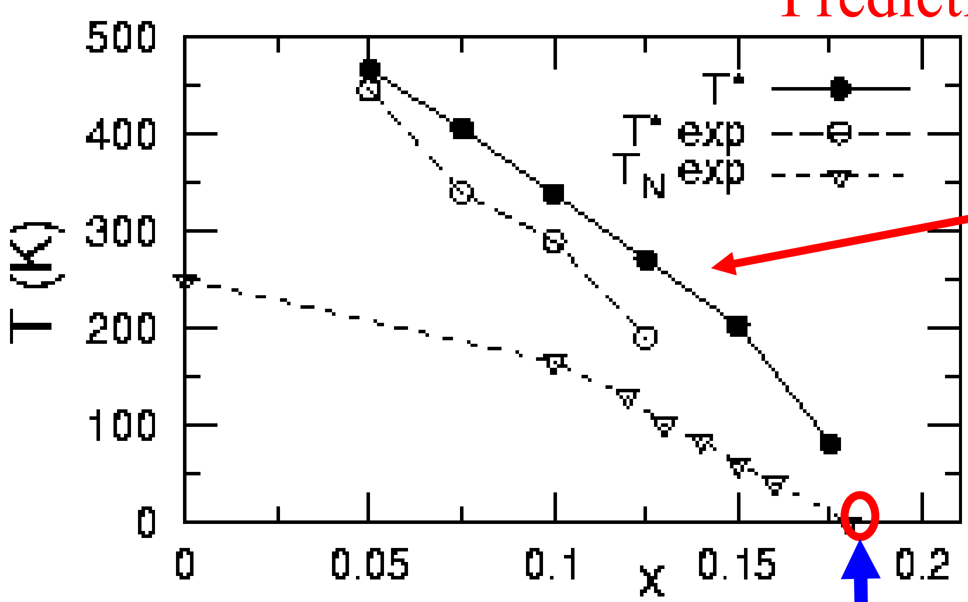


# AFM correlation length (neutron)




Hankevych, Kyung, A.-M.S.T., PRL, sept. 2004
Expt: P. K. Mang et al., cond-mat/0307093, Matsuda (1992).

# Pseudogap temperature and QCP




Prediction ➢ $\xi \approx \xi_{th}$ at PG temperature $T^*$, and $\xi > \xi_{th}$ for $T < T^*$

Prediction supports further AFM fluctuations origin of PG

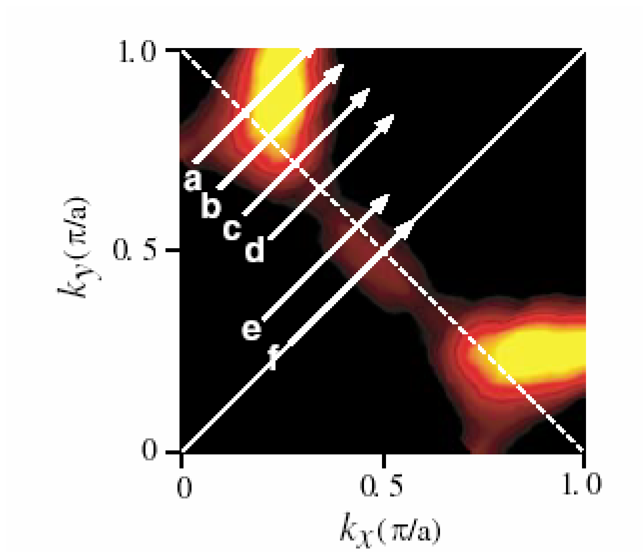
Matsui *et al.* PRL (2005)
Verified theo.T* at $x=0.13$
with ARPES

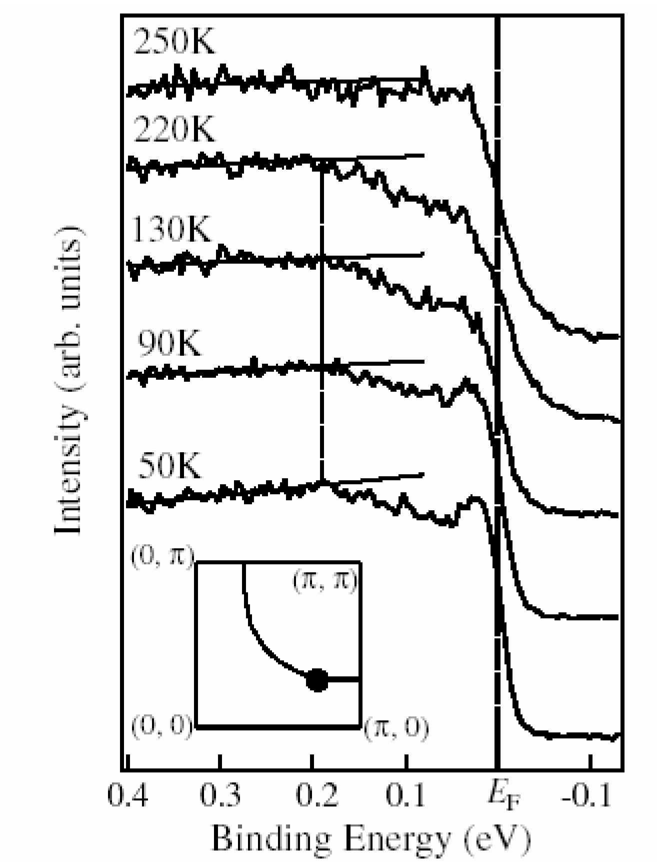
Prediction QCP
may be masked by 3D transitions

➢ $\Delta_{PG} \approx 10 k_B T^*$ comparable with optical measurements

Hankevych, Kyung, A.-M.S.T., PRL 2004 : Expt: Y. Onose et al., PRL (2001).

# Observation




Matsui et al. PRL **94,** 047005 (2005)

Reduced, *x=0.13*

AFM *110 K*, SC *20 K*

does not change with temperature. On further increasing the temperature, the pseudogap is totally filled in in the spectrum at 250 K, suggesting that the short-range AF correlation disappears at around this temperature. The

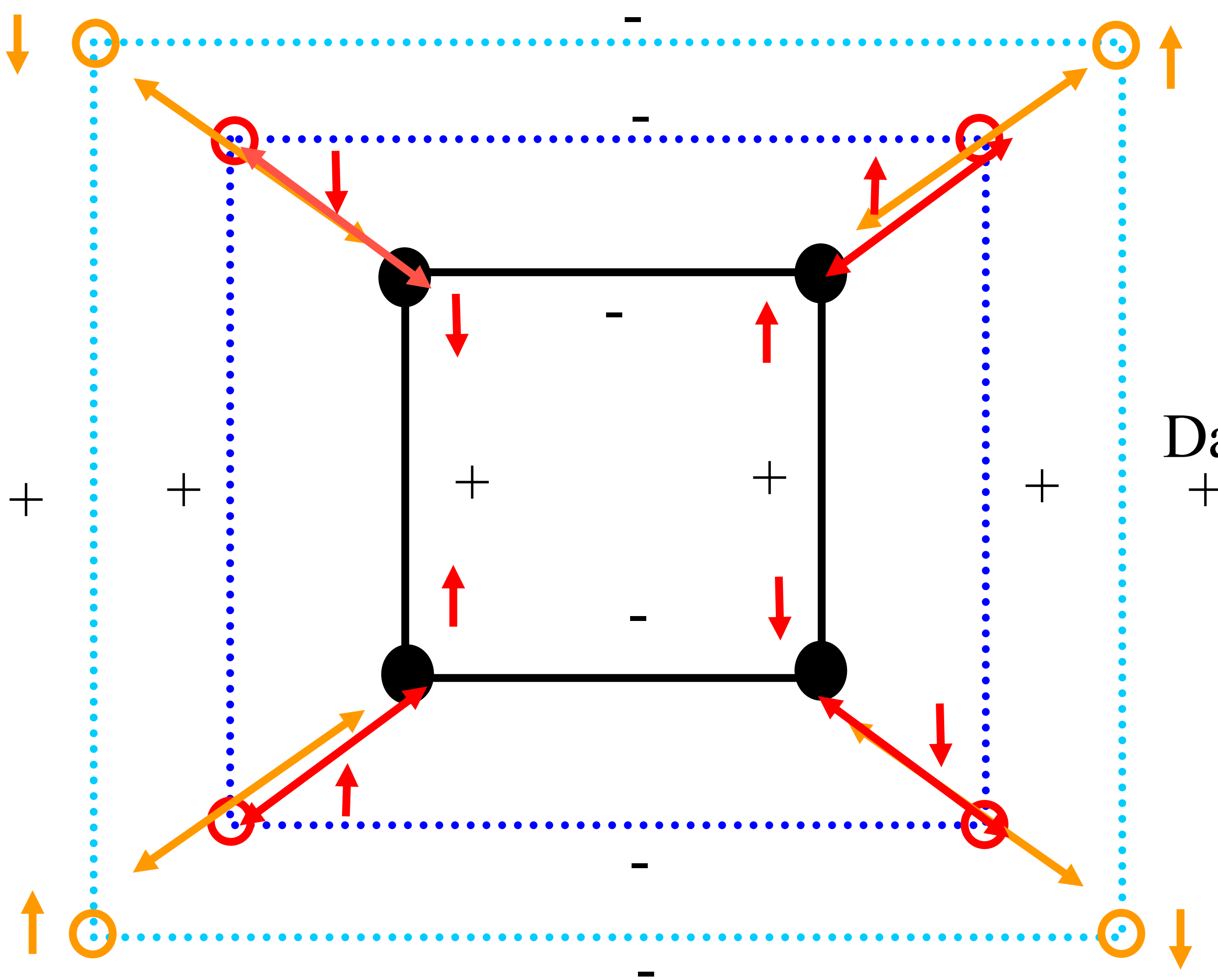
# Precursor of SDW state (dynamic symmetry breaking)

- Y.M. Vilk and A.-M.S. Tremblay, J. Phys. Chem. Solids **56**, 1769-1771 (1995).
- Y. M. Vilk, Phys. Rev. B 55, 3870 (1997).
- J. Schmalian, *et al.* Phys. Rev. B **60**, 667 (1999).
- B.Kyung *et al.*,PRB **68**, 174502 (2003).
- Hankevych, Kyung, A.-M.S.T., PRL, sept 2004
- R. S. Markiewicz, cond-mat/0308469.

# The phase diagram for high-temperature superconductors

# Competition between antiferromagnetism and superconductivity

# Competition AFM-dSC – using SFT



David Sénéchal

See also, Capone and Kotliar, cond-mat/0603227,
Macridin et al. DCA cond-mat/0411092

# Preliminary

$t' = -0.3\,t, \;\; t'' = 0.2\,t$
$U = 8t$

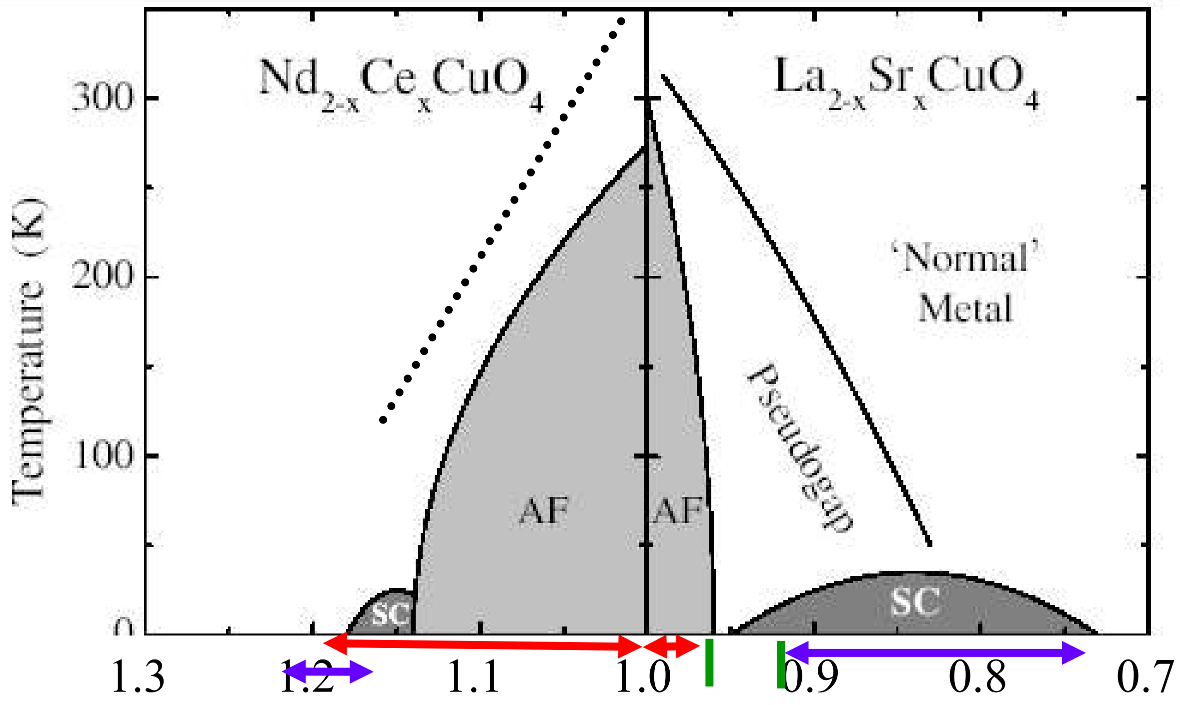



FIG. 1 Phase diagram of n and p-type superconductors.

*n*, electron density Damascelli, Shen, Hussain, RMP 75, 473 (2003)

# Anomalous superconductivity near the Mott transition

# Effect of proximity to Mott

Sarma Kancharla

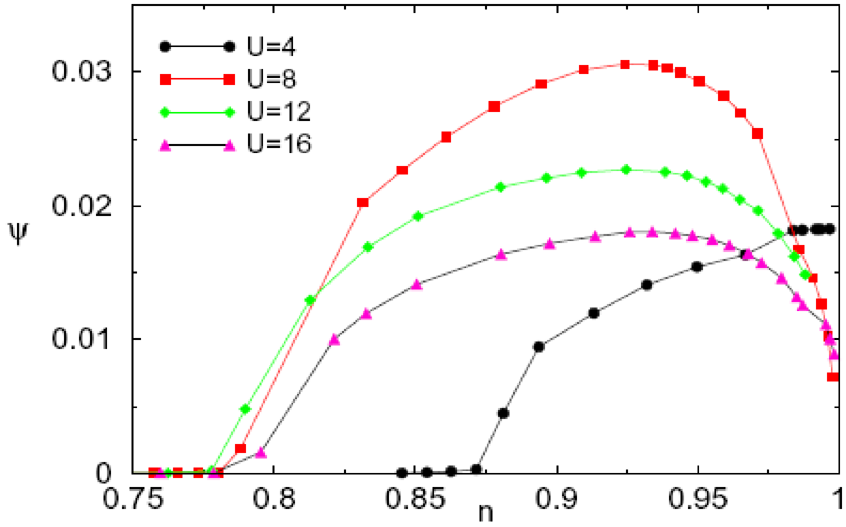



FIG. 1: SC order parameter $\psi$ as a function of filling $n$ and onsite Coulomb repulsion $U$, $t' = 0$.



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# Gap vs order parameter

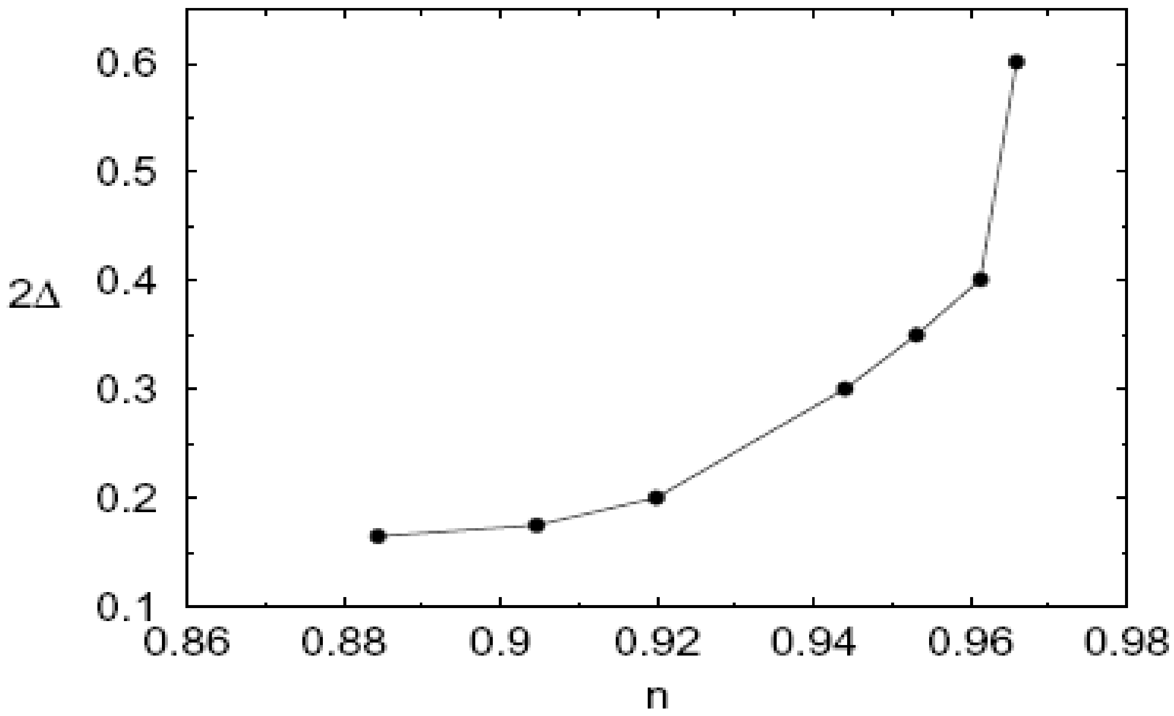
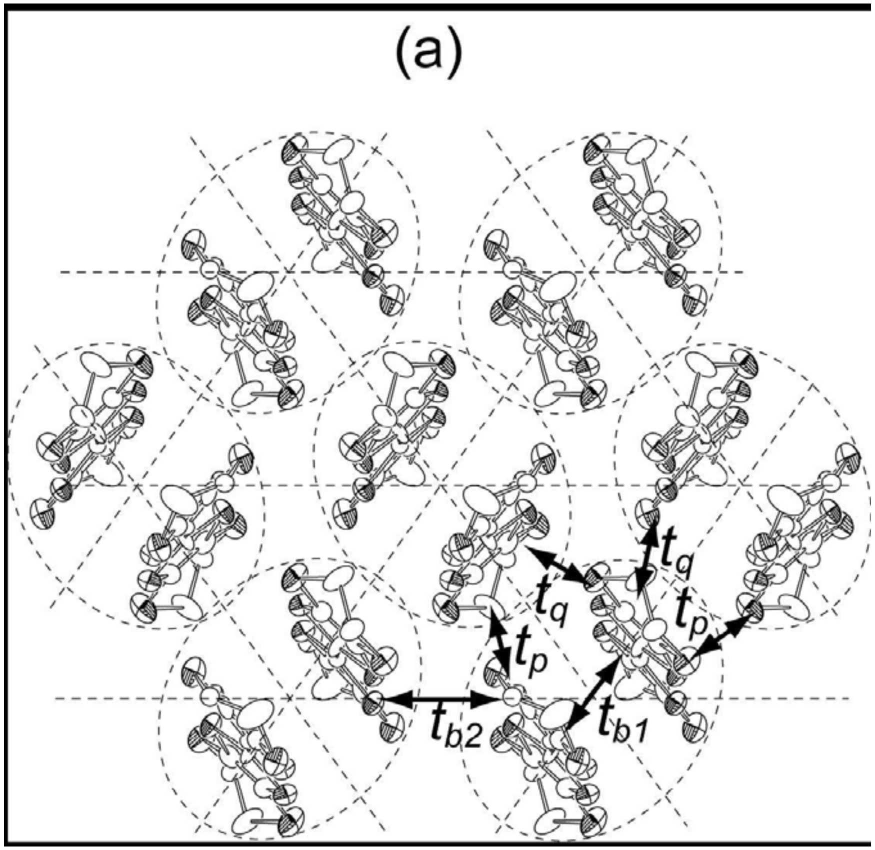


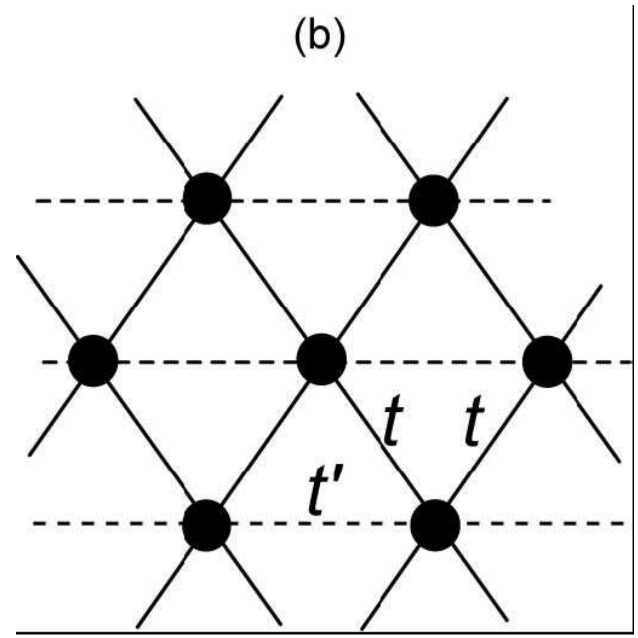

FIG. 2: The dSC gap as a function of filling, U=8t, $t' = -0.3t$.

# One-band Hubbard model for organics

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




Y. Shimizu, et al. Phys. Rev. Lett. **91**, 107001(2003)

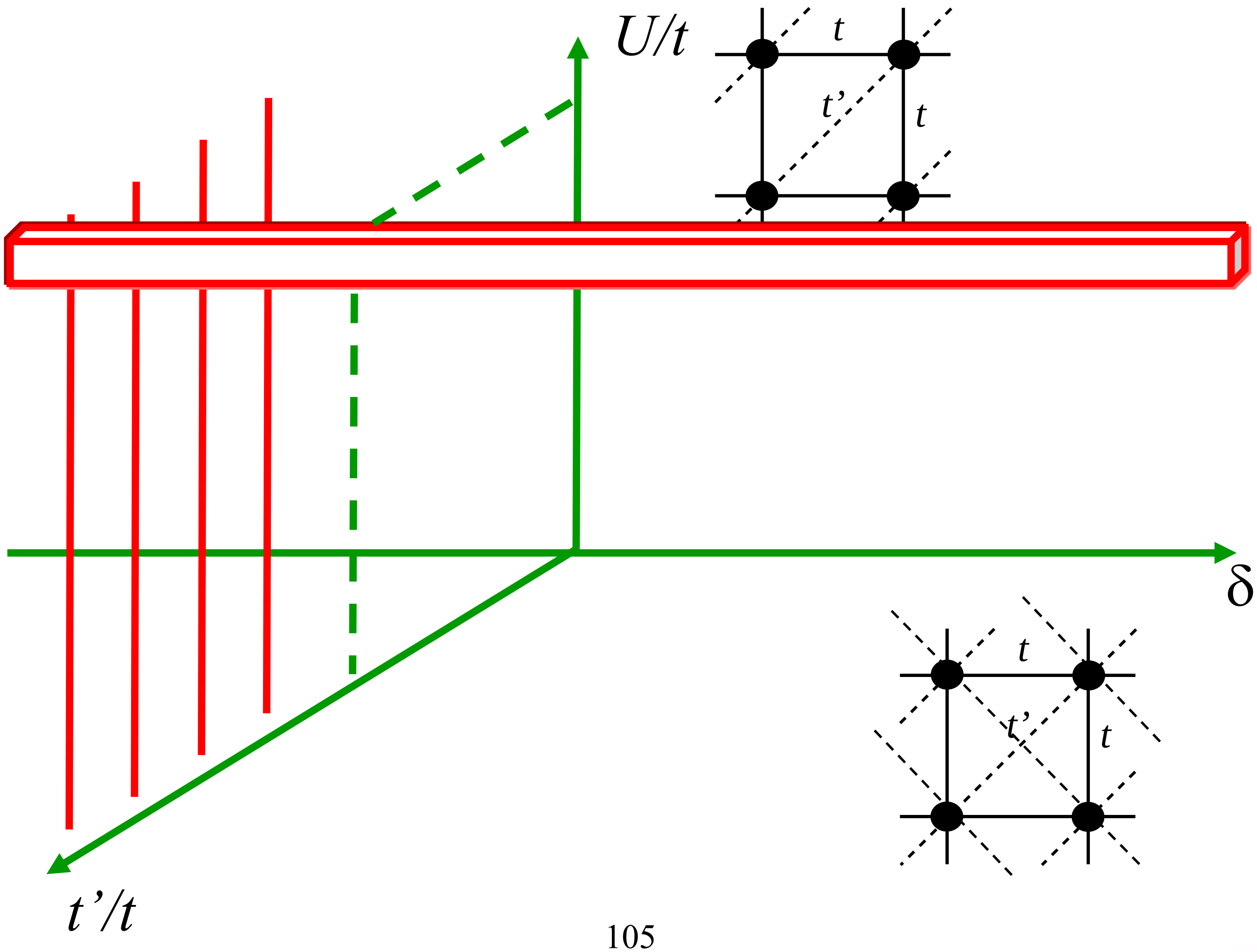



$$t \approx 50 \text{ meV}$$

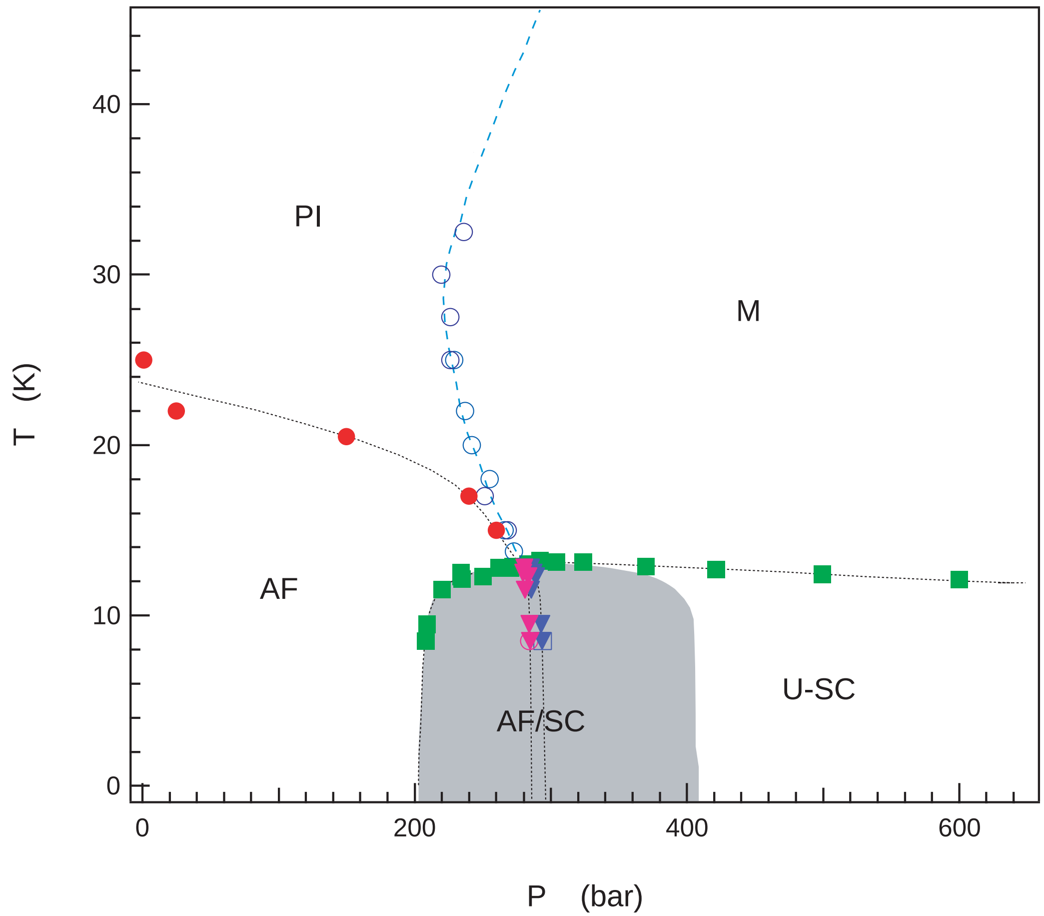
$$\Rightarrow U \approx 400 \text{ meV}$$

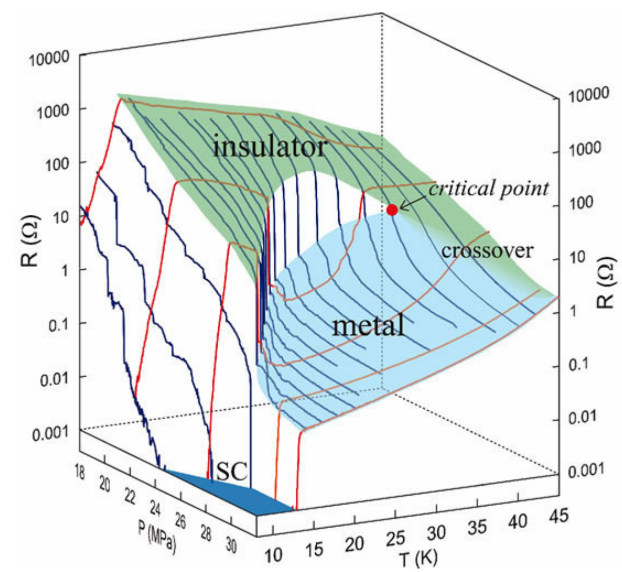
$t'/t \sim 0.6 - 1.1$

# Perspective



# Experimental phase diagram for Cl



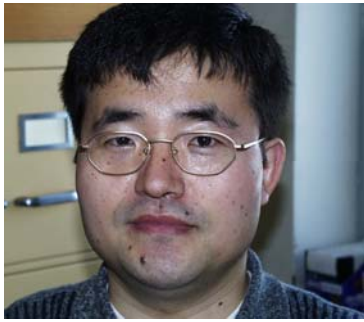




F. Kagawa, K. Miyagawa, + K. Kanoda
PRB **69** (2004) +Nature **436** (2005)

Diagramme de phase (X=$Cu[N(CN)_2]Cl$)

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

# Mott transition (C-DMFT)



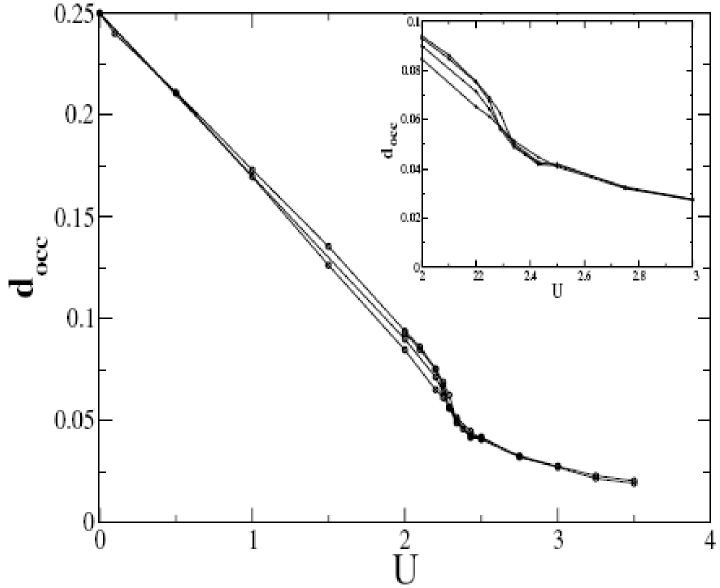
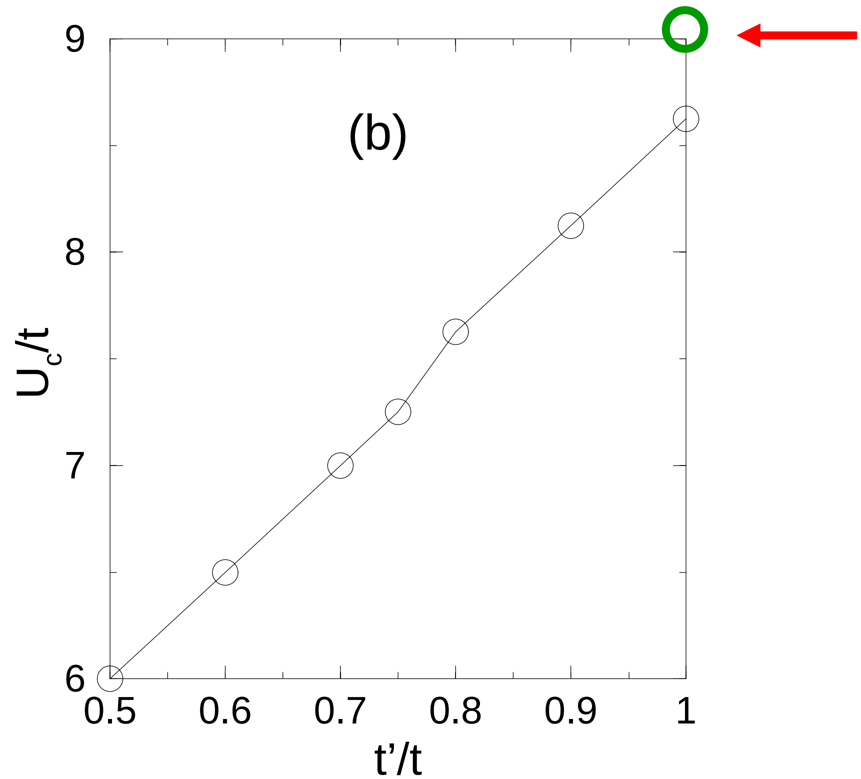



FIG. 3. Double occupancy as a function of $U/D$. The curves correspond (from bottom to top) to $T/D = 1/20, 1/30, 1/40, 1/44$.




Kyung, A.-M.S.T. (2006)

Parcollet, Biroli, Kotliar, PRL 92 (2004)

See also, Sénéchal, Sahebsara, cond-mat/0604057



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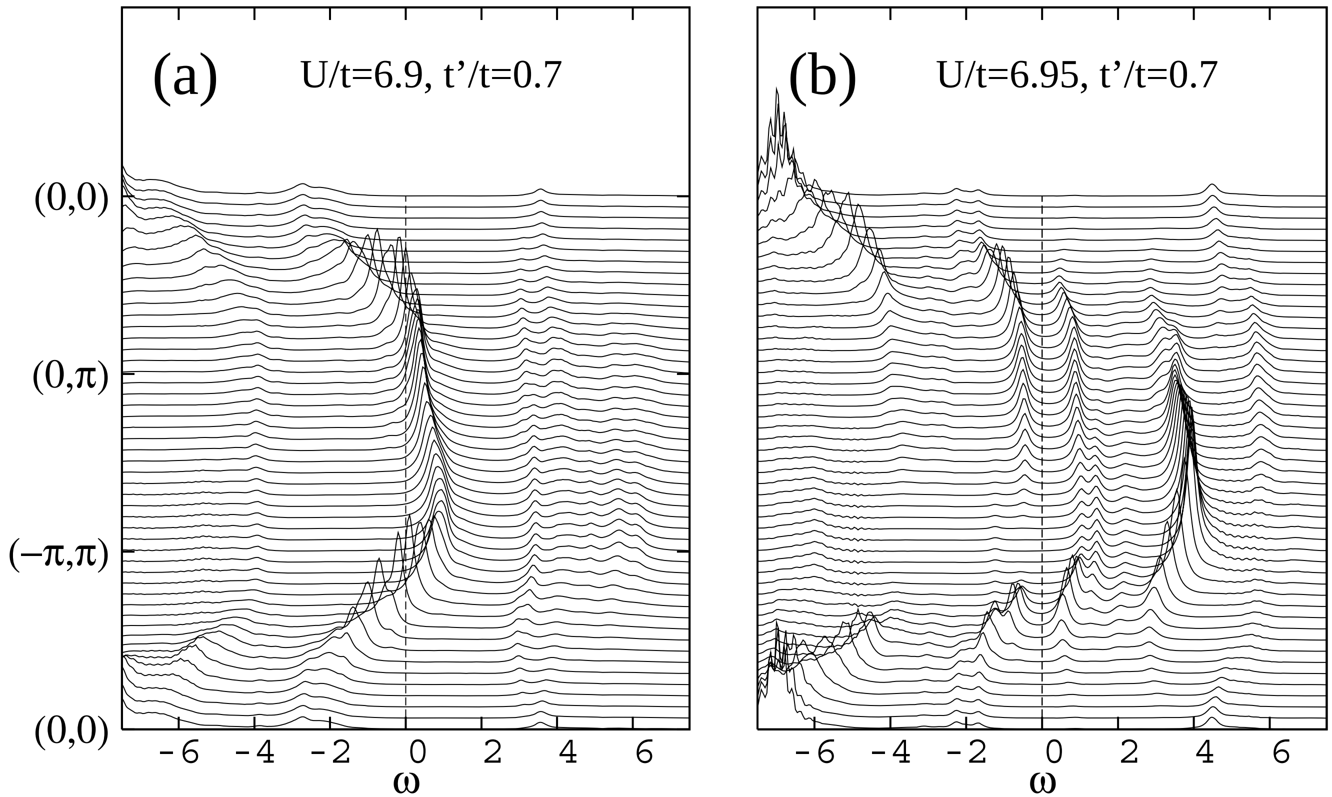
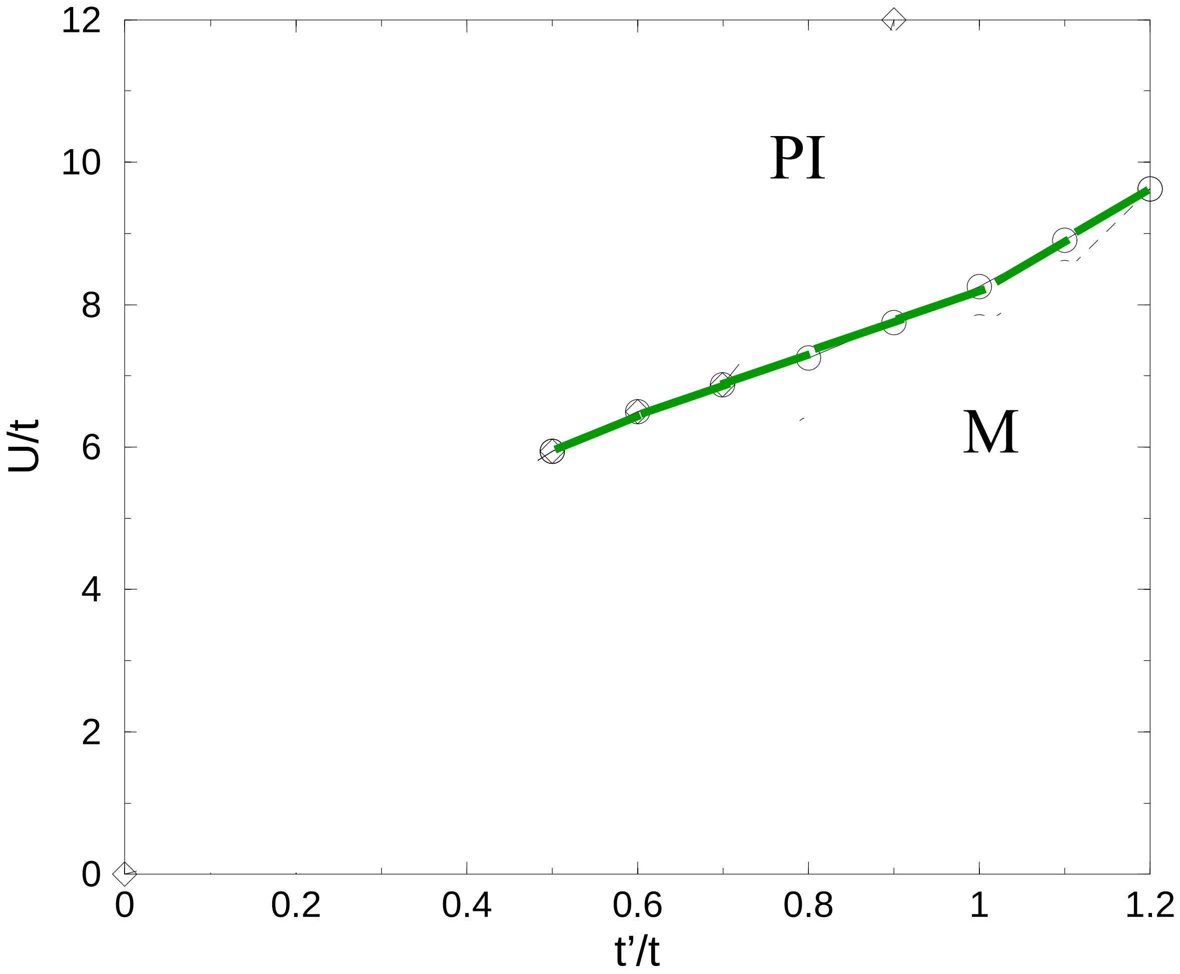
# Mott transition (C-DMFT)




Kyung, A.-M.S.T. (2006)

See also, Sénéchal, Sahebsara, cond-mat/0604057

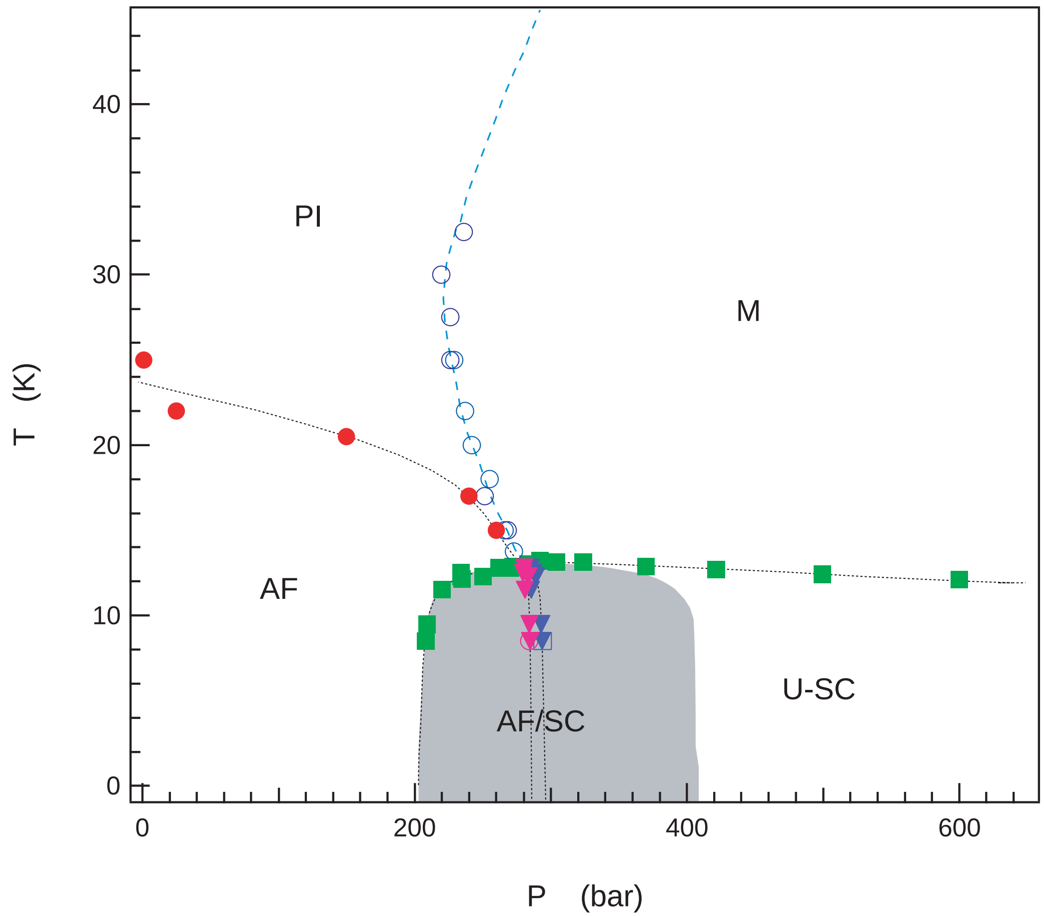
# Normal phase theoretical results for BEDT-X

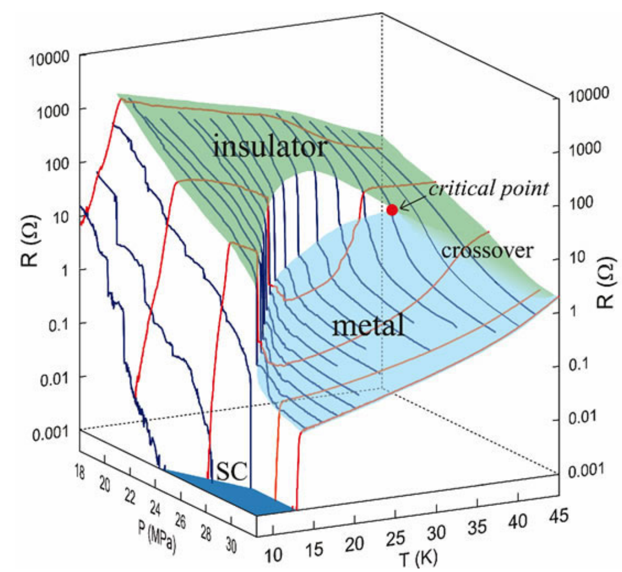





Kyung, A.-M.S.T. (2006)

# Experimental phase diagram for Cl




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

## Diagramme de phase (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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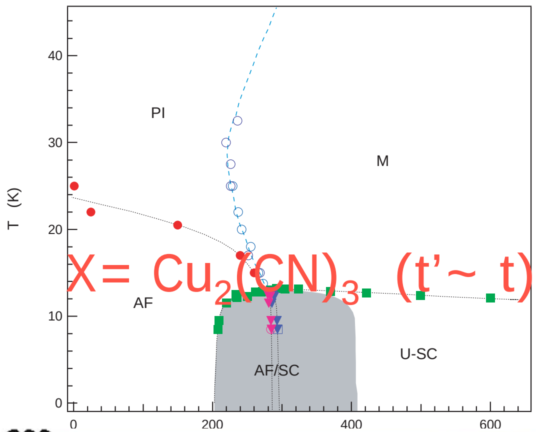
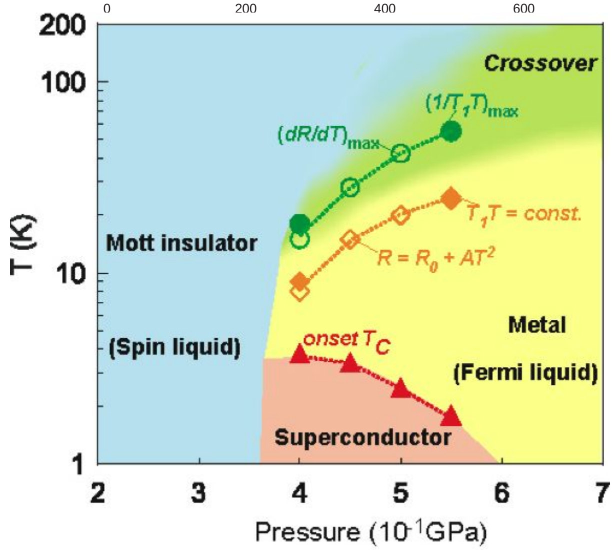
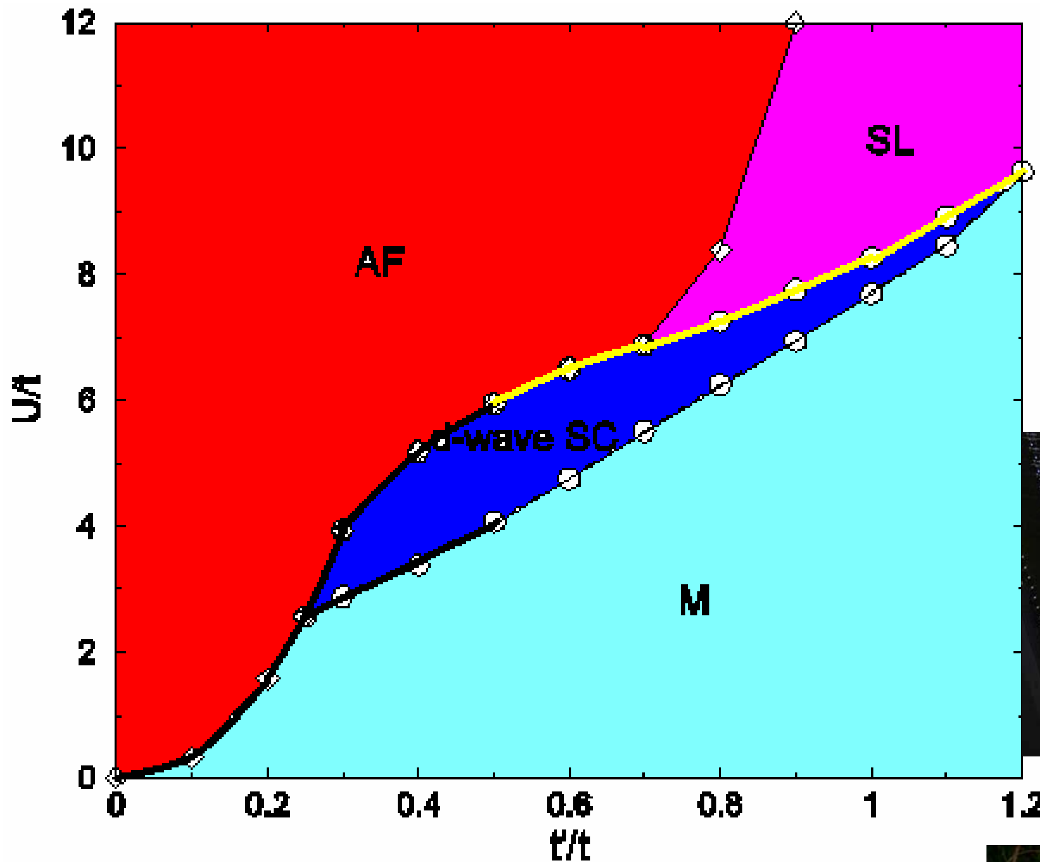
# Theoretical phase diagram BEDT




OP


Kyung, A.-M.S.T. cond-mat/0604377
Sénéchal, Sahebsara, cond-mat/0604057

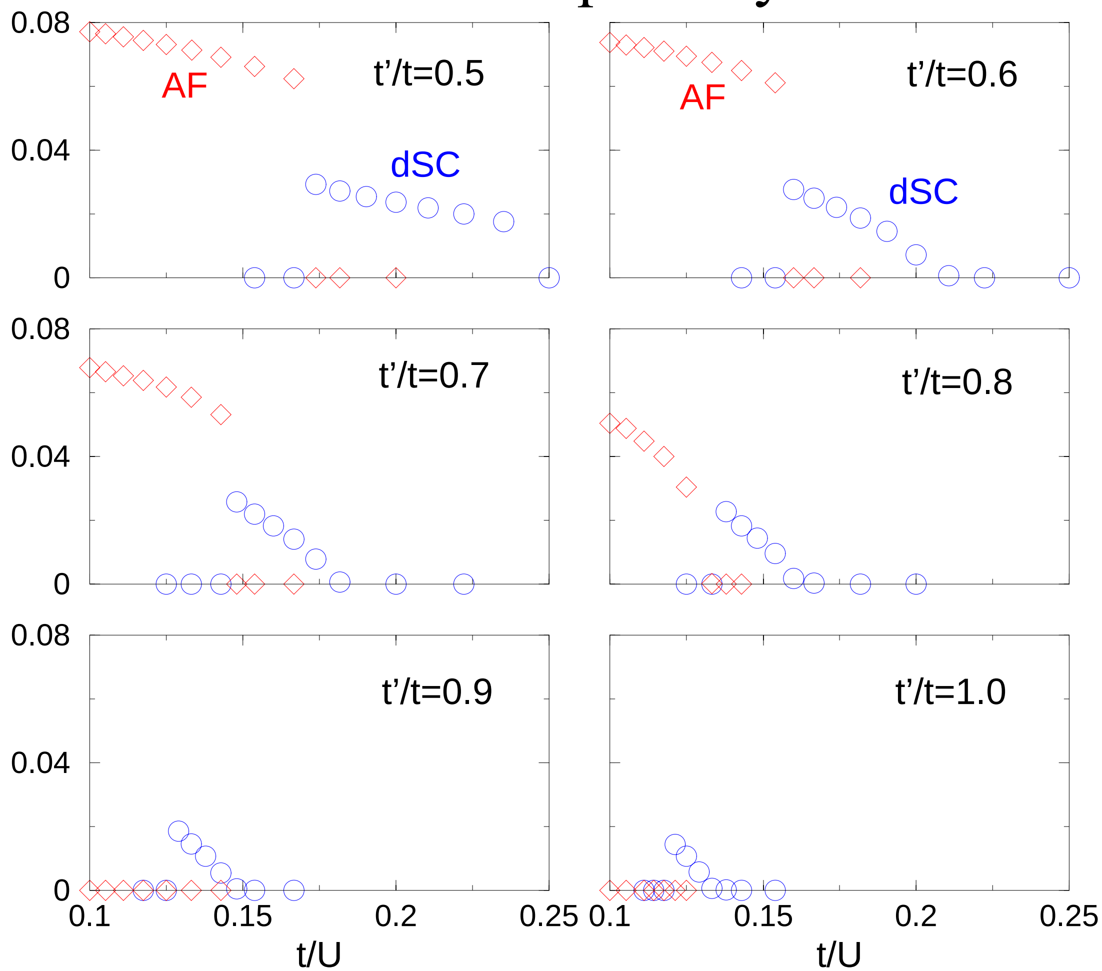
Y. Kurisaki, et al.
Phys. Rev. Lett. **95**, 177001(2005) Y. Shimizu, et al. Phys. Rev. Lett. **91**, (2003)

# AFM and dSC order parameters for various t'/t

- Discontinuous jump
- Correlation between maximum order parameter and Tc

| X | $Cu[N(CN)_2]Br$ | $Cu(NCS)_2$ | $Cu_2(CN)_3$ |
|---|---|---|---|
| t'/t | 0.68 | 0.84 | 1.06 |
| $T_c$ | 11.6 | 10.4 | 3.9 |

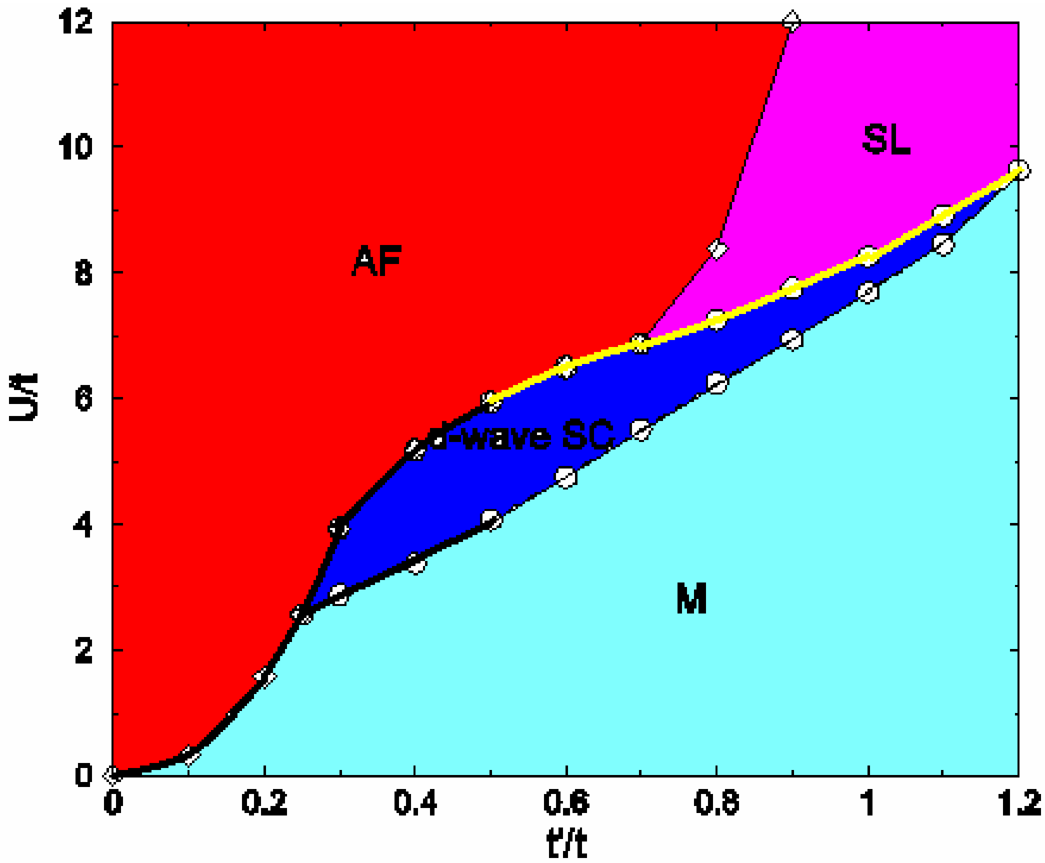
AF multiplied by 0.1






Kyung, A.-M.S.T. cond-mat/0604377

# d-wave

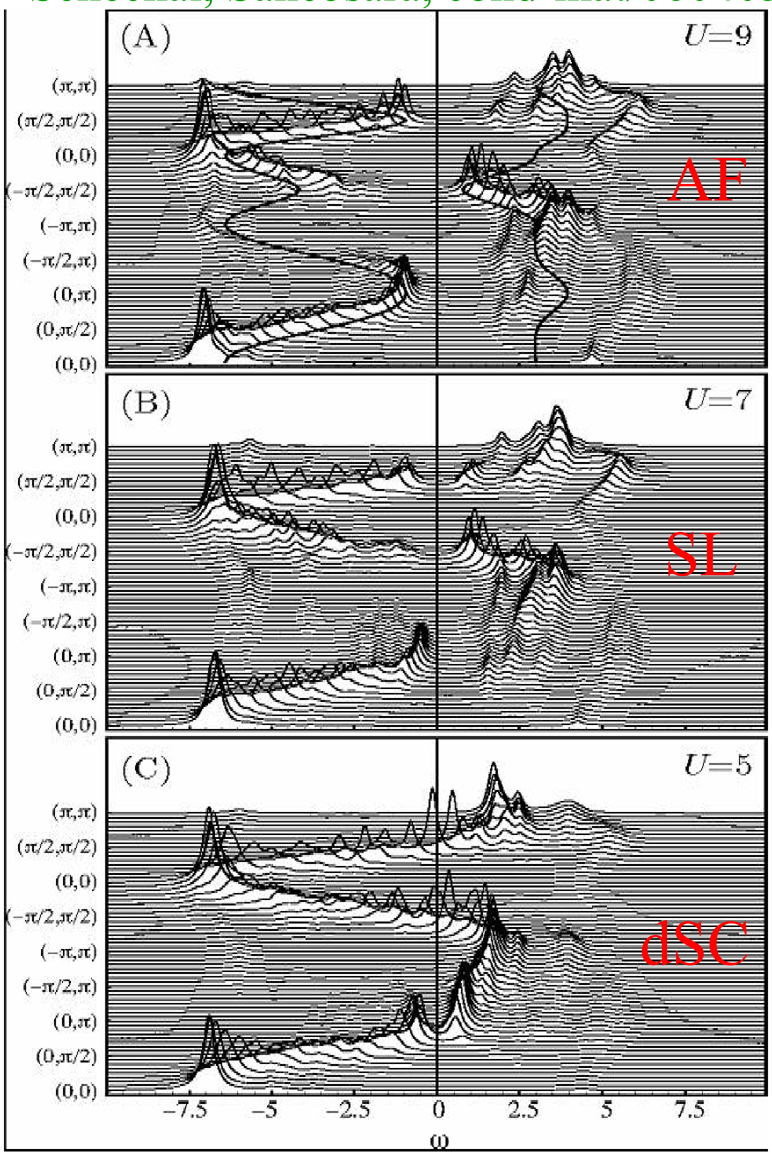



Kyung, A.-M.S.T. cond-mat/0604377

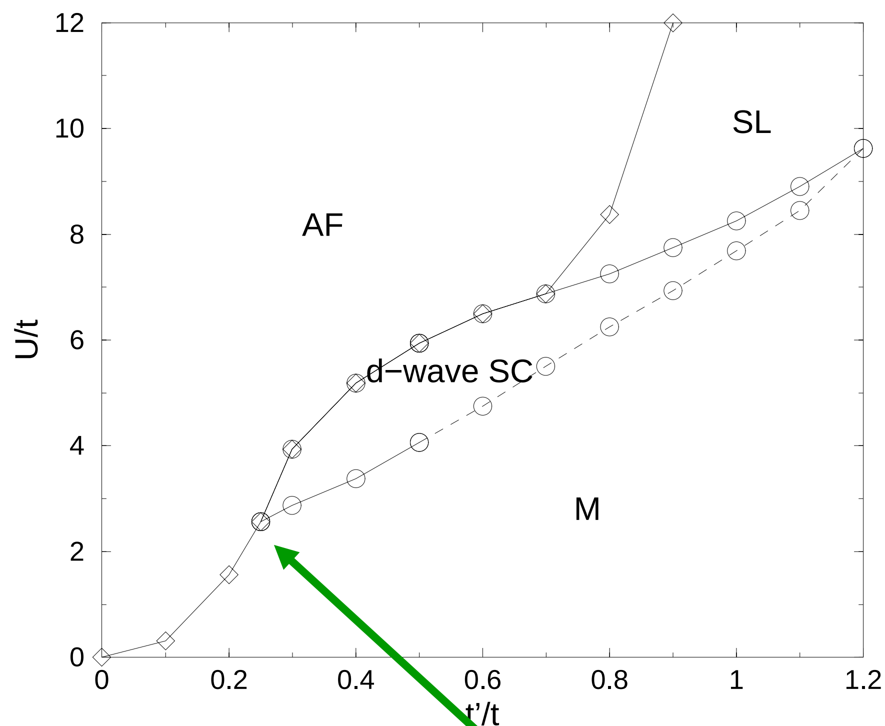
Sénéchal, Sahebsara, cond-mat/0604057

# Prediction of a new type of pressure behavior

Sénéchal, Sahebsara, cond-mat/0604057




Kyung, A.-M.S.T. cond-mat/0604377




•All transitions first order, except one with dashed line

*t'/t=0.8t*

•Triple point, not *SO(5)*

# Références on layered organics

H. Morita et al., J. Phys. Soc. Jpn. 71, 2109 (2002).

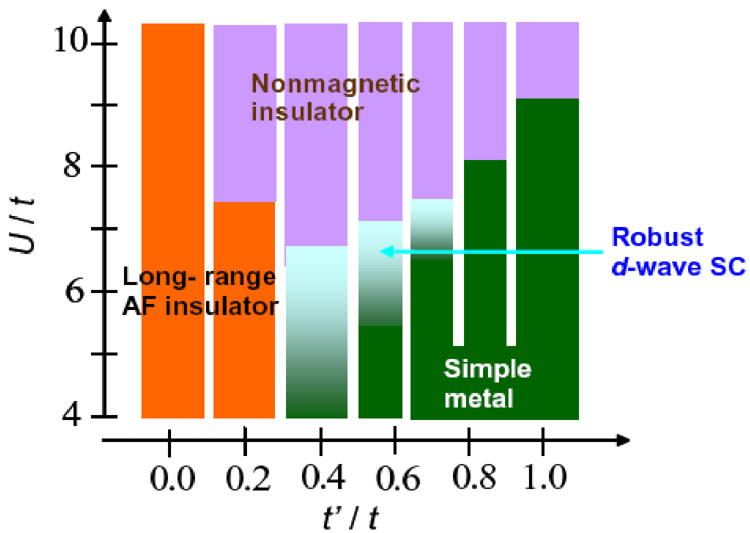
J. Liu et al., Phys. Rev. Lett. 94, 127003 (2005).

S.S. Lee et al., Phys. Rev. Lett. 95, 036403 (2005).

B. Powell et al., Phys. Rev. Lett. 94, 047004 (2005).

J.Y. Gan et al., Phys. Rev. Lett. 94, 067005 (2005).

T. Watanabe et al., cond-mat/0602098



# Summary - Conclusion

- Ground state of $CuO_2$ planes (h-, e-doped)
  - V-CPT, (C-DMFT) give overall ground state phase diagram with *U* at intermediate coupling.
  - Effect of *t'*.
- Non-BCS feature
  - Order parameter decreases towards $n = 1$ but gap increases.
  - Max dSC scales like *J*.
  - Emerges from a pseudogaped normal state (Z) (scales like *t*).

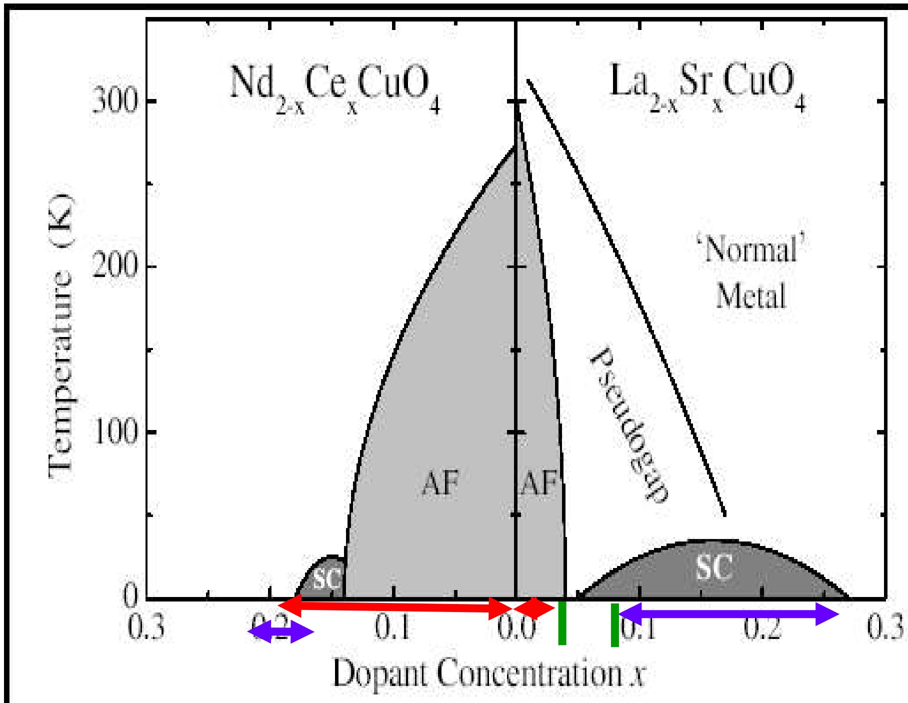
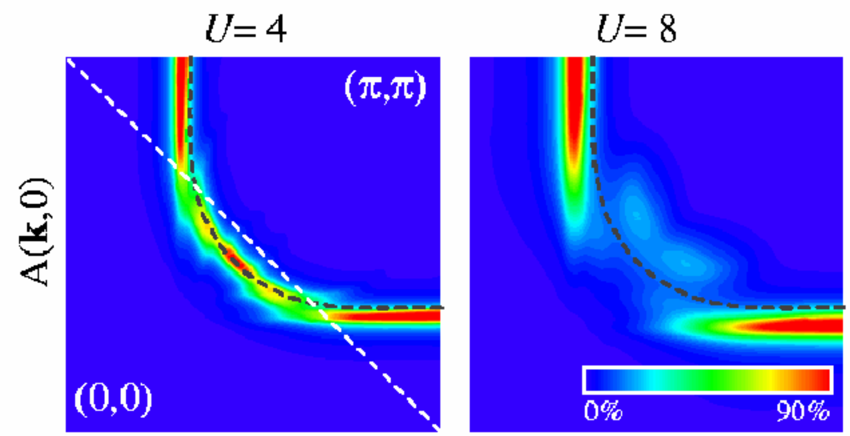


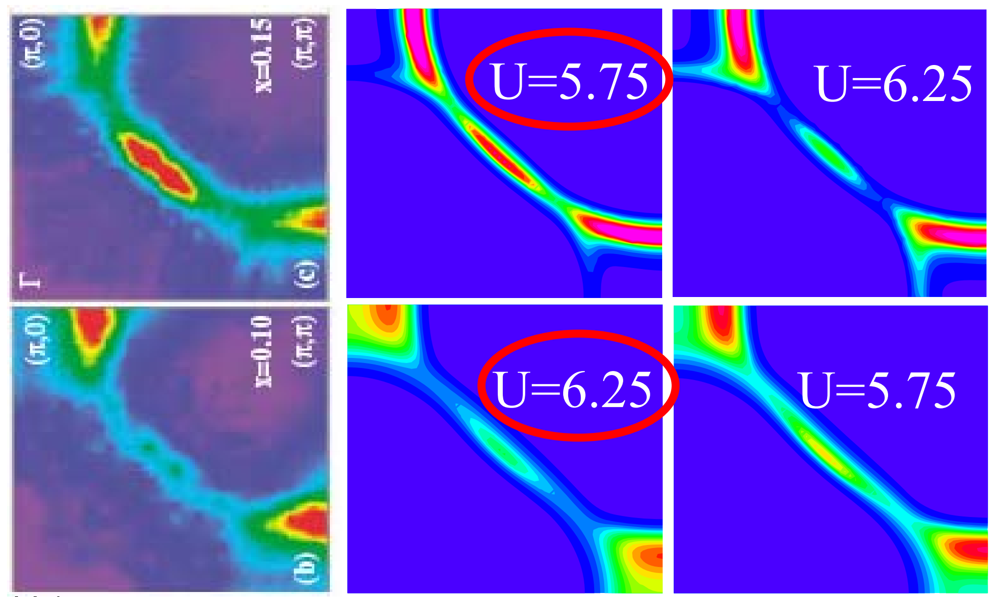

FIG. 1 Phase diagram of n and p-type superconductors.

Sénéchal, Lavertu, Marois, A.-M.S.T., PRL, 2005
Kancharla, Civelli, Capone, Kyung, Sénéchal, Kotliar, A-M.S.T. cond-mat/0508205

# Conclusion

- Normal state (pseudogap in ARPES)
  - Strong and weak coupling mechanism for pseudogap.
  - CPT, TPSC, slave bosons suggests *U ~ 6t* near optimal doping for e-doped with slight variations of U with doping.



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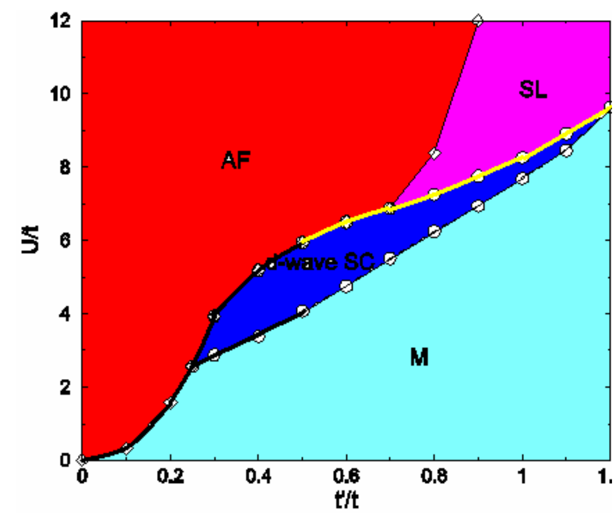
# Conclusion

- The Physics of High-temperature superconductors is in the Hubbard model (with a very high probability).

- We are beginning to know how to squeeze it out of the model!

- Insight from other compounds




- Numerical solutions … DCA (Jarrell, Maier) Variational QMC (Paramekanti, Randeria, Trivedi).

- Role of mean-field theories : Physics

- Lot more work to do.

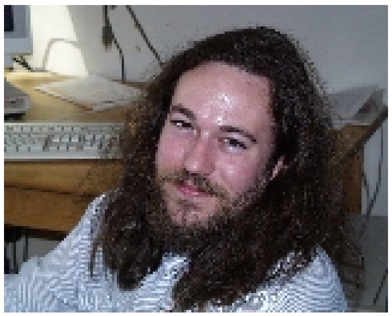
# Conclusion, open problems

- Methodology:
  - Response functions
  - $T_c$
  - Variational principle
  - First principles
  - …
- Questions:
  - Why not 3d?
  - Best « mean-field » approach.
  - Manifestations of mechanism
  - Frustration *vs* nesting

Steve Allen

Liang Chen

Yury Vilk



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Samuel Moukouri

David Poulin

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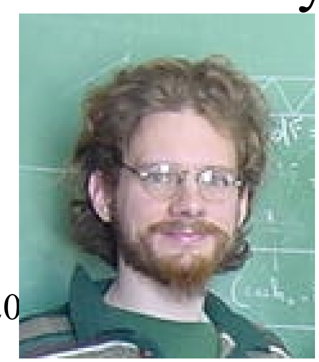

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Alexis Gagné-Lebrun

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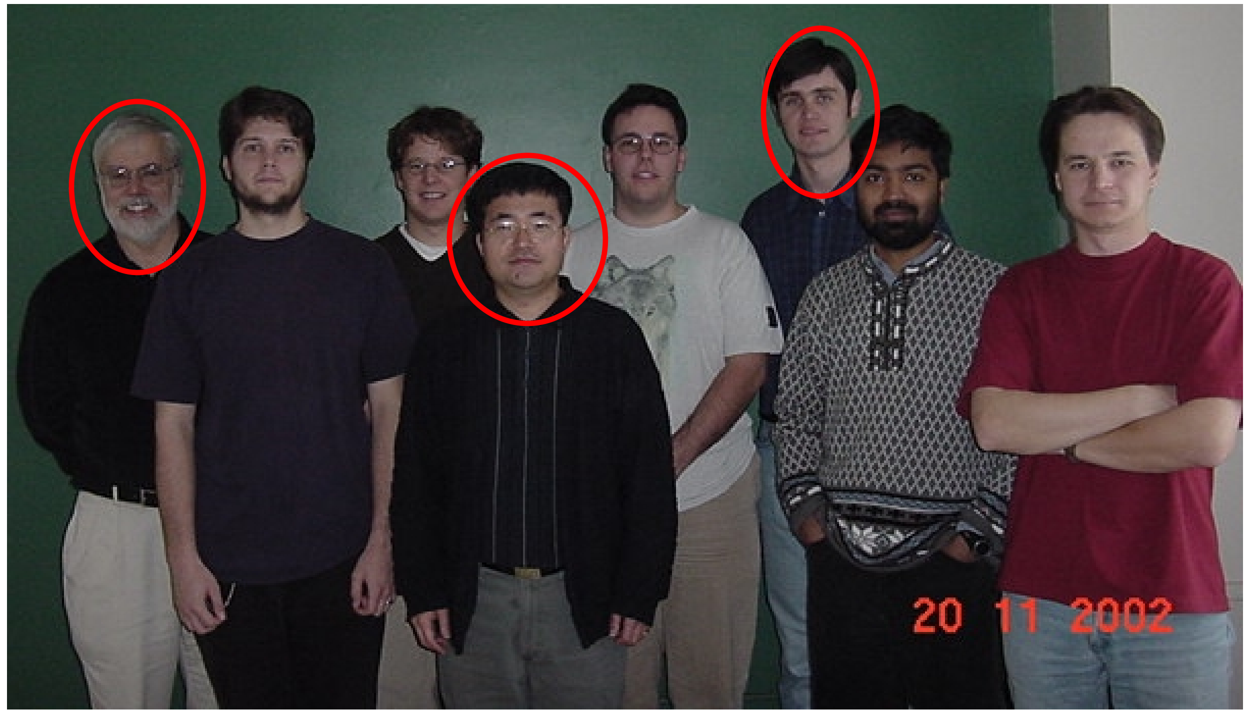


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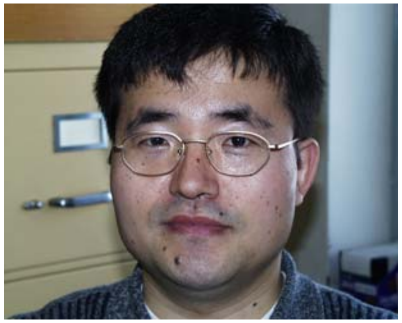
Bumsoo Kyung Maxim Mar'enko



Bumsoo Kyung

David Sénéchal

Sarma Kancharla

u

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Outside collaborators


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Marcello Civelli

Massimo Capone



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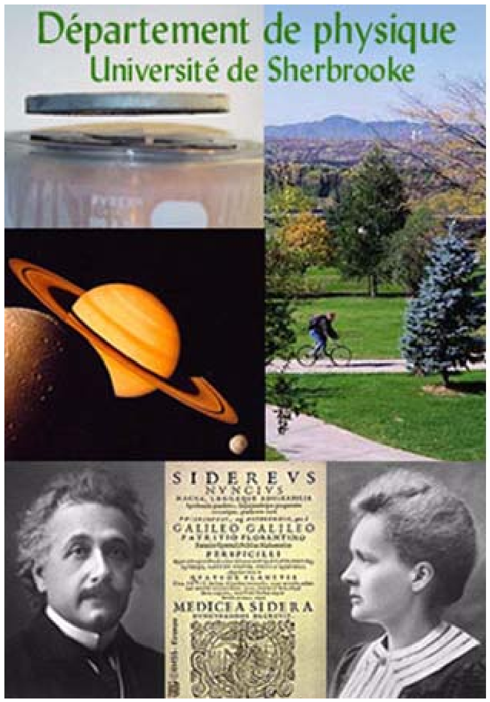


# André-Marie Tremblay

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- A.-M.S. Tremblay, B. Kyung et D. Sénéchal, Fizika Nizkikh Temperatur, **32**,561 (2006).
- T. Maier, M. Jarrell, T. Pruschke, and M. H. Hettler, Rev. Mod. Phys. **77**, 1027 (2005)
- G. Kotliar, S. Y. Savrasov, K. Haule, V. S. Oudovenko, O. Parcollet, and C.A. Marianetti, cond-mat/0511085 v1 3 Nov 2005

C'est fini...

Merci