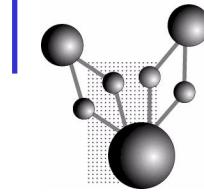


André-Marie Tremblay



CENTRE DE RECHERCHE SUR LES PROPRIÉTÉS
ÉLECTRONIQUES
DE MATERIAUX AVANÇÉS



Sponsors:



Fondation canadienne pour l'innovation



Why is the high- T_c problem so difficult?

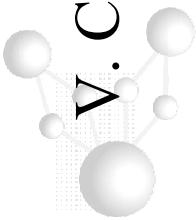
I. Standard paradigm

II. Why is there a problem with standard approaches?

III. Microscopic model

IV. Theoretical difficulties (and what can be done sometimes...)

- (a) Straight numerical approaches
- (b) Inadequacies of mean-field theory in low dimension
- (c) Approaching from weak coupling
- (d) Approaching from strong coupling
- (e) Phonons
- (f) Inhomogeneities



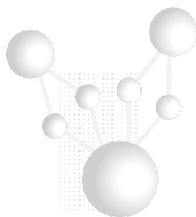
V. Conclusion

I. Standard Paradigm

Theory of solids

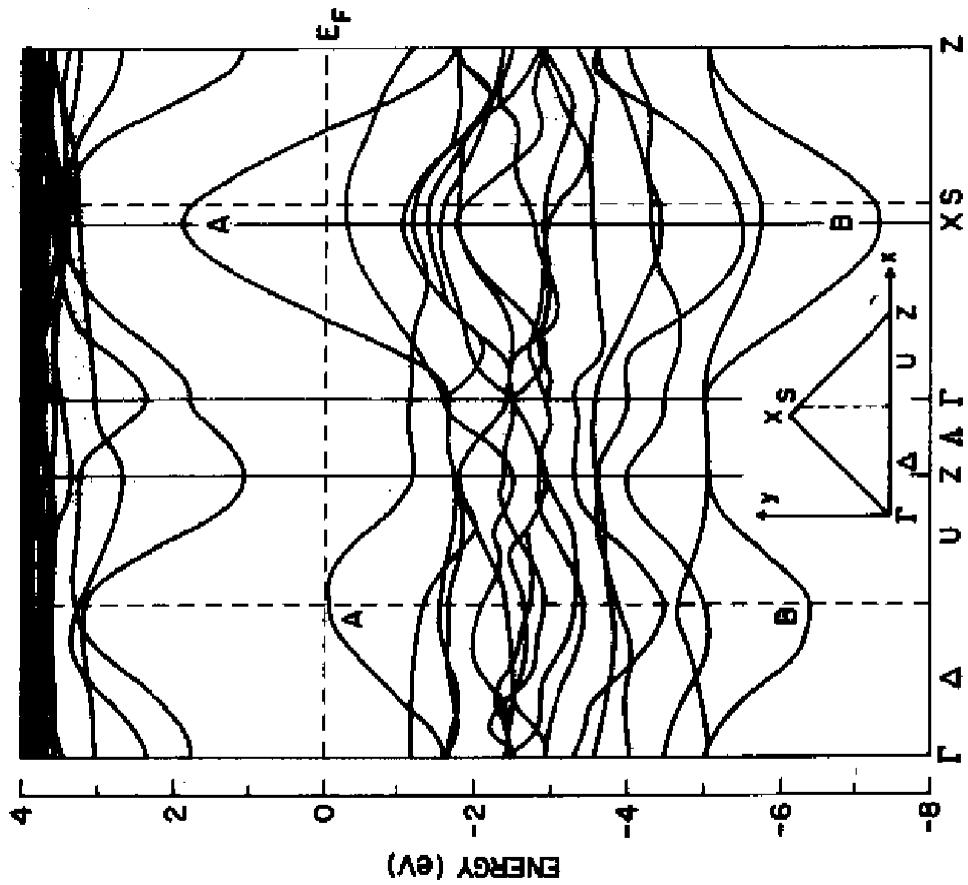
$$H = \text{Kinetic} + \text{Coulomb}$$

- Many new ideas and concepts needed for progress
(Born-Oppenheimer, H-F, Bands...)
- Successful program
 - Semiconductors, metals *and superconductors*
 - Magnets
- Is there anything left to do?
 - Unexplained materials: High T_c, Organics...
 - Strong correlations:
 - strong interactions, low dimension

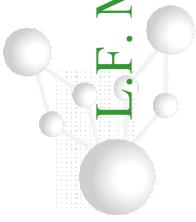


The standard approaches :

- A. Quasiparticles, Fermi surface
and Fermi liquids
- LDA (Nobel prize 1998)



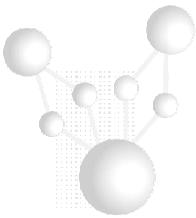
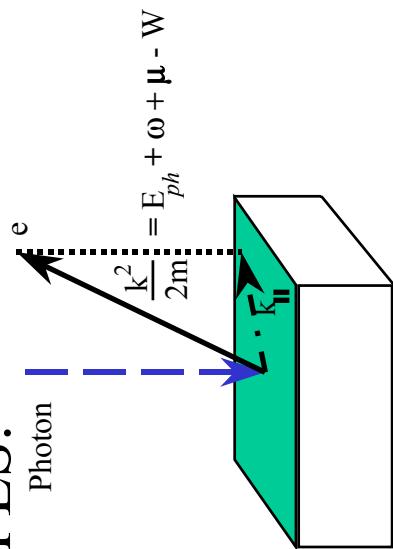
L.F. Mattheiss, Phys. Rev. Lett. 58, 1028 (1987).



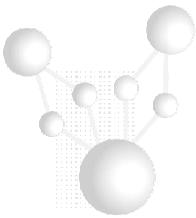
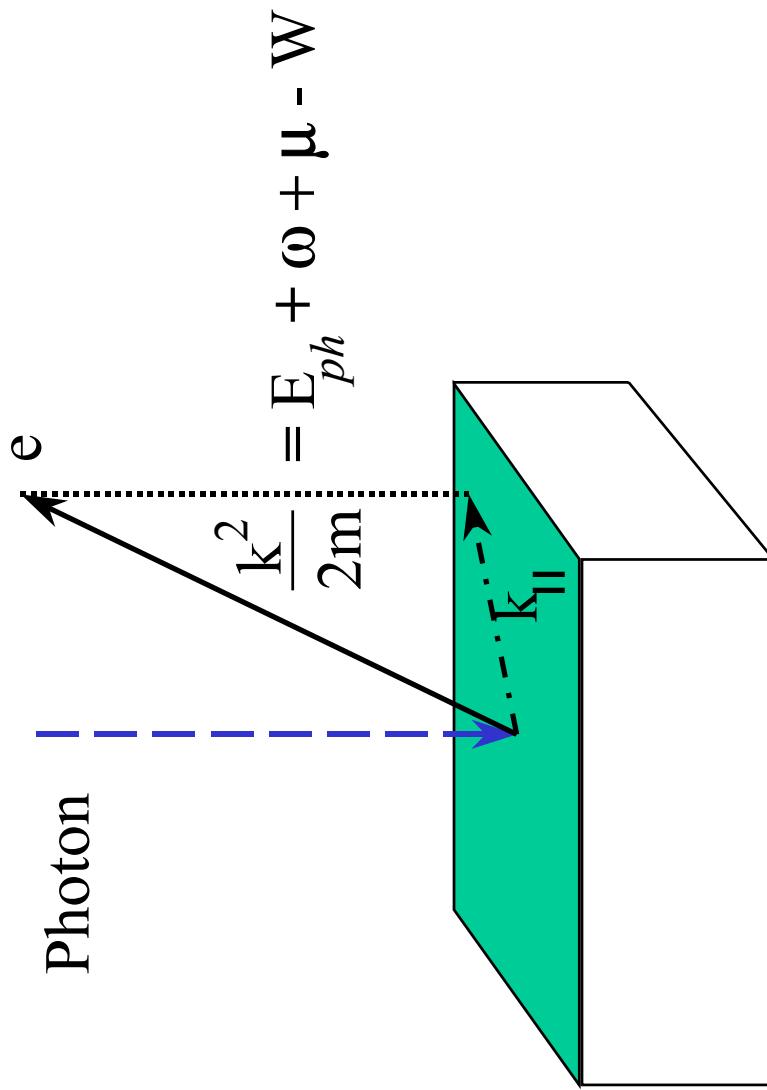
The standard approaches :

- Matrix elements of H in LDA basis
- In practice, from general considerations:
 - Short range
 - Single Slater determinant not eigenstate
- Phase space + Pauli restricts possible scatterings:
 - Quasiparticles m^* , effective fields,

- «See» the quasiparticles with ARPES:



Photoemission



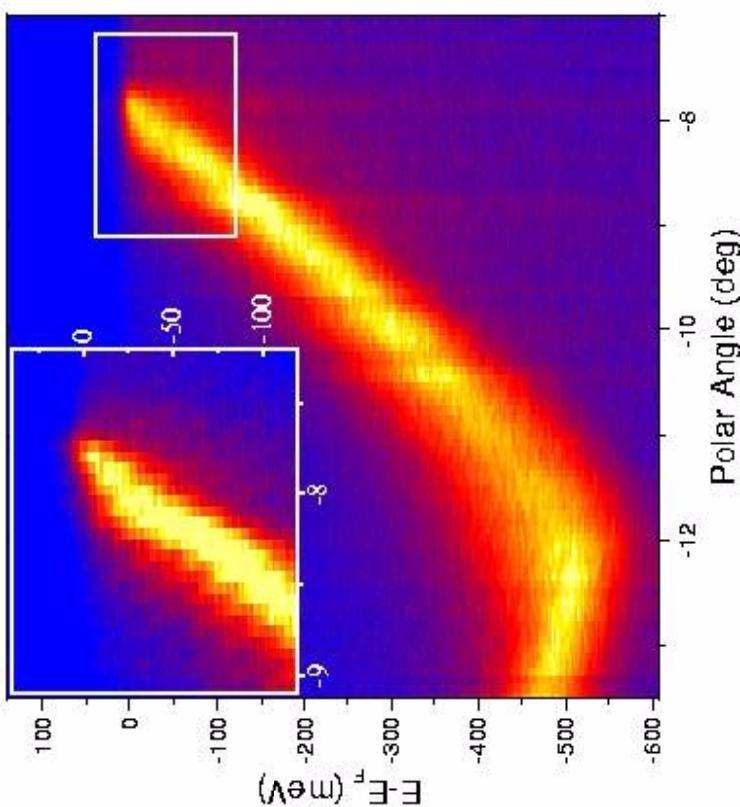


FIG. 1. ARPES intensity plot of the Mo(110) surface recorded along the $\bar{\Gamma}$ – \bar{N} line of the SBZ at 70 K. Shown in the inset is the spectrum of the region around k_F taken with special attention to the surface cleanliness.

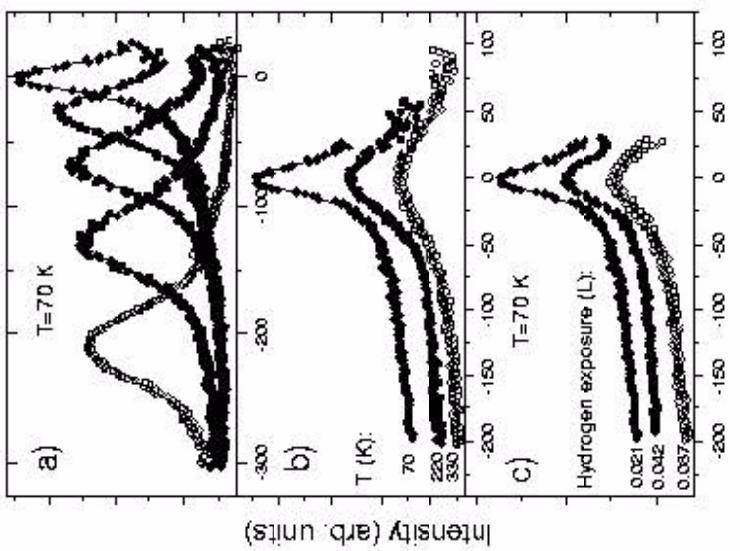


FIG. 2. Spectral intensity as a function of binding energy for constant emission angle, normalized to the experimentally determined Fermi cut-off. Data are symbols, while lines are fits to the Lorentzian peaks with a linear background. The dependence on the binding energy (a), temperature (b), and hydrogen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

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



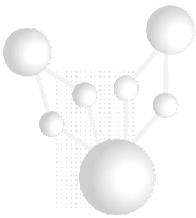
The standard approaches :

B. Thermodynamics and phase transitions

- Thermodynamics of Fermi liquids
 - particle-hole excitations
- Phase transitions
 - $\chi \sim N(0) / (1 + F_0^a)$
 - Superconducting transition

C. Heisenberg model and related models

- Band for $s-p$
- Localized (often) for $d-f$
 - Only spin degrees of freedom
 - Use symmetry to write H

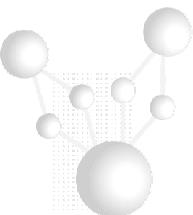
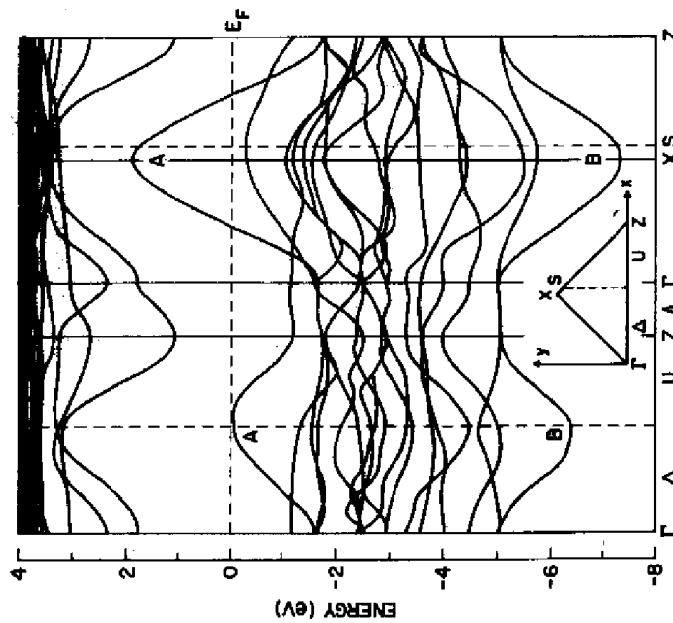
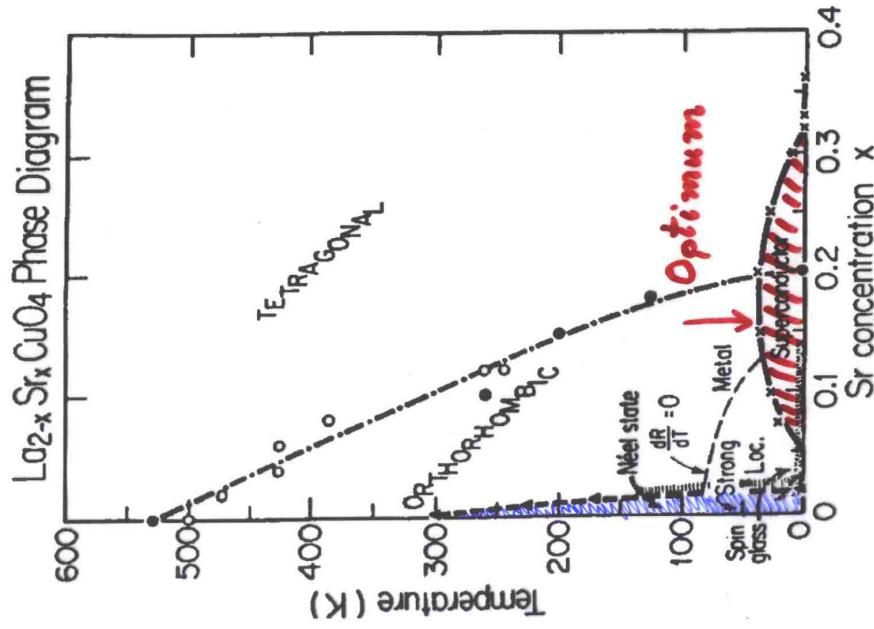


$$n = I,$$

Metal according to band

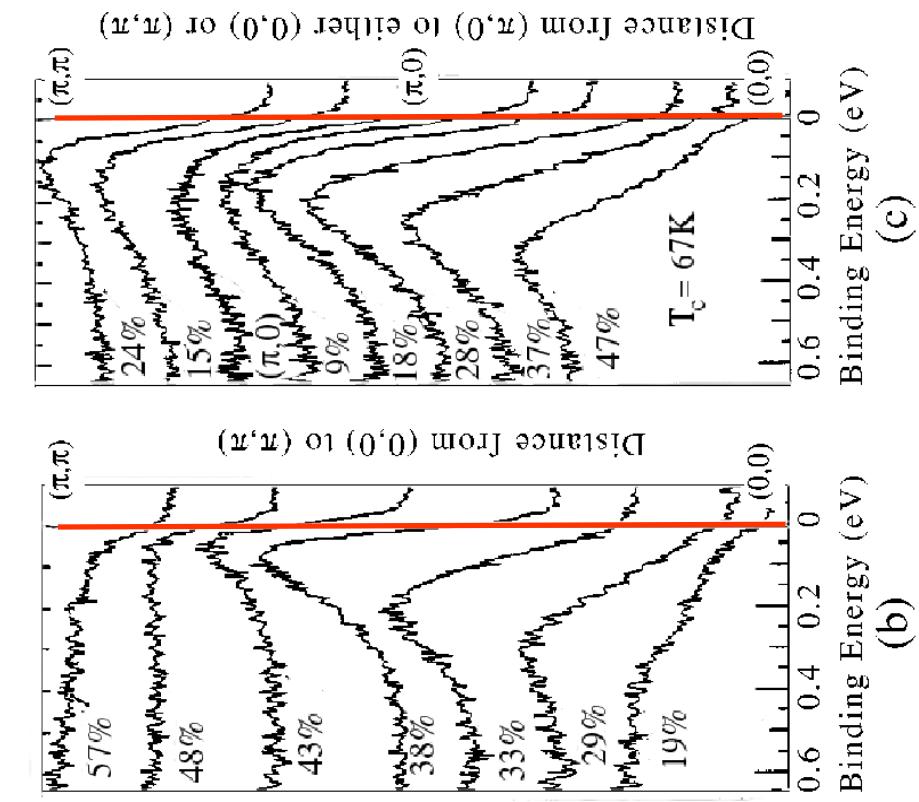
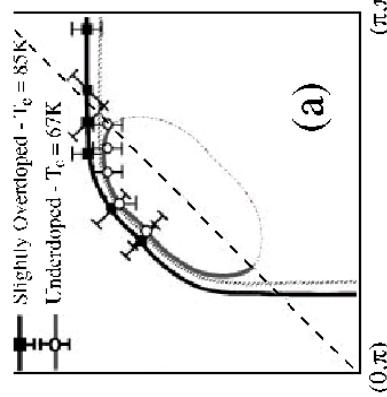
II. Failure of standard paradigm

AFM insulator in reality

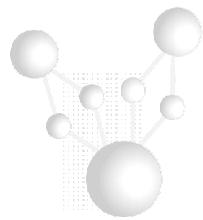


Experimental evidence for failure :

- $d=2$ partial vanishing act
of the Fermi surface away
from $n = 1$.



D.S. Marshall, D.S. Dessau, A.G.
Loeser, C.-H. Park,
A.Y. Matsuura, J.N. Eckstein, I.
Bozovic, P. Fournier,
A. Kapitulnik, W.E. Spicer, and
Z.X. Shen, Phys. Rev.
Lett. 76, 4841 (1996).



H. Ding *et al.*
 Nature, 382, 51 (1996).
 P.R.L. 78, 2628 (1997)

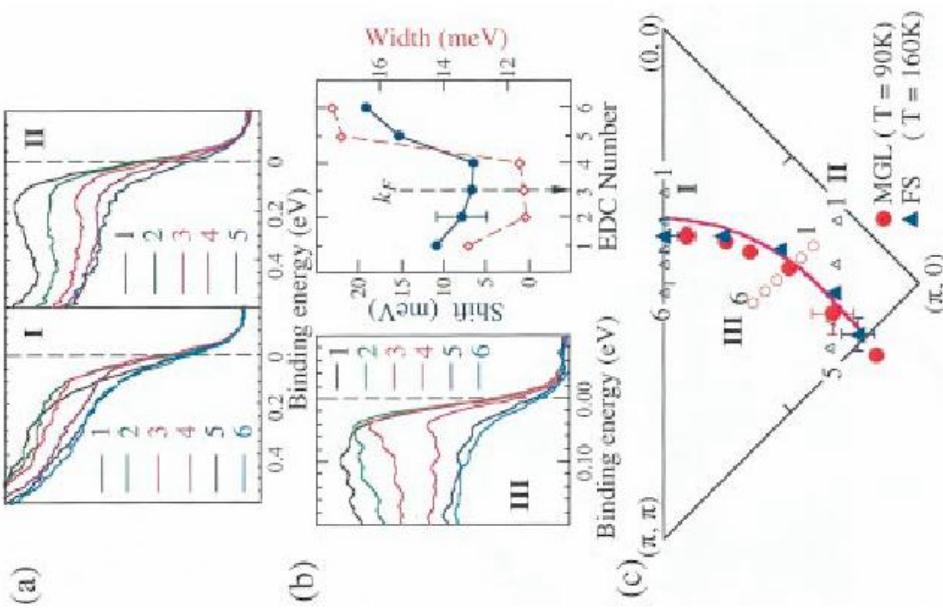
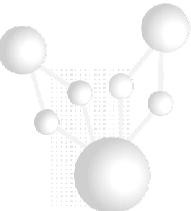


FIG. 1(color). Measurements of the 83 K sample. (a) EDCs at a photon energy of 19 eV at 160 K along cuts I and II in (c). (b) EDCs at a photon energy of 22 eV at 90 K along cut III in (c) (left panel). Midpoint shifts (blue dots) and widths (red diamonds) of this cut (right panel). (c) Fermi surface (FS) at 160 K (solid blue triangles) and minimum gap locus (MGL) at 90 K (solid red dots). Cuts I, II (open blue triangles), and III (open red dots) are locations of EDCs in (a) and (b). Notice that the two surfaces coincide within error bars. The error bars represent uncertainties of Fermi crossings as well as possible sample misalignment. The red curve is a rigid band estimate of the Fermi surface.



III. Establishing a microscopic model

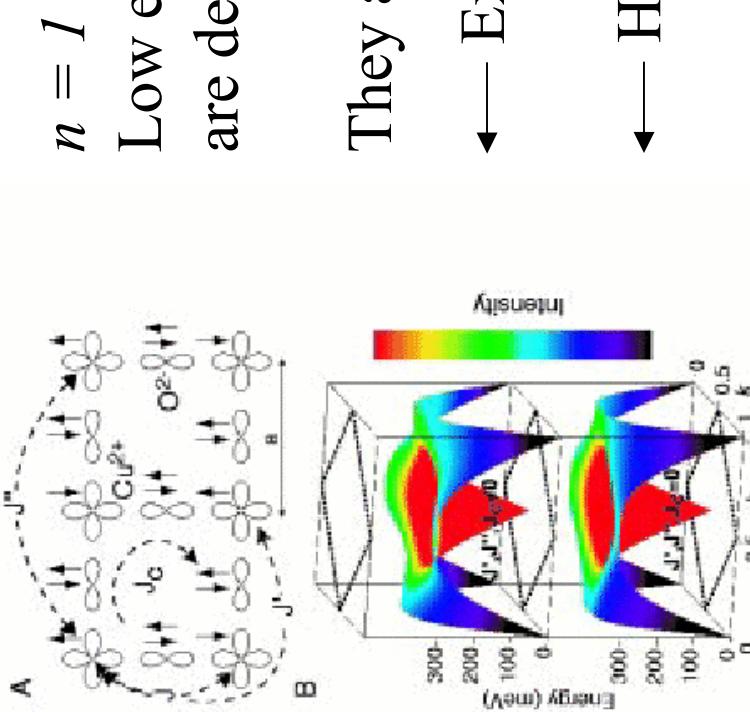
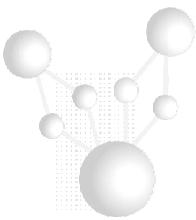
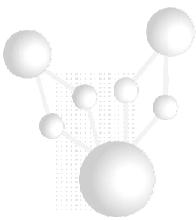
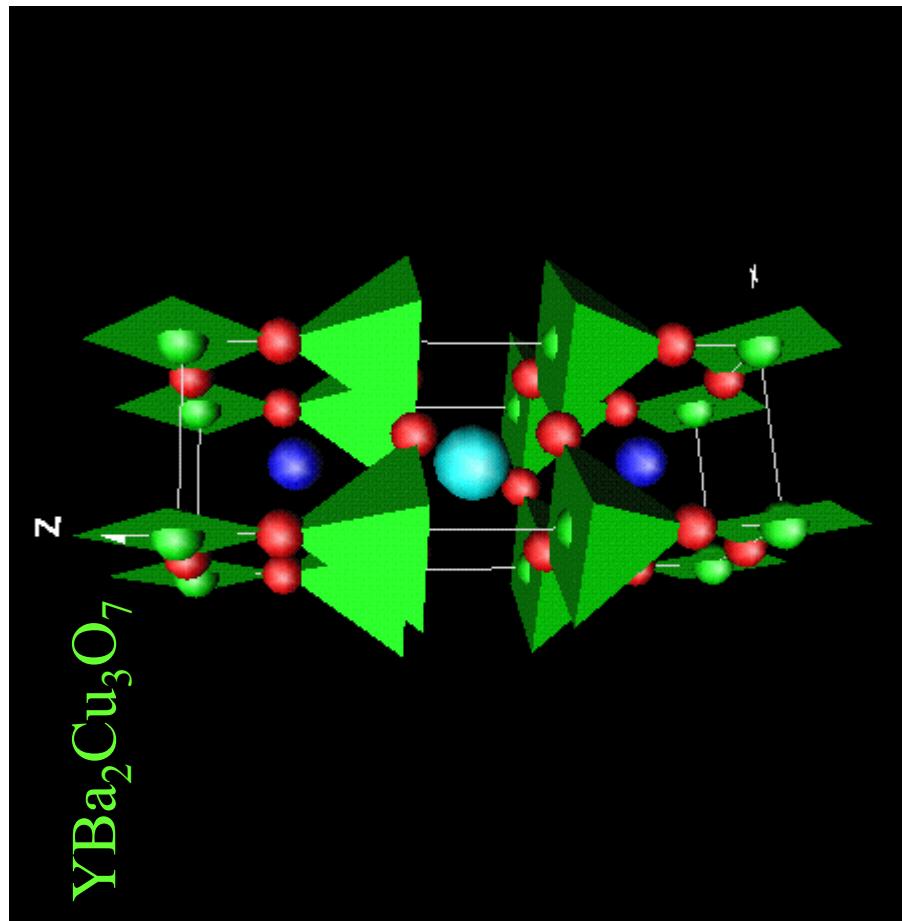


FIG. 1. (color) **A** The CuO₂ plane showing the atomic orbitals (Cu $3d_{x^2-y^2}$ and O $2p_{x,y}$) involved in the magnetic interactions. J , J' and J'' are the first-, second- and third-nearest-neighbor exchanges and J_c is the cyclic interaction which couples spins at the corners of a square plaquette. 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.

R. Coldea cond-mat/ 0006384

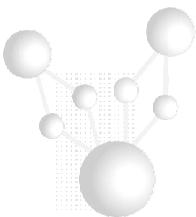


Unit cell



Introduction : Structure du $YBaCuO$

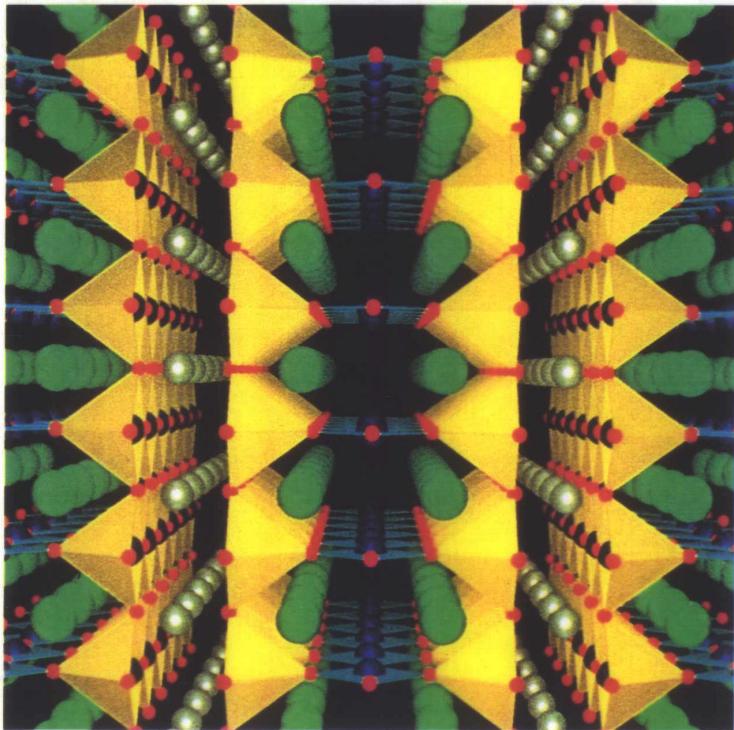
Yttrium
Baryum
Cuivre
Oxygène



SCIENTIFIC AMERICAN

JUNE 1988
\$3.50

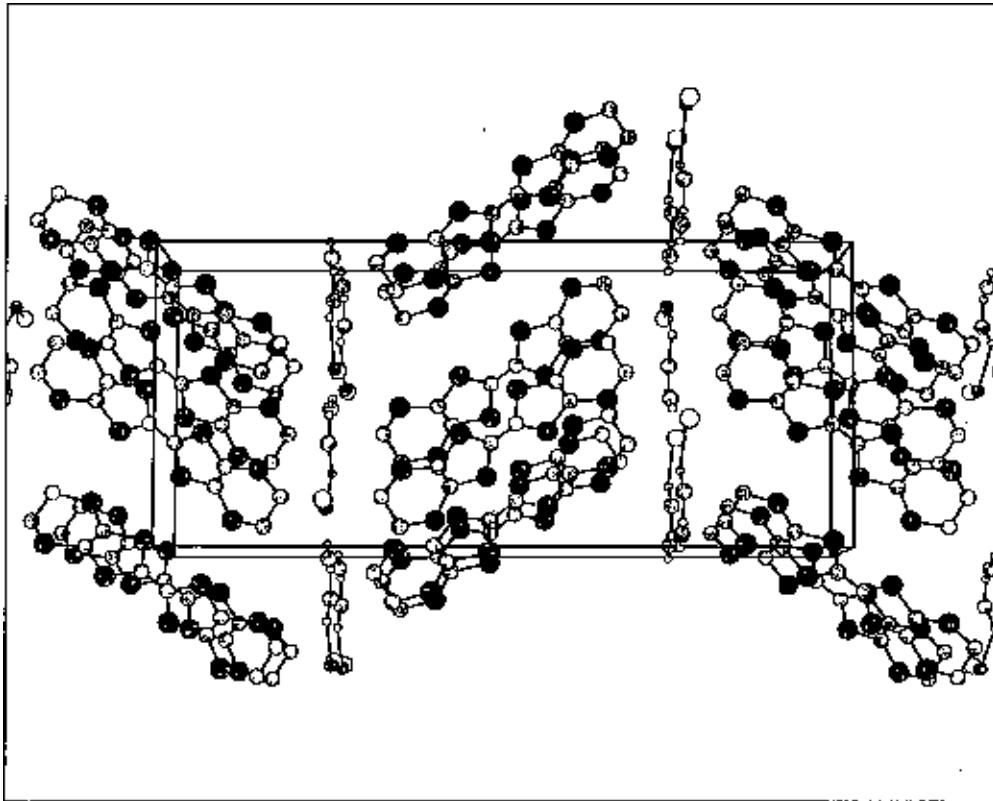
How nonsense is deleted from genetic messages.
R₂ for economic growth: aggressive use of new technology.
Can particle physics test cosmology?



$\gamma\text{-Ba}_2\text{Cu}_3\text{O}_{7-\delta}$

High-temperature Superconductor belongs to a family of materials that exhibit exotic electronic properties.

92 - 37



$\kappa\text{-(BEDT)}_2\text{X}$

- **Atomic Physics** CuO_2 plane.

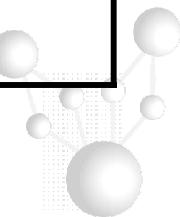
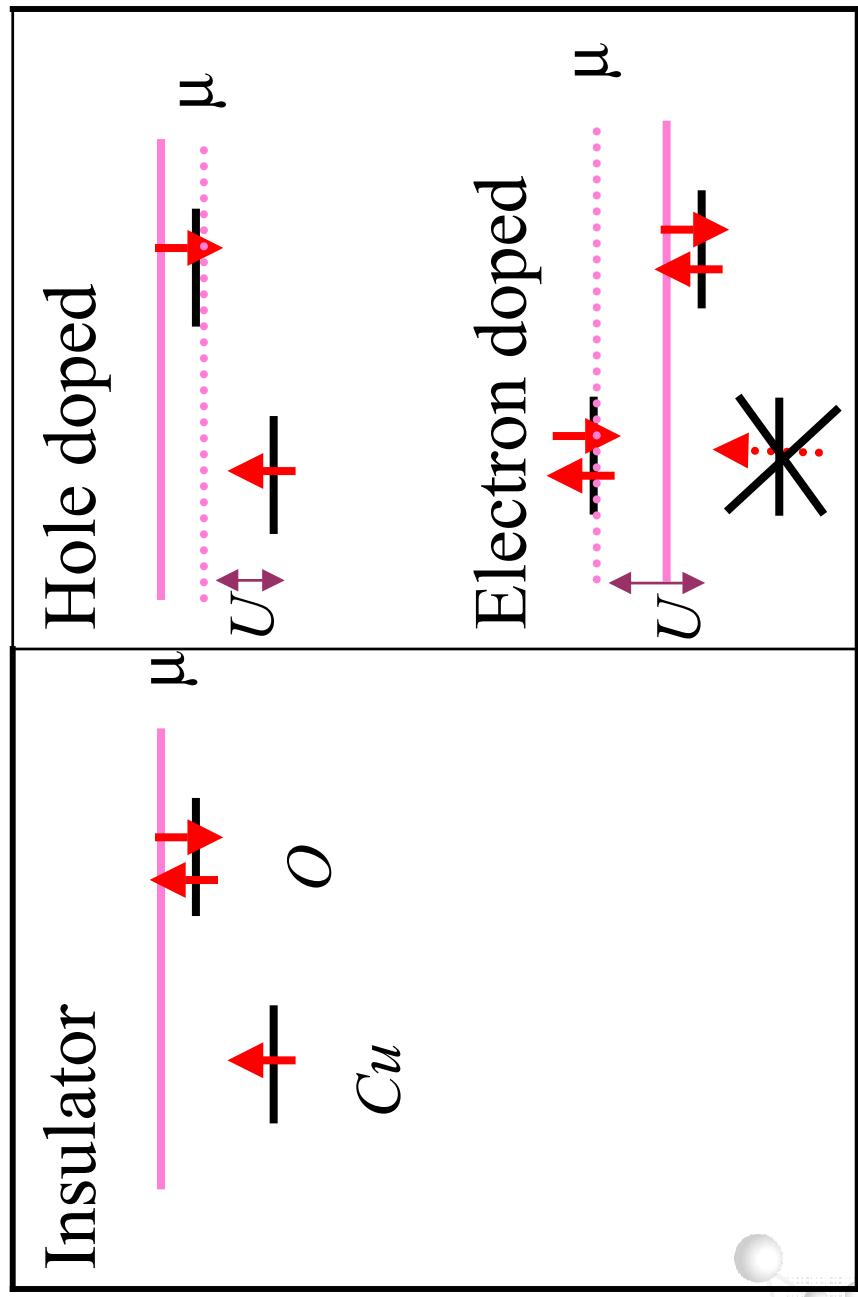
- Cu is $3d^{10}4s^1$.

- In high T_c , Cu^{++}

- $3d_{x^2-y^2}$ has one hole

- Four other levels are filled

Zhang-Rice singlet



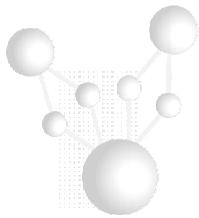
Insulator



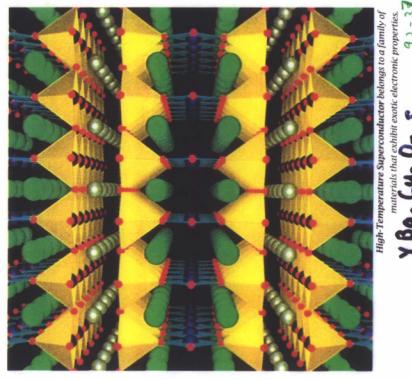
Doped system : Doping δ



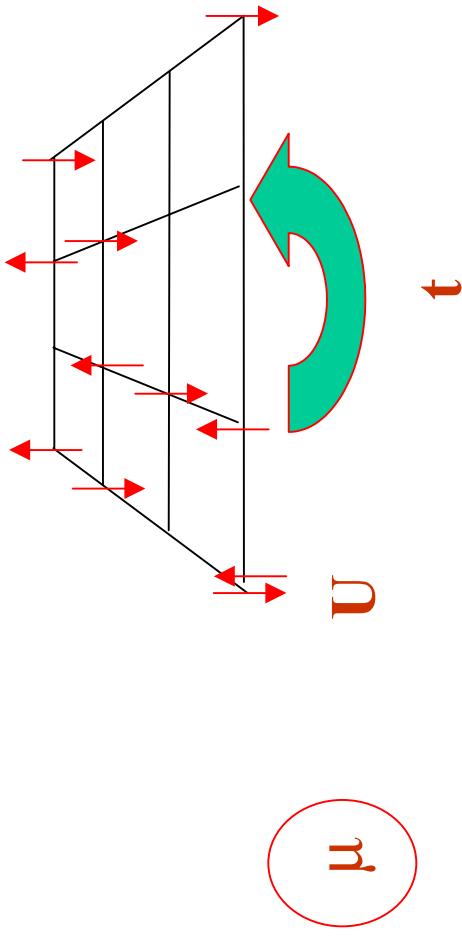
- UHB loses δ states
- LHB gains 2δ states



Observable experimentally (XPS)



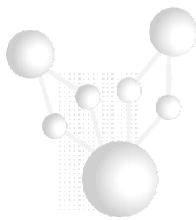
Simplest microscopy model for Cu O planes.



$$(N = 16)$$

•Size of Hilbert space : 4^N

$$\frac{Tr[Oe^{[-H/k_B T]}]}{Tr[e^{[-H/k_B T]}]}$$

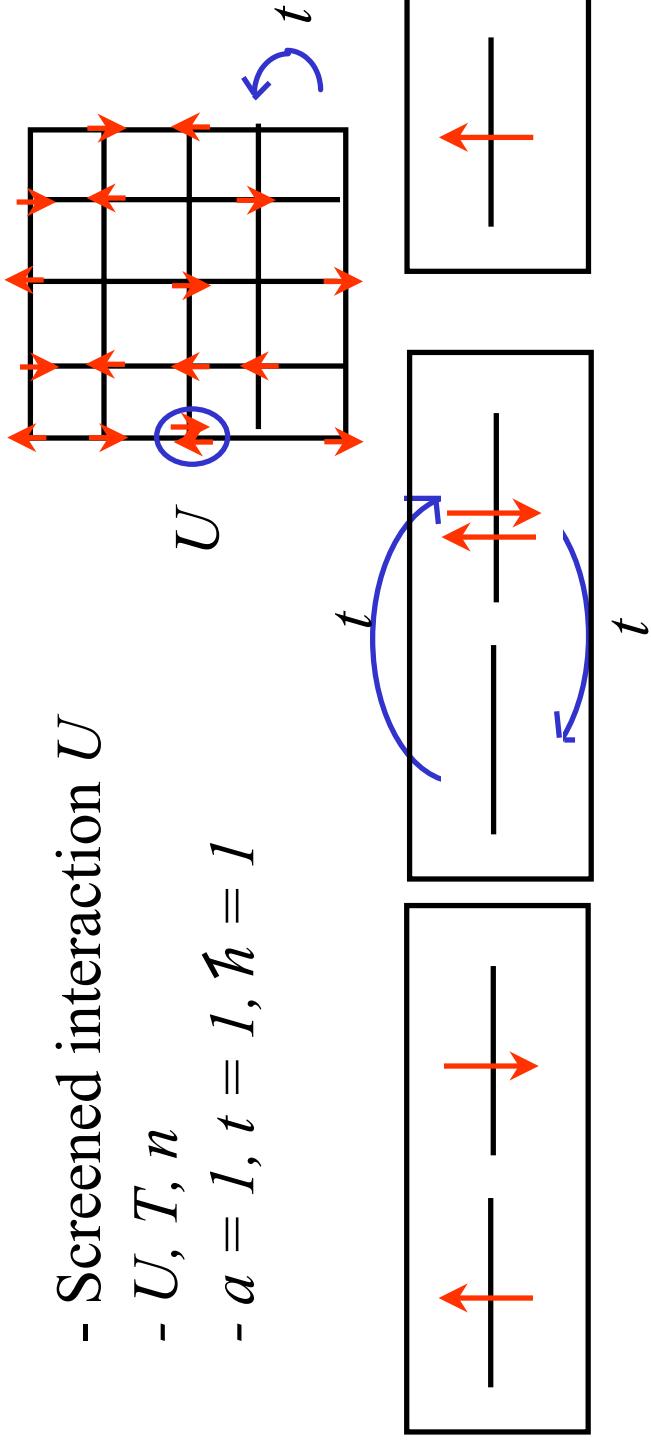


Hubbard model (Kanamori, Gutzwiller, 1963) :

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

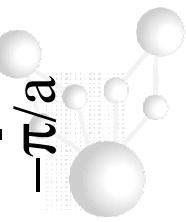
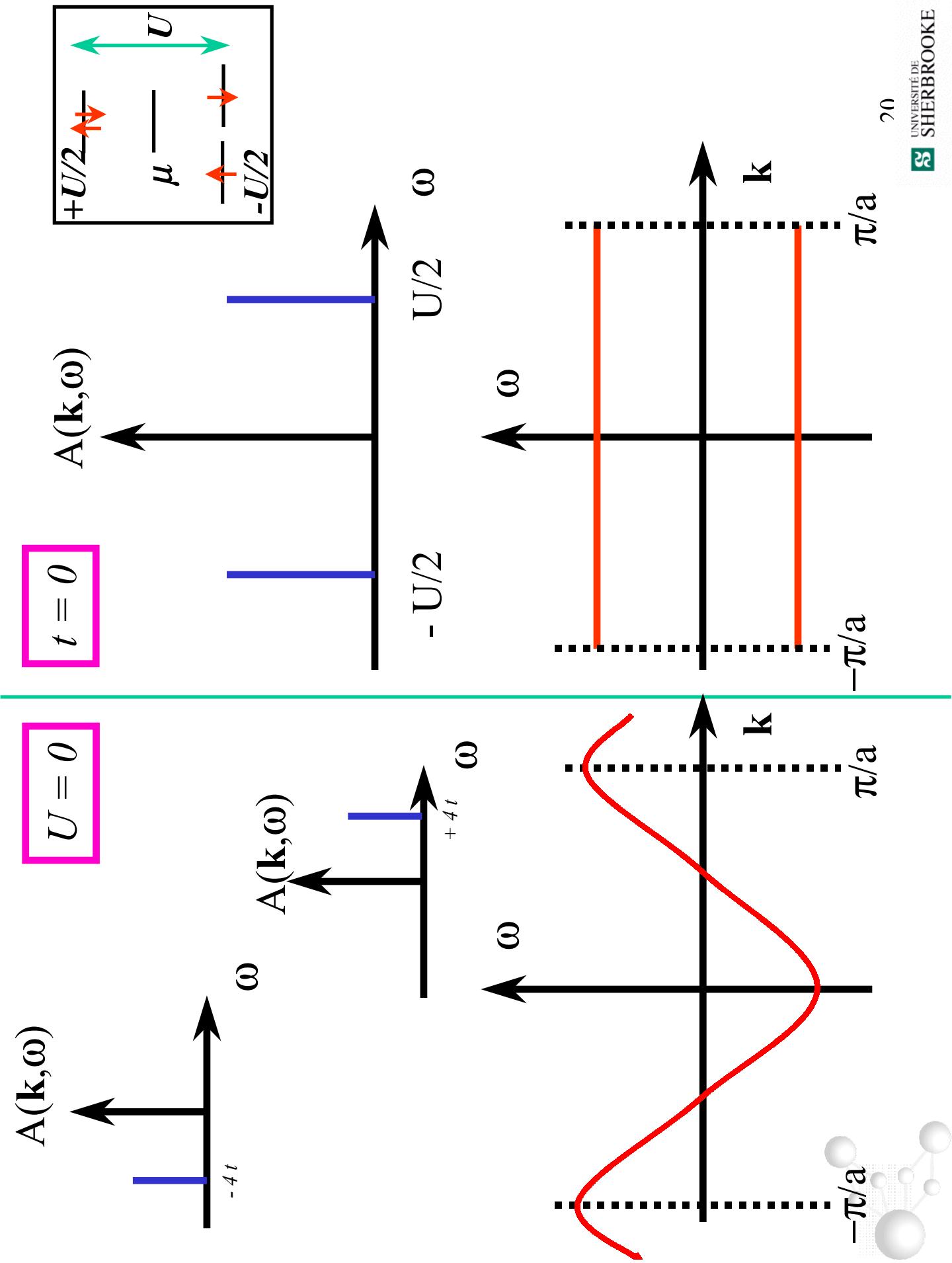
- Screened interaction U

- U, T, n
 - $a = 1, t = 1, \hbar = 1$

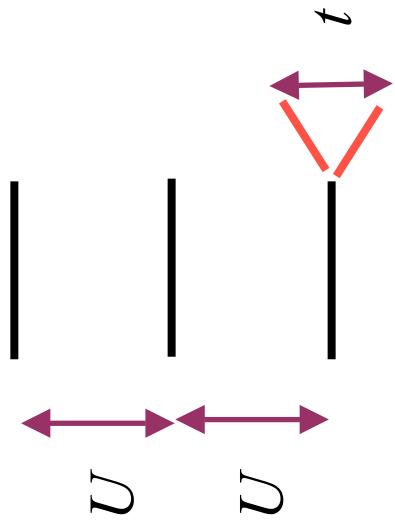


- 2001 vs 1963: Numerical solutions to check analytical approaches



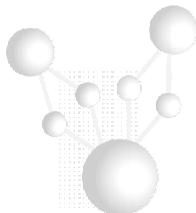


• $t-J$



•Number of states : 3^N

- Problems
- Poor screening
- Phonons



IV. Theoretical difficulties

(a) Straight numerical approaches

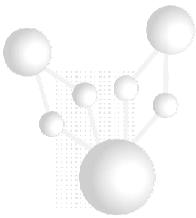
- $2^{30} \sim 1 \text{ GB}$. Compare with 4^{16} for 16 site lattice!

- Exact diagonalizations of $t\text{-}J$ for one hole suggest:

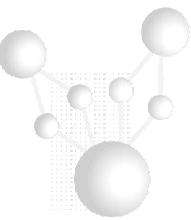
- One peak in $A(\mathbf{k}, \omega)$ plus incoherent background
- Peak disperses with width of J . Thus
 - Number of carriers small.
 - Effective mass finite.

- Cluster Perturbation Theory (New method)

- D. Senechal, D. Perez, M. Piioro-Ladriere Phys. Rev. Lett. 84 (2000) 522.



- Quantum Monte Carlo (**S.R. White et al.** Phys. Rev. B **40**, 506 (1989))
 - AFM at $n = 1$. Away from half-filling problems with BC
 - Pseudogap in weak to intermediate coupling
 - Temperature not low enough to establish *d-wave* superconductivity
 - Useful as a benchmark for analytical approaches.
- Main drawback: « fermion sign problem » and instabilities
- Density Matrix Renormalization Group
 - People are working on $d = 2$ generalizations.



(b) Inadequacy of mean field in low dimension

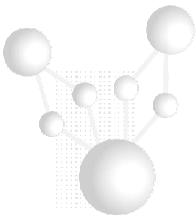
- Fluctuations dominate the physics

- $d = 1$ Spin-Charge separation (*Luttinger liquid Behavior*)
(Quantum fluctuations at $T = 0$)

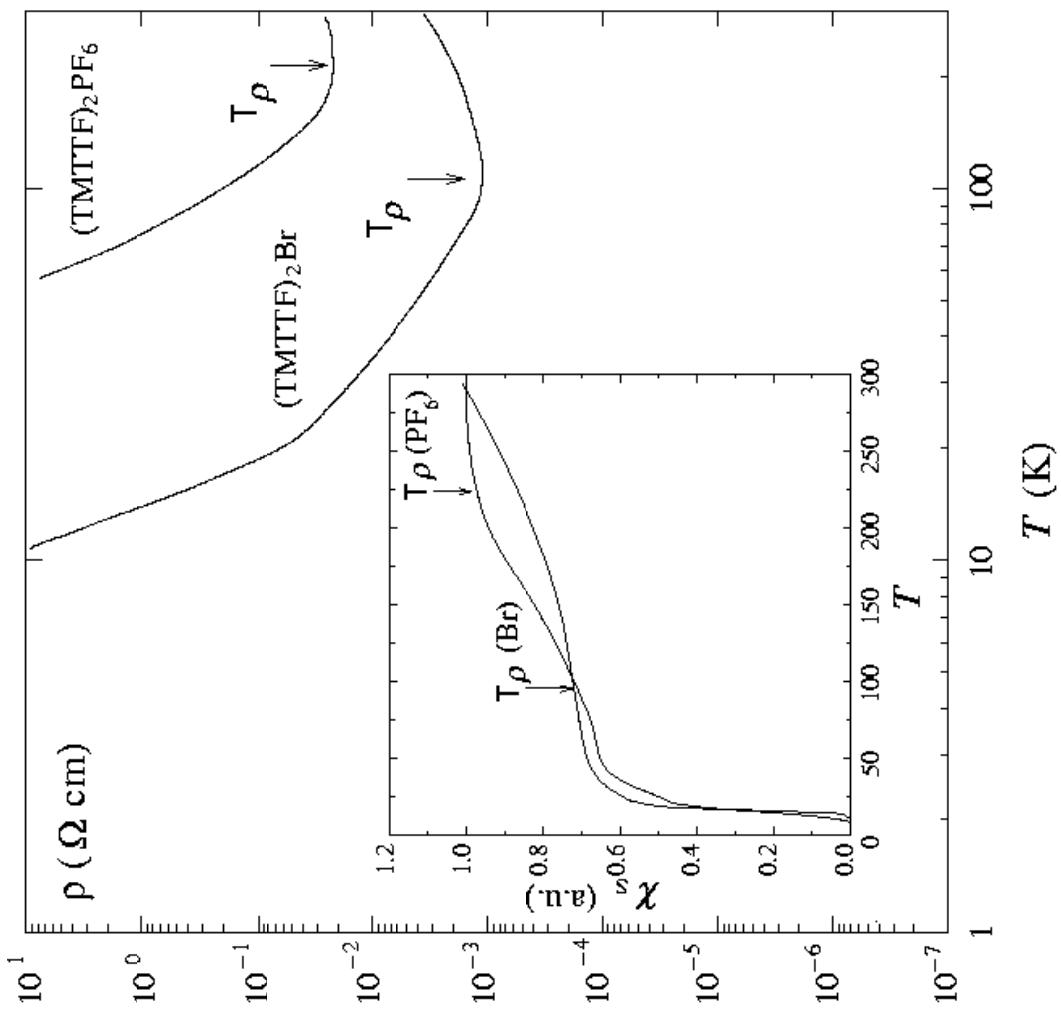
- $d = 2$ Thermal fluctuations :

- *Hohenberg-Coleman-Mermin-Wagner theorem.*

And the strong interactions complicate all that.



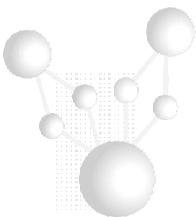
- $d=1$ Spin-charge separation



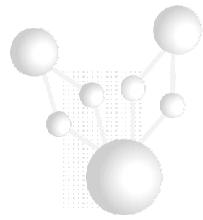
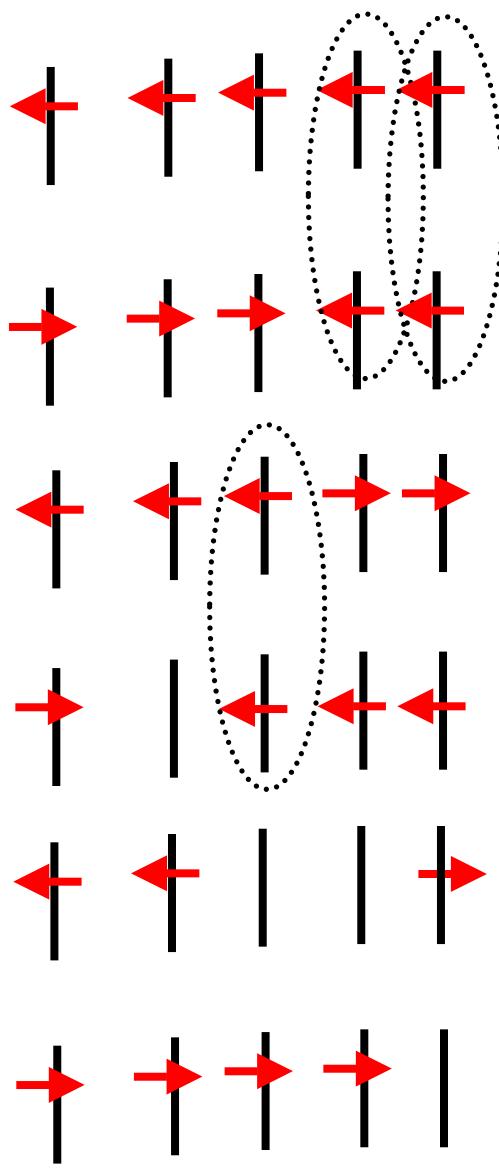
Claude Bourbonnais



C. Bourbonnais
et al.
(cond-
mat/9903101).



Spin-charge separation



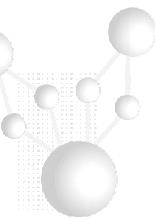
- Straight perturbation theory for nested $d=2$ Fermi surface gives non-trivial results (F. Lemay PhD thesis, 2000)
- Thermal and quantum fluctuations in $d = 2$

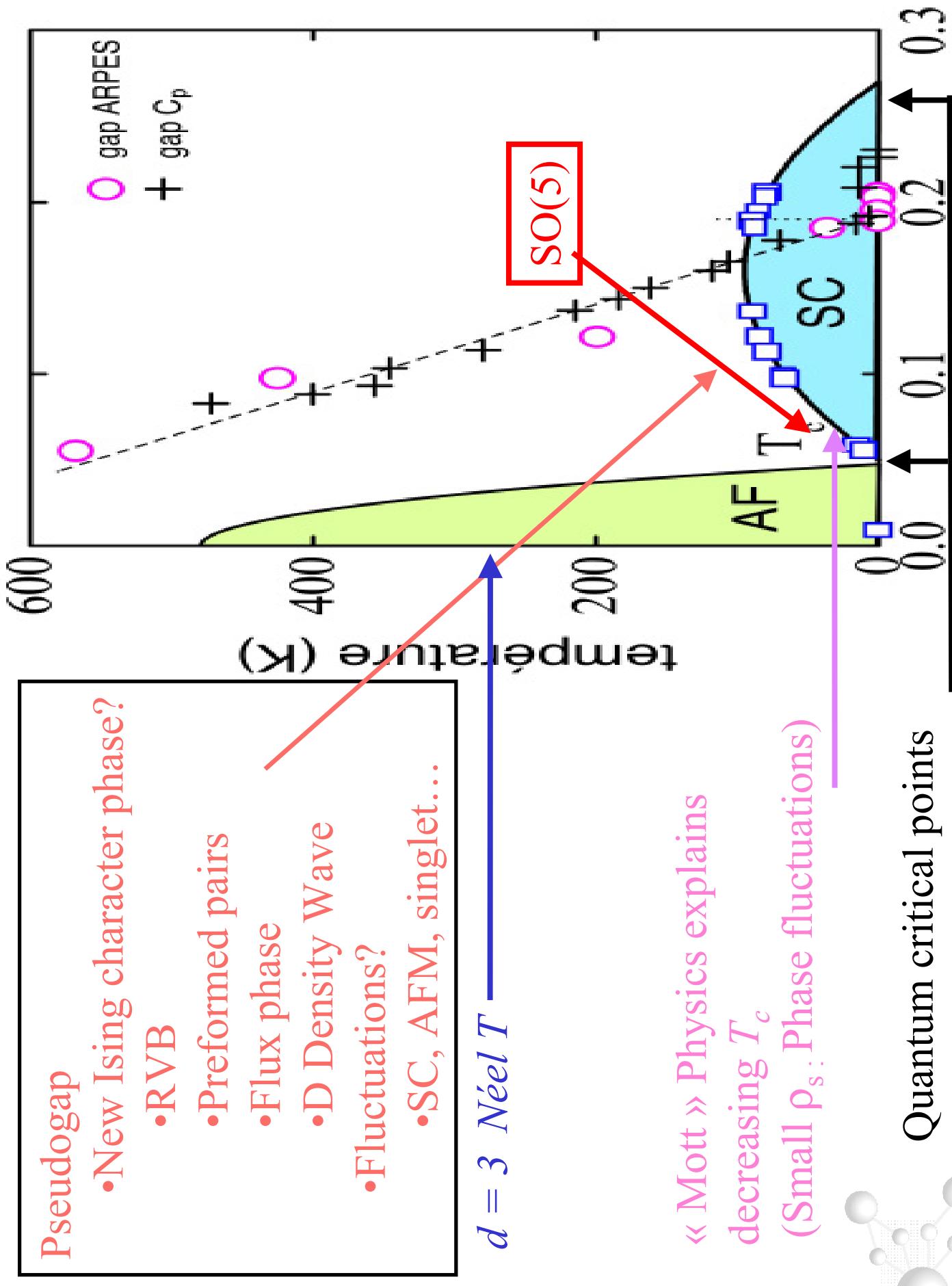
$d = 2$, Mermin-Wagner

$$(\nabla \theta)^2 \rightarrow q^2 \theta_{\mathbf{q}} \theta_{-\mathbf{q}} \sim kT$$

$$\langle \theta^2 \rangle \propto \int d^2 q \frac{kT}{q^2} \rightarrow \infty$$

- $d = 1$: R.G., Bosonization, Conformal Field Theory...
 $d = 2$: Slave bosons, R.G., strong coupling p.t., TPSC





Would help decide
 « What type » of fluctuations
 are important. (See later)

Loram and Tallon, cond-mat/0005063

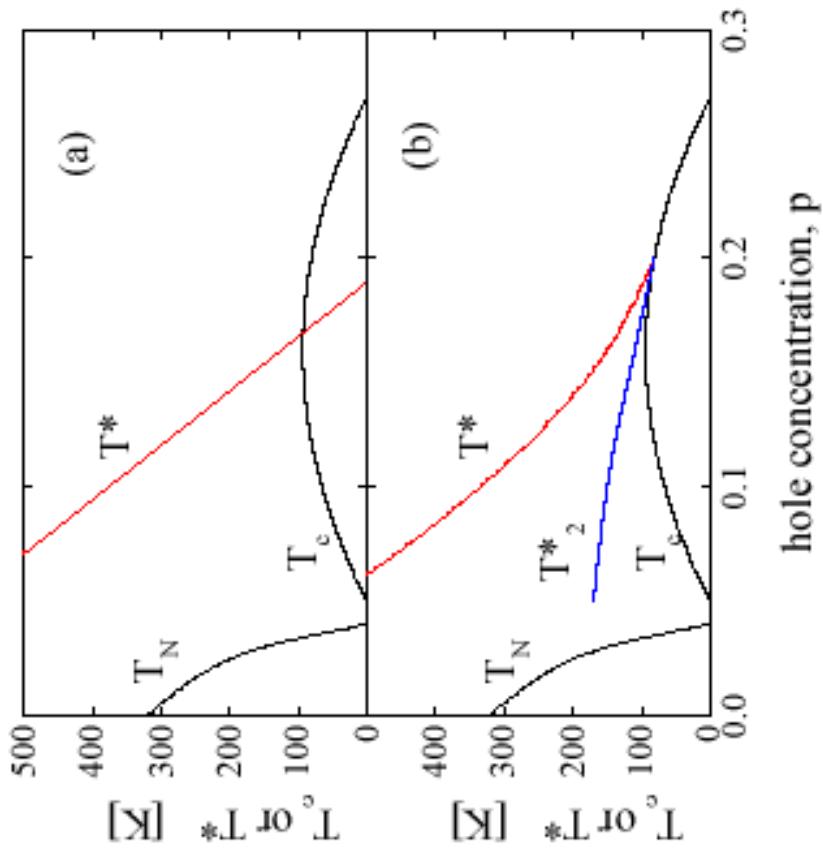
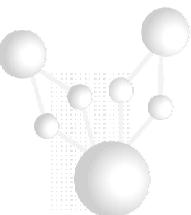
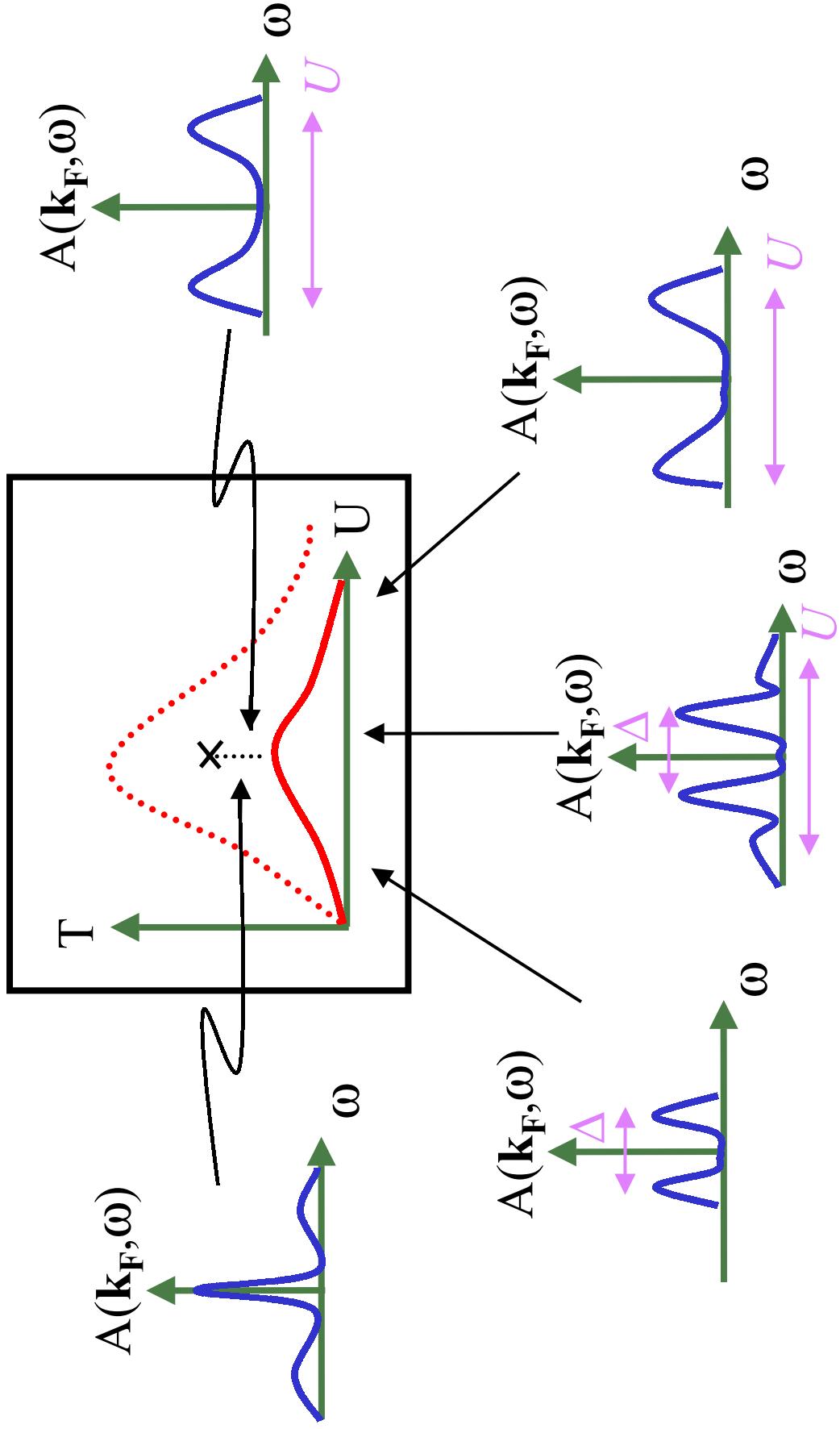


Fig. 1. Two scenarios for the “phase diagram” for HTS cuprates. In (a) T^* represents and energy scale which falls abruptly to zero at a critical doping, $p=0.19$. In (b) T^* merges with T_c on the overdoped side and often a lower T^*_2 associated with a small pseudogap or a spin gap is invoked. T_N is the Neel temperature for the 3-D AF state.



Weak vs strong coupling



High T_c are at « intermediate » coupling:
 $U = 8t$ $t \sim 300 \text{ meV}$

R. Coldea
cond-mat/0006384

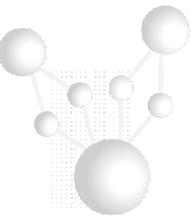
30

(c) Approaching from weak coupling

- Perturbation theory (Wick's theorem)
- Finding « effective interactions »
- RPA with long range interaction *vs* Hubbard
- Notion of « channel »
- RG and « interference »
- Problem with Pauli principle (Parquet, Bickers)
- Self-consistent treatments
- Migdal's theorem *vs* theory of « ordinary » superconductors

- Alternative: satisfy sum-rules
- Conservation laws
 - Pauli principle
 - Mermin-Wagner theorem

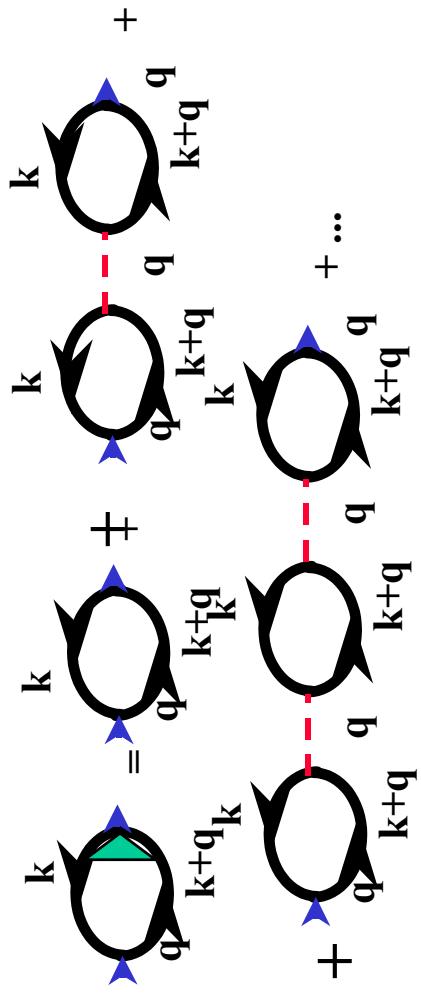
Fluctuation-induced pseudogap?



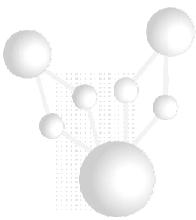
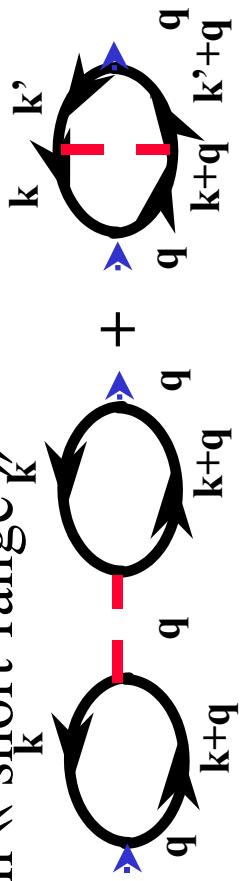
- Perturbation theory:

$$\frac{1}{(X+Y)} = \frac{1}{X} - \frac{1}{X} \frac{Y}{X+Y} \frac{1}{X+Y}$$

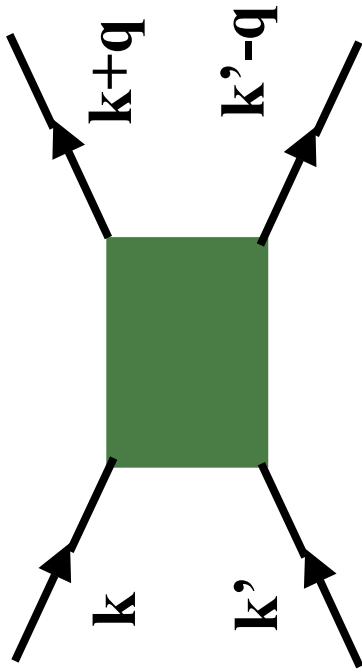
- Effective interaction (Screening in usual solids)



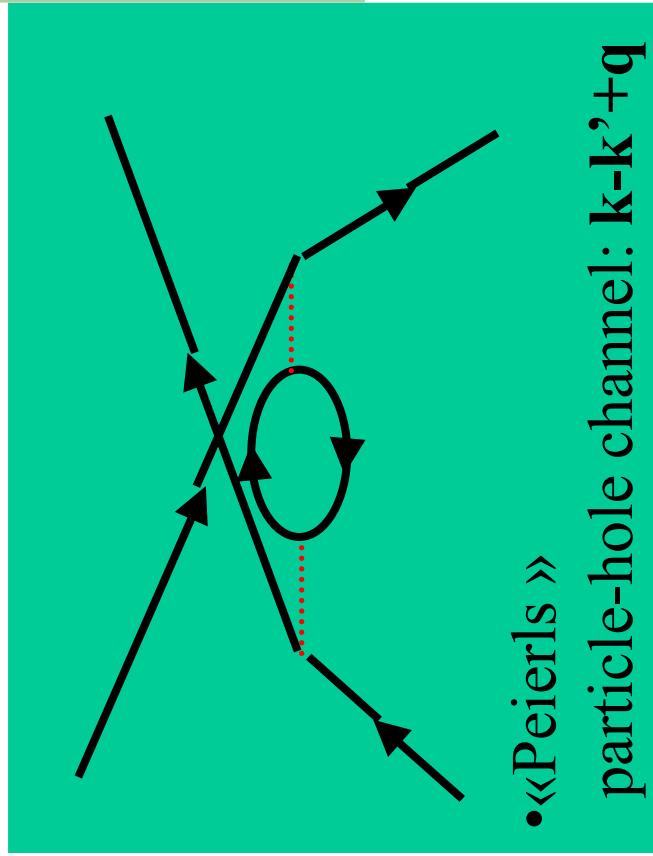
- Problem with « short-range »



•Notion of « channel »

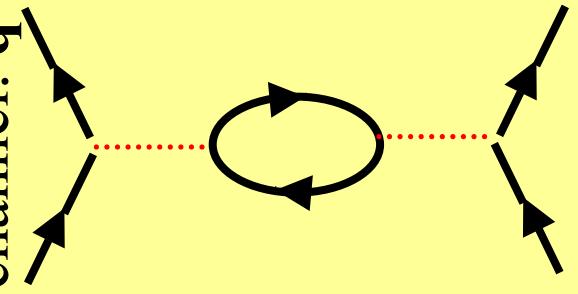


•Particle – particle
channel: $\mathbf{k} + \mathbf{k}'$



•«Peierls»
particle-hole channel: $\mathbf{k} - \mathbf{k}' + \mathbf{q}$

•« Landau »
p-h channel: \mathbf{q}



- Renormalization group : « interference »

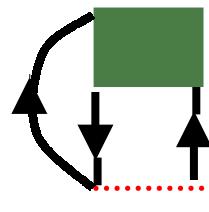
Zanchi, Schultz... Recent: C. Honerkamp *et al.* Phys. Rev. B **63** 035109 (2001)

- Problem with Pauli principle when summing infinite sets of diagrams
 - Need to include all crossed diagrams: in practice, impossible
 - Can be done approximately with Parquet approximation (Bickers) (with self-consistency, unsatisfactory)

- « Self-consistency » and conservation laws

$$\rightarrow = \rightarrow + \rightarrow \Sigma$$

$$\Sigma = \text{---} + \text{---} + \text{---}$$



- Self-consistency in conventional « Eliashberg » superconductivity
- Take phonons as « given »

$$\Sigma = \Sigma_{\text{irr}} + \Sigma_{\text{int}}$$

$$\Sigma = \delta F / \delta G$$

$$\Gamma_{\text{irr}} = \delta \Sigma / \delta G$$

Migdal's theorem:

can be dropped because $(m/M)^{1/2} \ll 1$

Not so for spin-fluctuation exchange

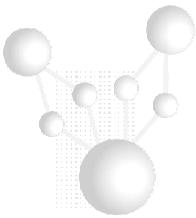
Conservation laws, but:
no Pauli, infinite number of theories, assumes Migdal



Non perturbative but from weak coupling:

- Pauli
- Conservation laws
- Mermin-Wagner

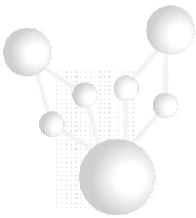
• Main result: Fluctuation-induced pseudogap



How it works...

$$1 - \begin{array}{c} 2 \\ \diagup \quad \diagdown \\ 1 \quad 3 \end{array} - 2 = - \begin{array}{c} 1 \quad 2 \\ \diagup \quad \diagdown \\ 3 \end{array} + \begin{array}{c} 1 \quad 2 \\ \diagup \quad \diagdown \\ 3 \end{array} + \begin{array}{c} 1 \quad 2 \\ \diagup \quad \diagdown \\ 3 \end{array} =$$

The diagram illustrates the decomposition of a loop with vertices 1, 2, and 2 into two smaller loops. The first part shows a red square with vertices 1, 2, 4, and 5. A green triangle at vertex 2 has arrows pointing from 2 to 4 and from 2 to 5. The second part shows a red rectangle with vertices 1, 2, 4, and 5. A green triangle at vertex 1 has an arrow pointing from 1 to 5. Below these, a purple circle contains a black Greek letter sigma (Σ), with dashed lines connecting it to the vertices 1, 2, and 2.



A non-perturbative approach for both $U > 0$ and $U < 0$

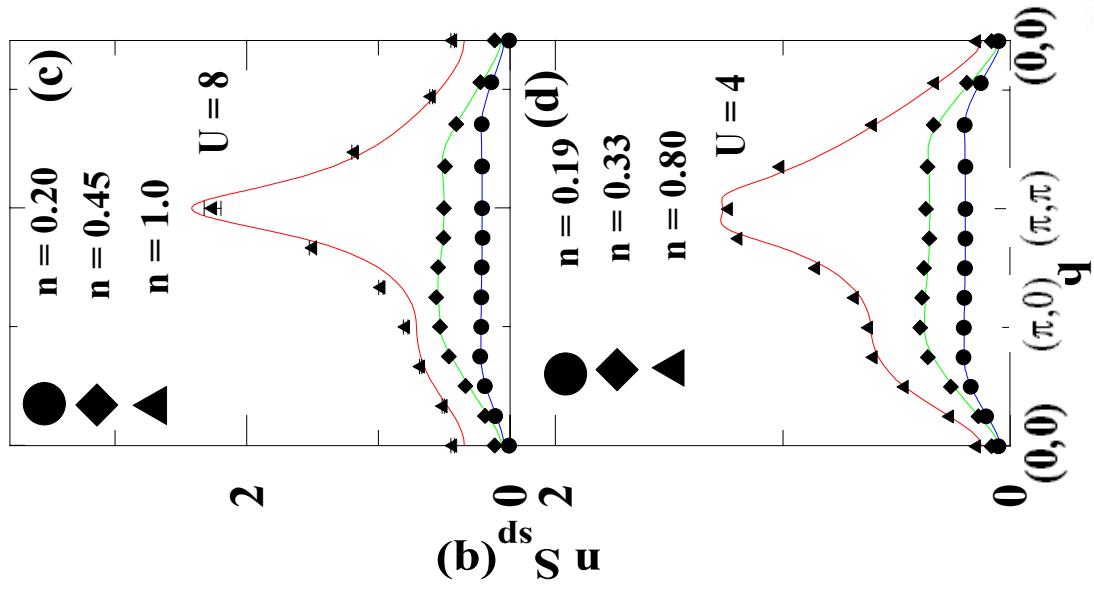
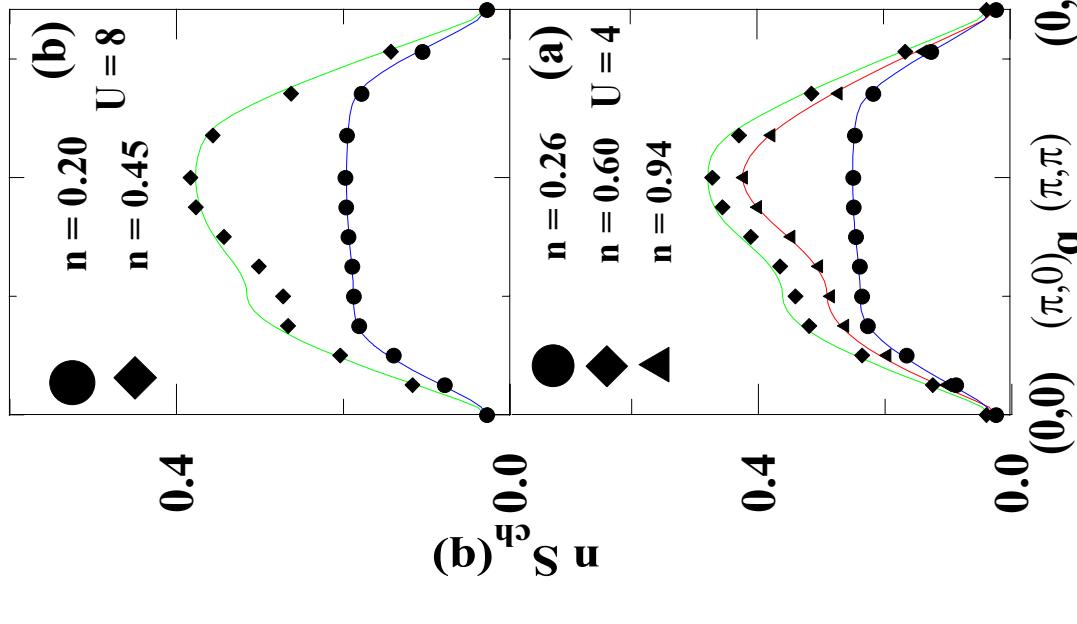
- Proofs that it works

Notes:

-F.L.

parameters

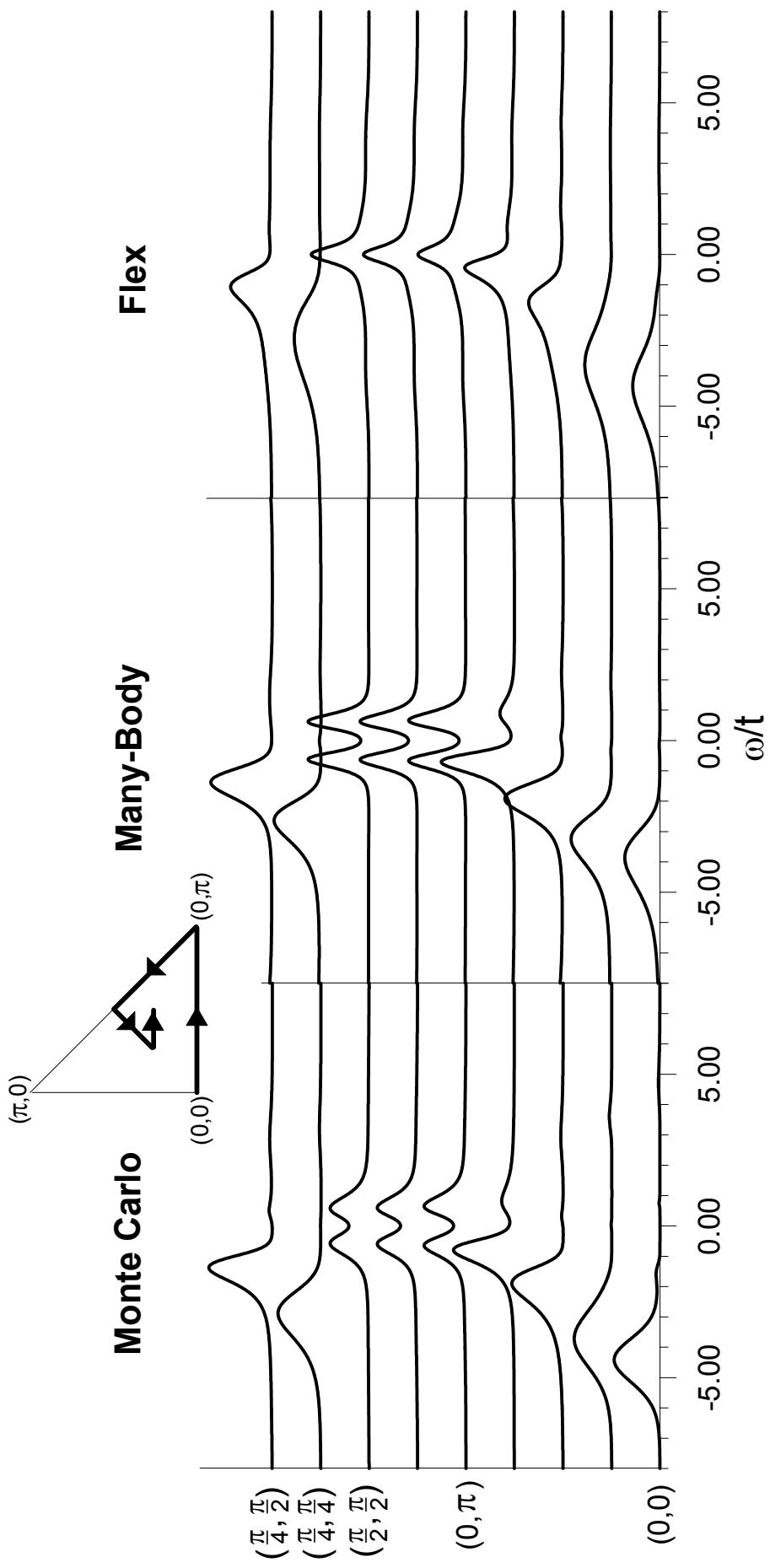
-Self also
Fermi-liquid



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



U = + 4



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

U = + 4

FLEX

Many-Body $\Sigma(s)$

Monte Carlo

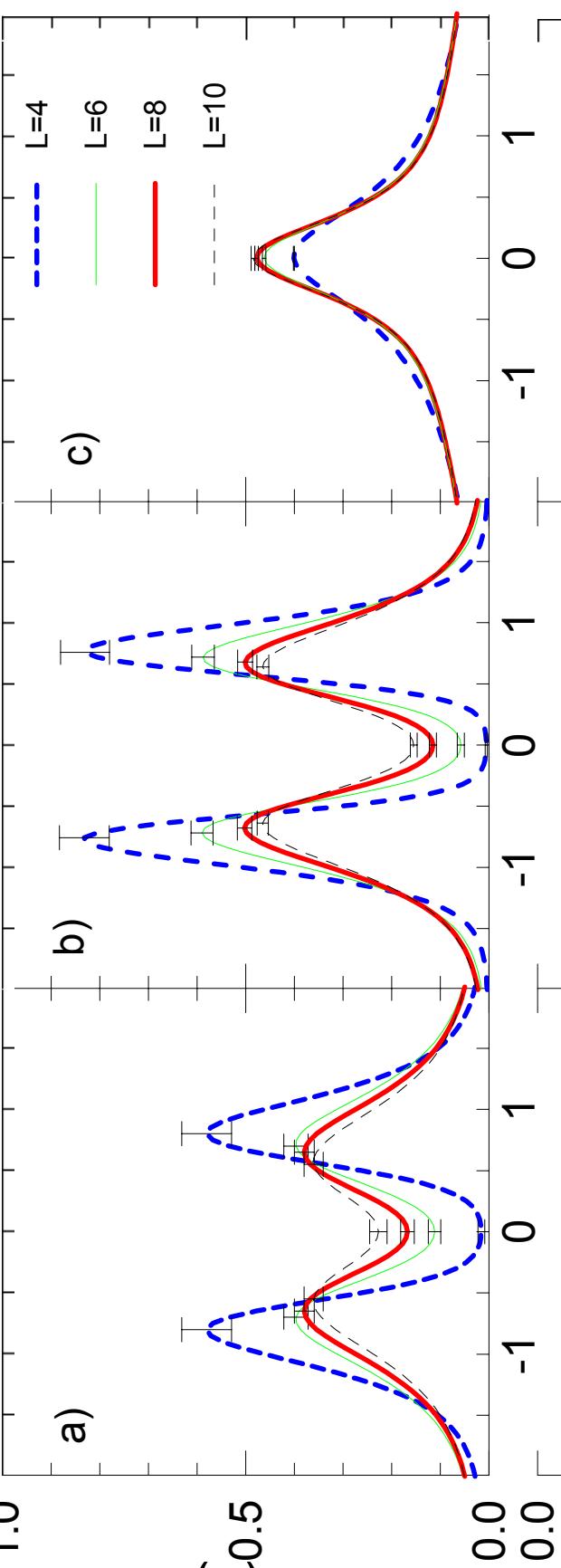
1.0

($\frac{G}{\beta}$)^{0.5}

a)

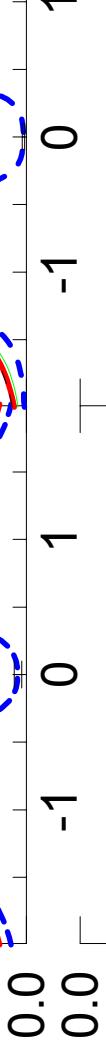
c)

b)



0.0

($\frac{G}{\beta}$)^{0.5}



-0.5

($\frac{G}{\beta}$)^{0.5}

-0.5

($\frac{G}{\beta}$)^{0.5}

0

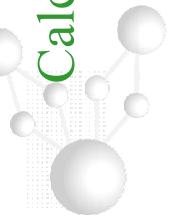
($\frac{G}{\beta}$)^{0.5}

0.5

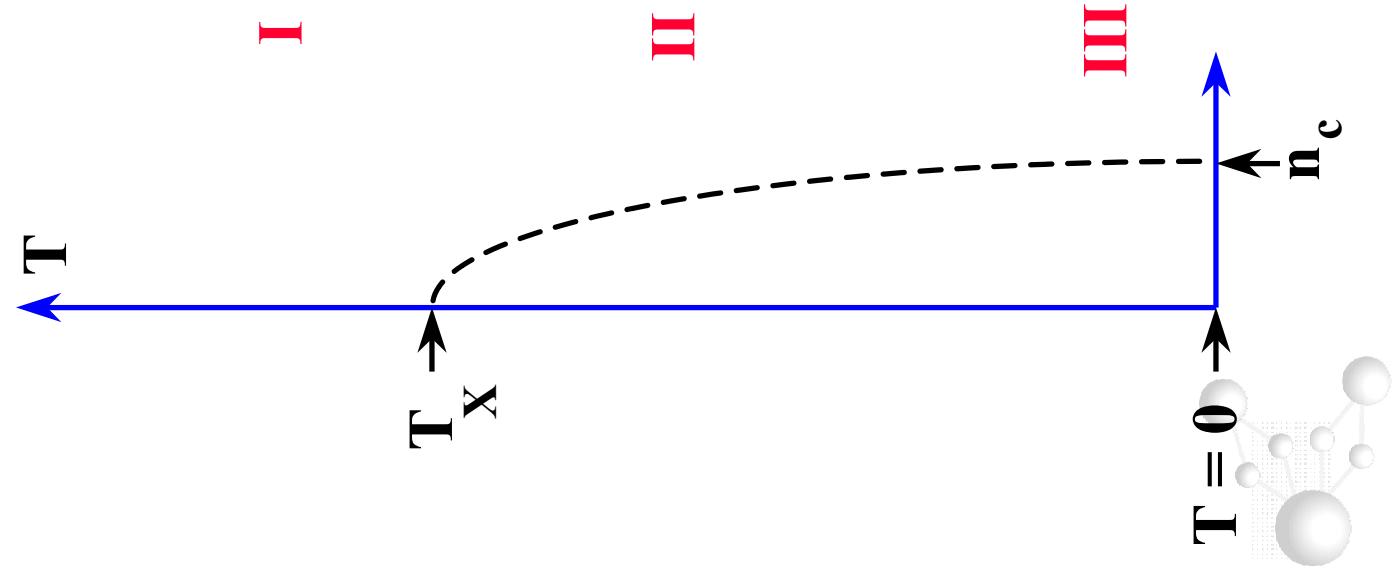
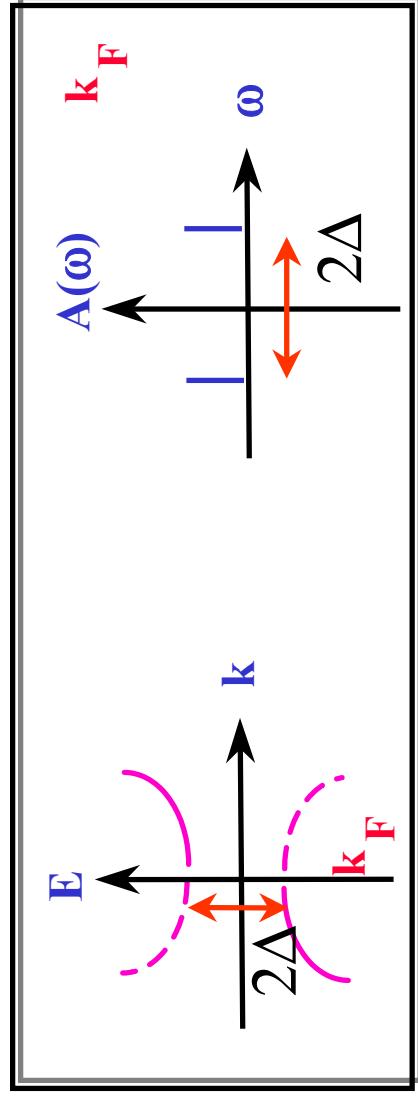
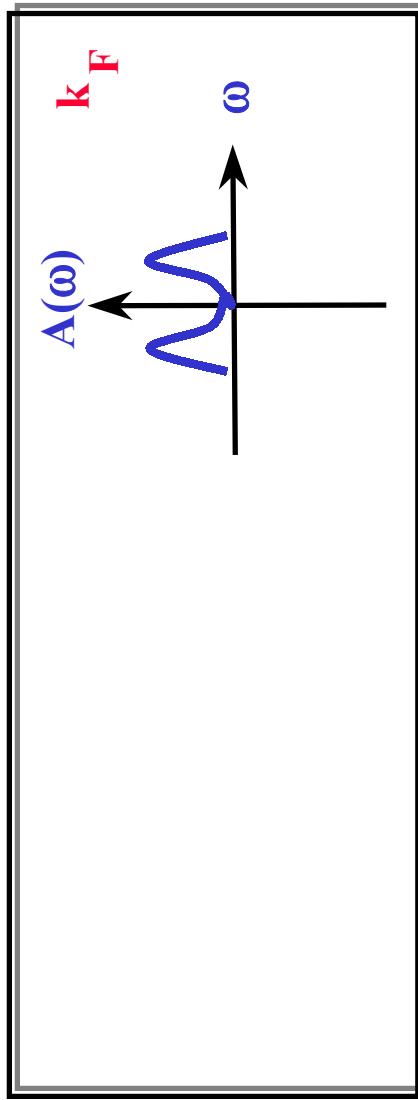
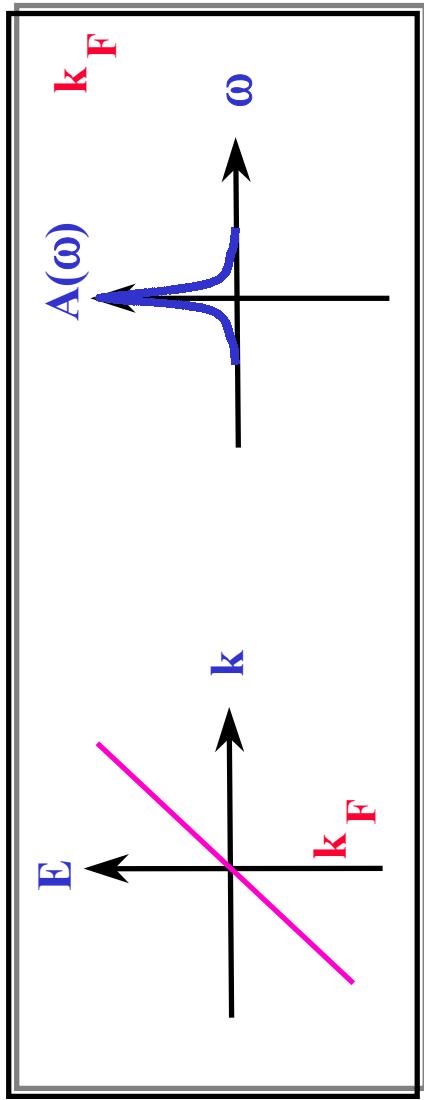
($\frac{G}{\beta}$)^{0.5}

1.0

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



40



41

$U > 0$

- Evidence against renormalized classical regime for spin fluctuations in pseudogap regime.

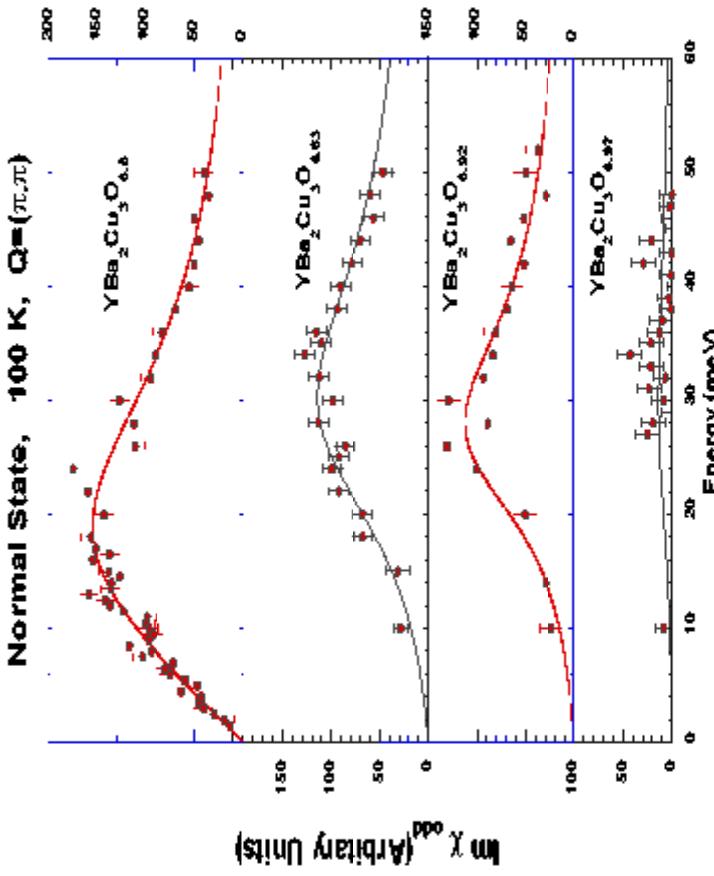
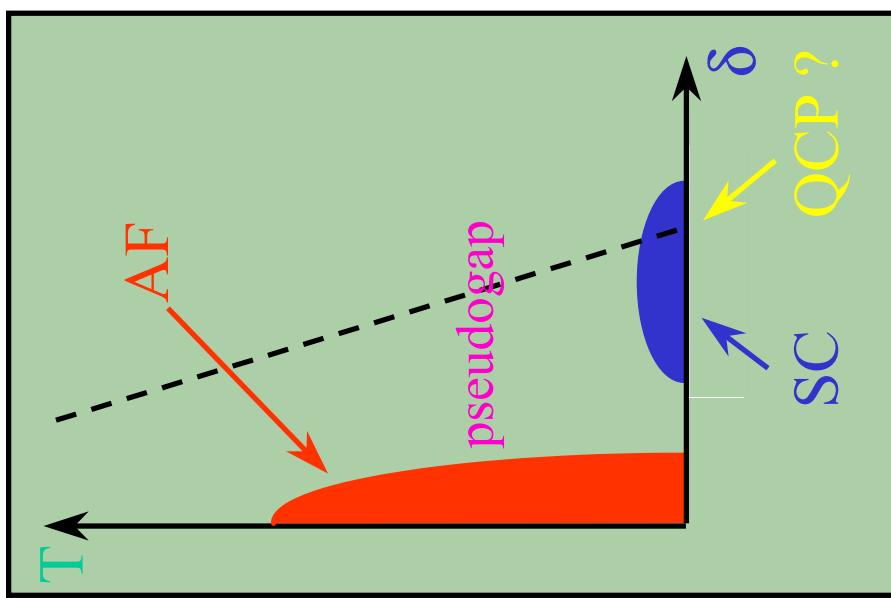


Figure 2: Normalized imaginary part of the spin susceptibility at the AF wavevector in the normal state, at $T = 100$ K, for four oxygen contents in YBCO ($T_c = 15, 19, 22, 25$ K for $x = 0.5, 0.52, 0.52, 0.57$, respectively). These curves have been normalized to the same units using standard phonon calibration.¹⁴ (100 counts in the vertical scale roughly correspond to $\sim 350 \mu_B^2/\text{eV i absolute units}$) [from ¹⁰].

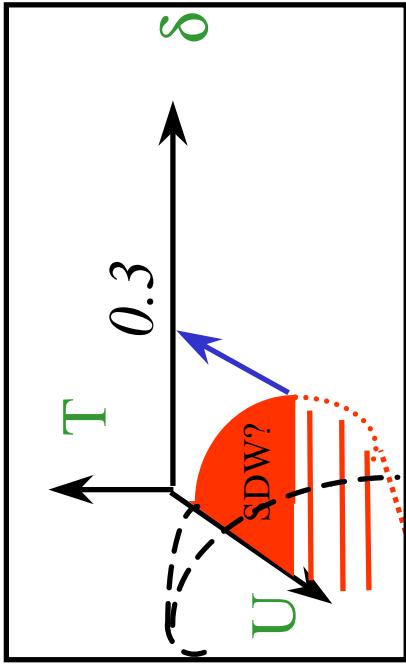


U > 0

- Quantum critical point, $d = 2$:

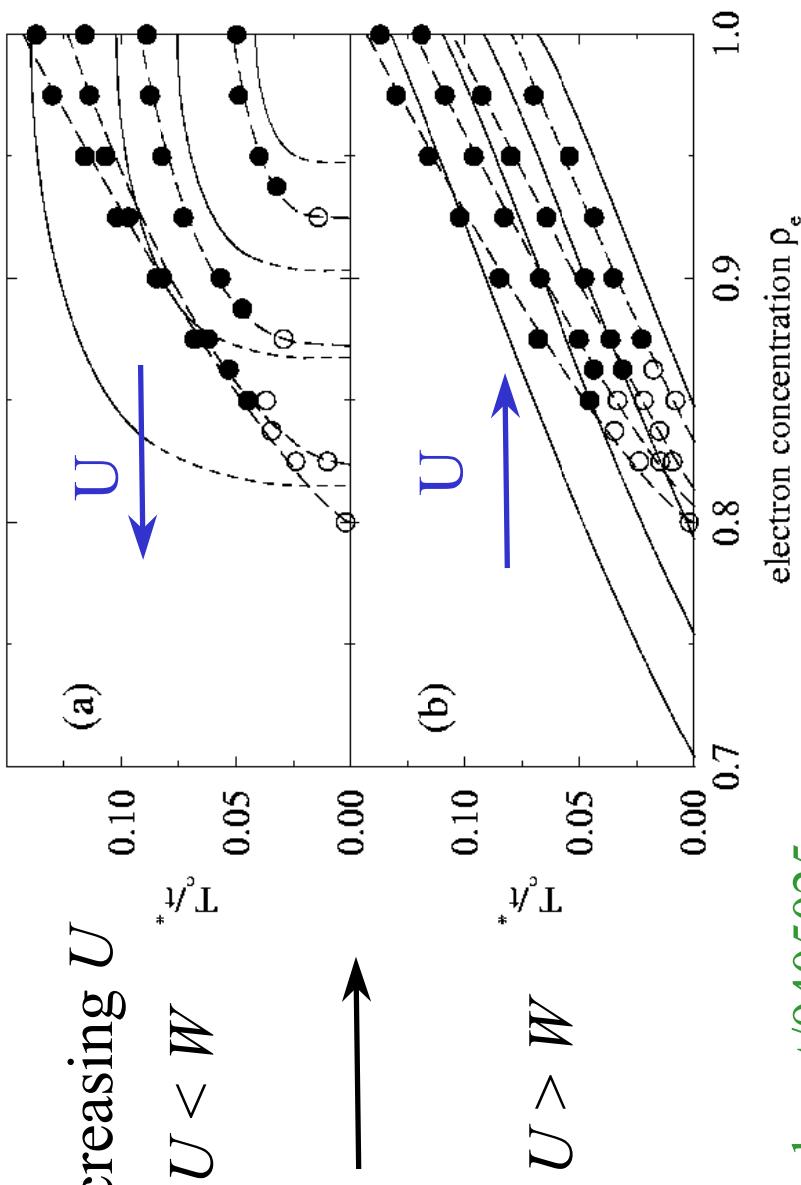
- Instability at incommensurate q
- Largest doping : 0.315

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



- Decreases with increasing U
 $U < W$

$d = \text{infinity}$



Freericks, Jarrell cond-mat/9405025

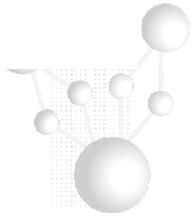
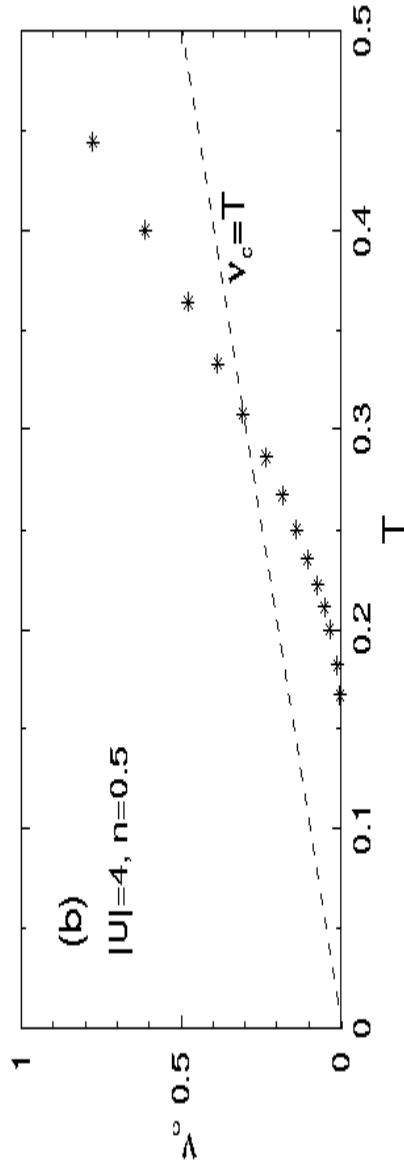
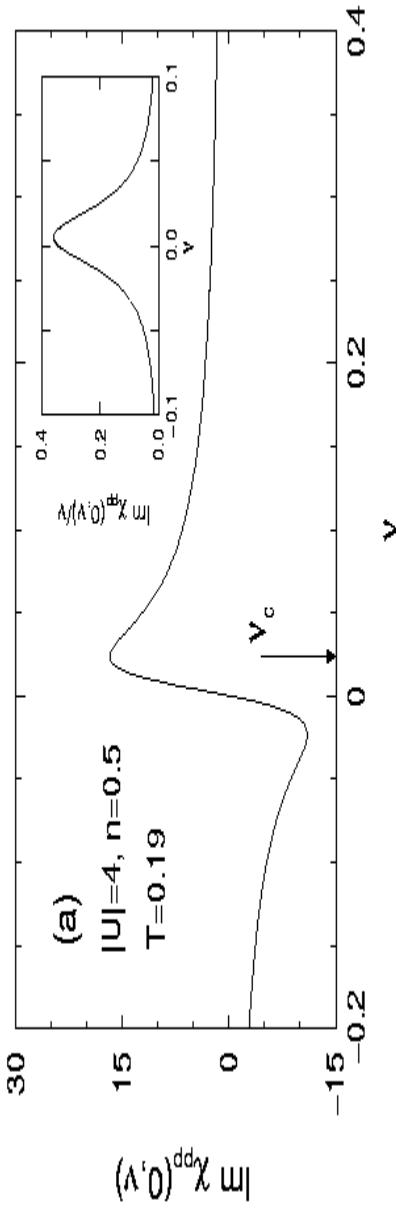


Mechanism for pseudogap, $U < 0$

$$U = -4$$

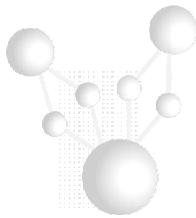
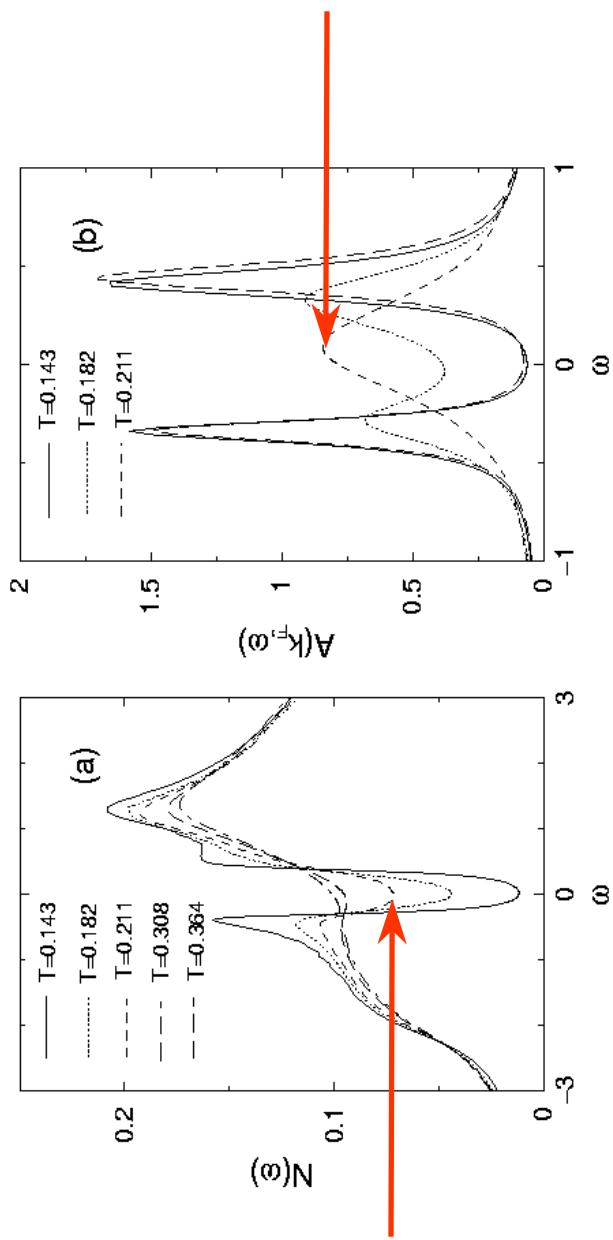
- (analogous to $U > 0$) : Vilk *et al.* Europhys. Lett. 33, 159 (1996)
Pines, Schmalian (98)

- Enter the renormalized-classical regime. N.B. $d = 2$



Mechanism for pseudogap, $U < 0$

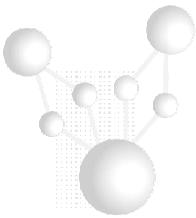
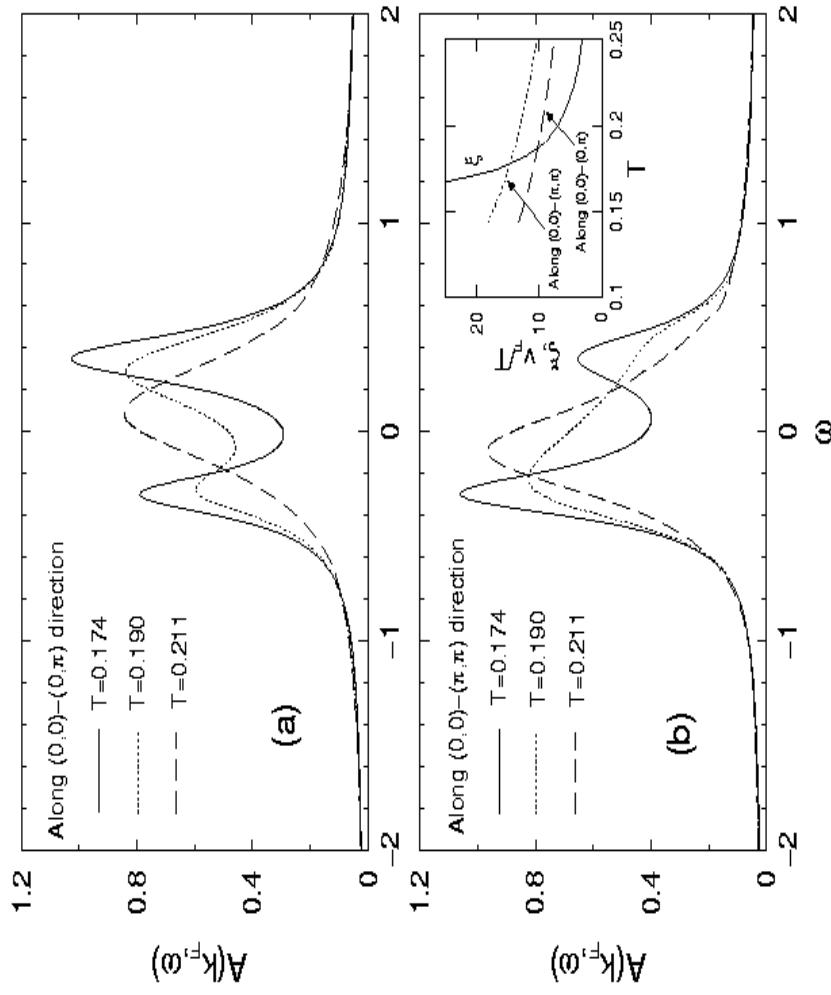
- Pseudogap appears first in total density of states
- Fills in instead of opening up
- Rearrangement over huge frequency scale compared with either T or ΔT . ($\Delta T \sim 0.03$, $T \sim 0.2$, $\Delta\omega \sim 1$)



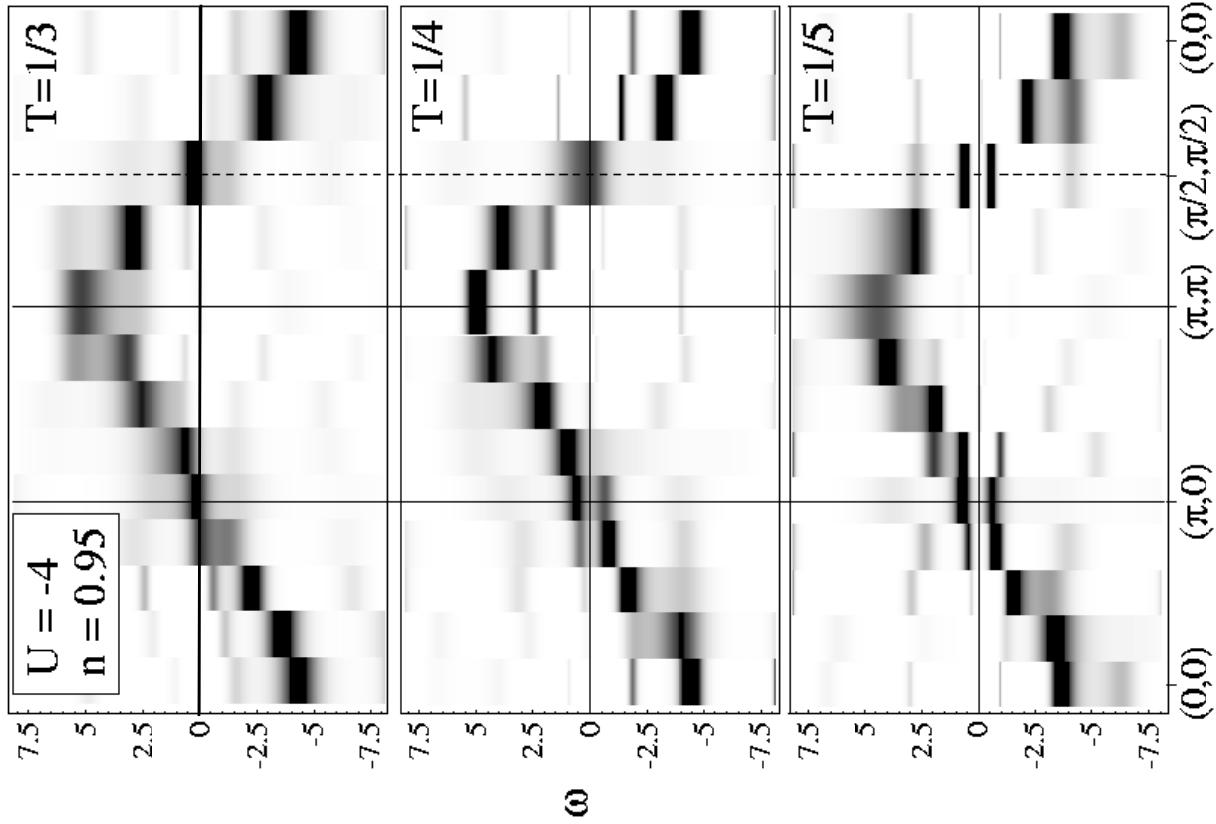
Mechanism for pseudogap, $U < 0$

U = -4

- Pairing correlation length larger than single-particle thermal de Broglie wavelength (v_F / T)

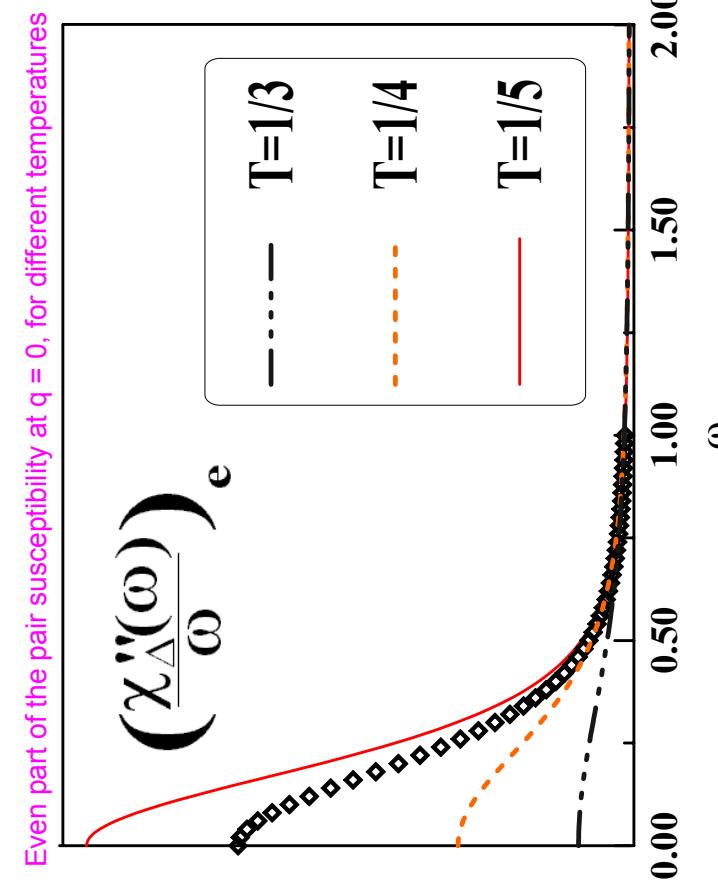


Mechanism for pseudogap, $U < 0$



$U = -4$

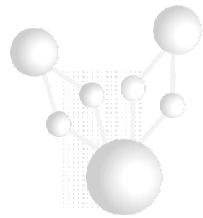
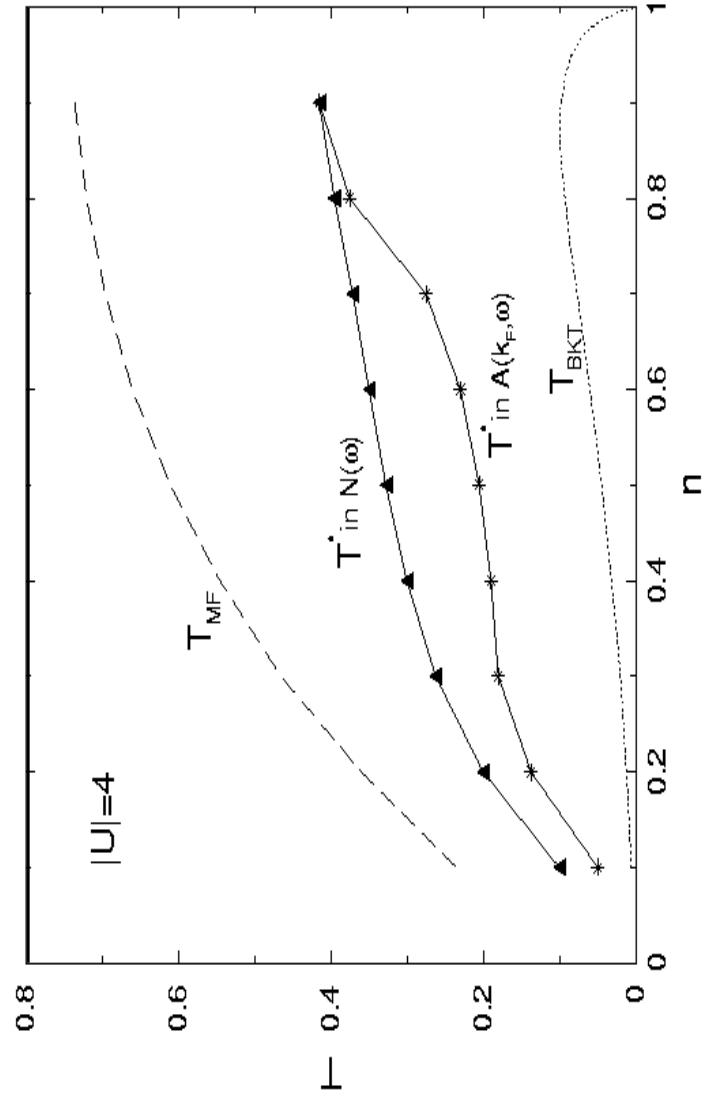
$d = 2$ is crucial



Allen, et al. P.R. L 83, 4128 (1999)

Crossover diagram

$U = -4$



$$U < 0$$

Pairing-fluctuation induced pseudogap

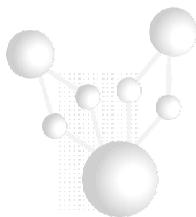
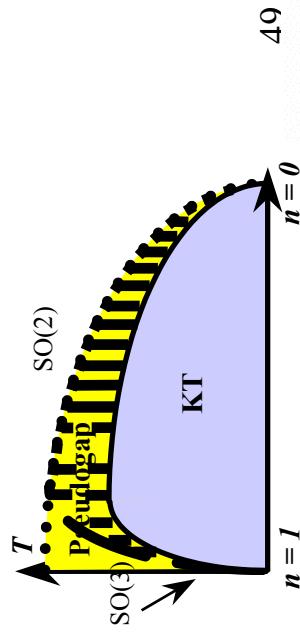
- Slightly Overdoped High-Tc Superconductor $TlSr_2CaCu_2O_{6.8}$
Guo-qing Zheng *et al.*, P. R. L. **85, 405 (2000)**
 - Pseudogap in Knight shift and NMR relaxation strongly H dependent, contrary to underdoped (up to 23 T).

- Underdoped in a range $\Delta T \sim 15 K$ near T_c see evidence for renormalized classical regime (KT behavior).

Corson *et al.* Nature, **398, 221 (1999).**

- Higher symmetry group creates large range of T where there is a pseudogap.

Allen et al. P.R.L. **83, 4128 (1999)**



(d) Approaching from strong coupling



D. Sénéchal

- Straight perturbative treatment is difficult:

- No Wick's theorem

- Non-causality

- (S. Pairault, D. Senechal, A.-M. S. T. Eur. Phys. J. B 16, 85 (2000))

- Slave bosons and slave fermions

$$\bullet c_{\uparrow}^{+}(1 - n_{\downarrow}) \rightarrow f_{\downarrow} b_{\uparrow}^{+} \quad \text{or} \quad f_{\uparrow} b_{\uparrow}^{+}$$

$$\bullet \text{Constraint: } (\sum_{\sigma} f_{\sigma}^{+} f_{\sigma}) + b^{+} b = I$$

- Mean field : constraint with Lagrange multiplier

- Gauge theory

$$\bullet f_{\uparrow}^{+} \rightarrow e^{i\theta} f_{\uparrow}^{+}$$

$$\bullet b \rightarrow e^{-i\theta} b$$



$$\bullet \lambda \rightarrow \lambda + \delta \theta / \delta \tau$$

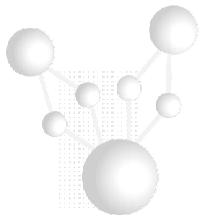
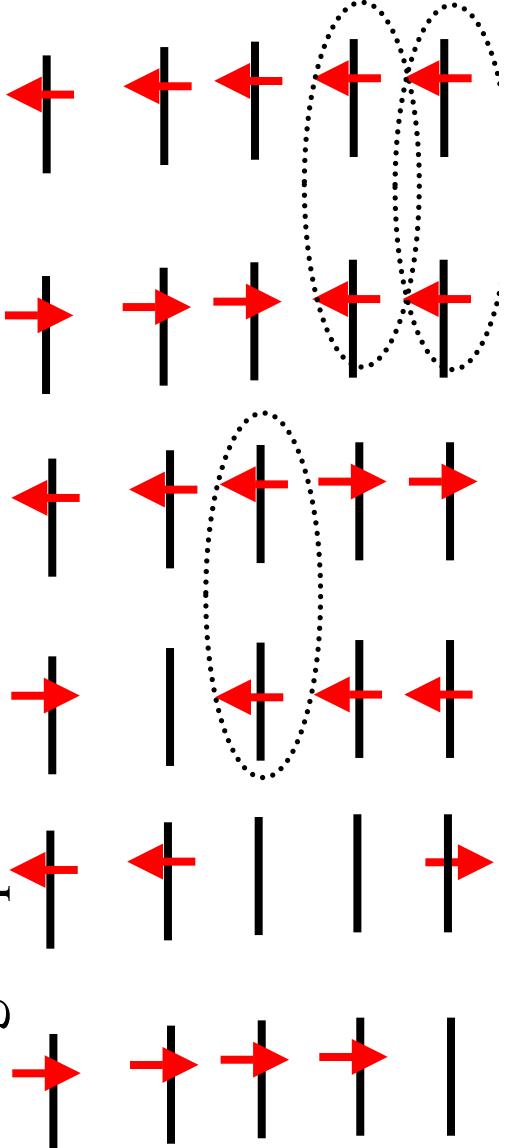
- Gauge theory:
 - Break Gauge symmetry
 - Look for mass of gauge field (stable if mass)
 - Find topological excitations
 - (charge carriers prop. to δ)

• There are ambiguities (Slave-fermions vs slave-bosons)

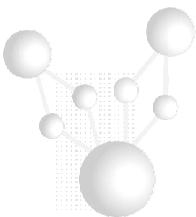
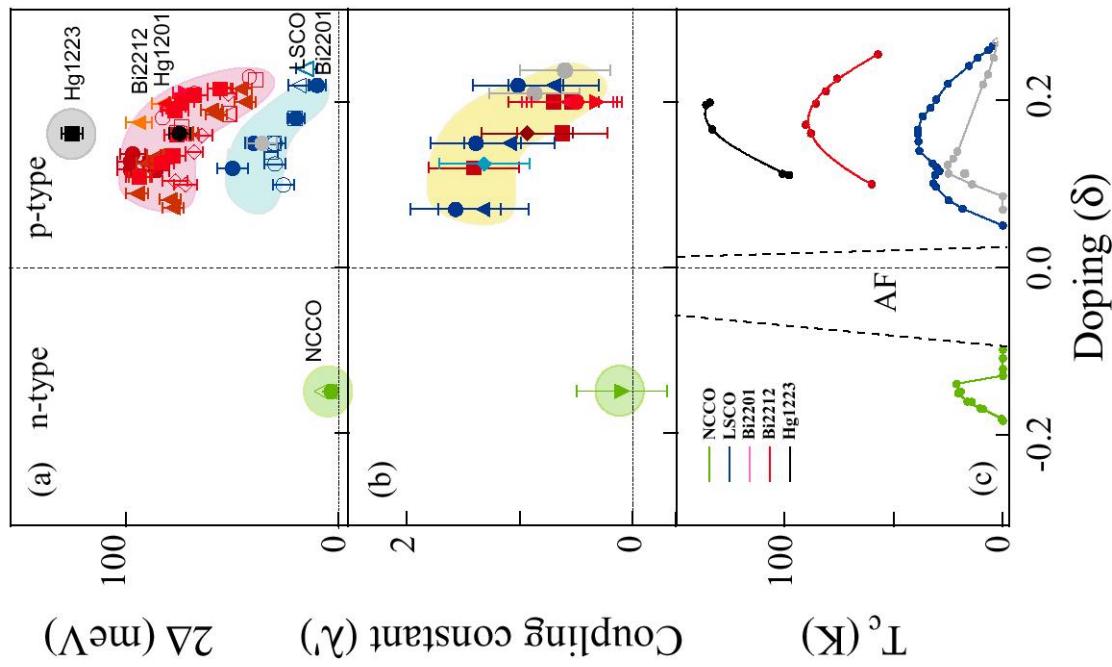
- e.g. limit $J = 0$ (Nagaoka)

*(Daniel Boies, F. Jackson and A.-M.S. T. Int. J. Mod. Phys. **9**, 1001 (1995))*

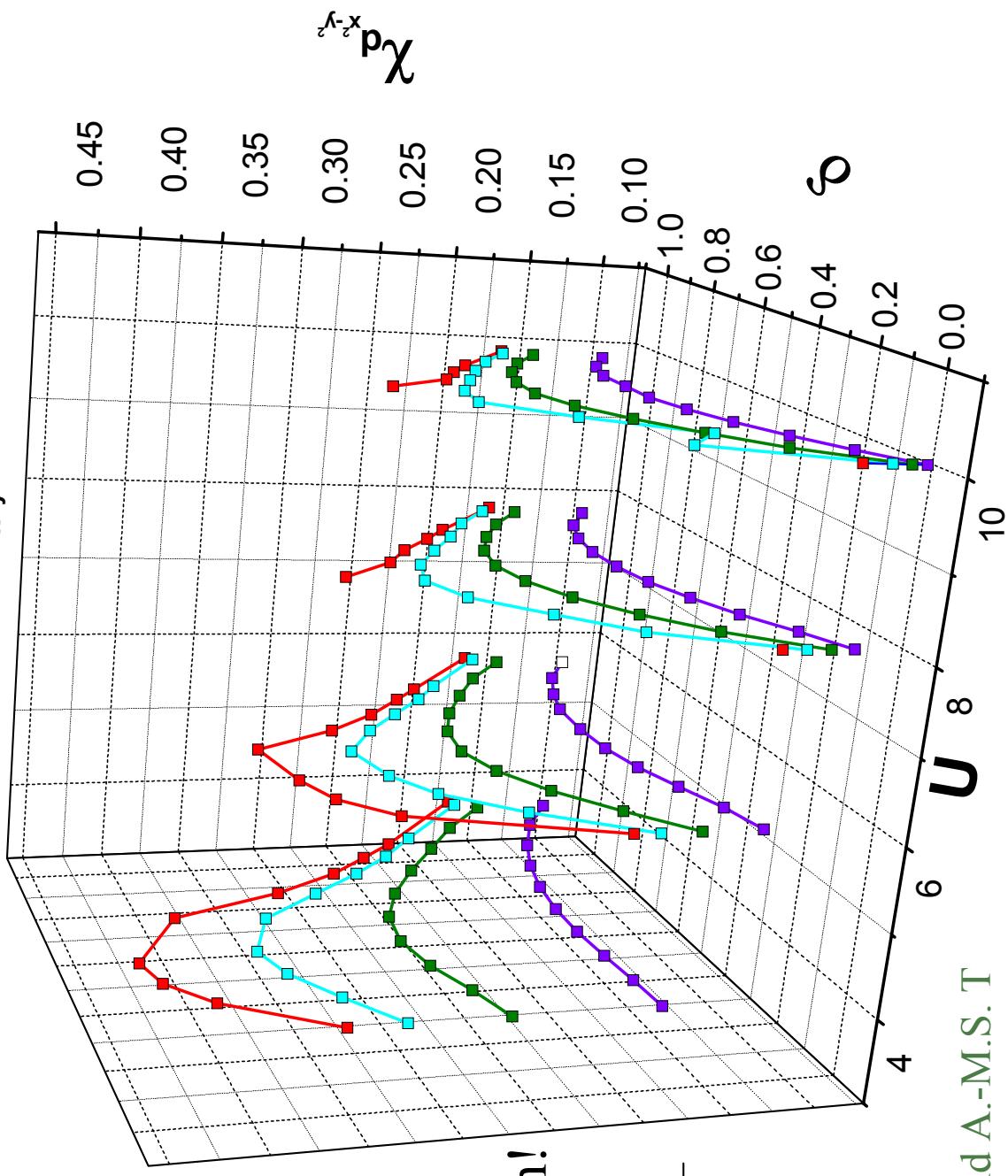
• Spin-charge separation



(e) Phonons



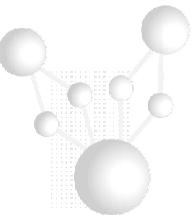
Susceptibilité de paires de type $d_{x^2-y^2}$ pour un réseau 6×6



$$\begin{aligned}\beta &= 1 \\ \beta &= 2 \\ \beta &= 3 \\ \beta &= 4\end{aligned}$$

Would need oxygen!

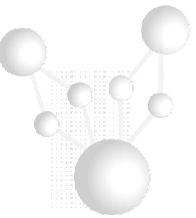
$$\chi_d = \frac{\chi_d}{1 - V \chi_d}$$



J.-S. Landry and A.-M.S. T

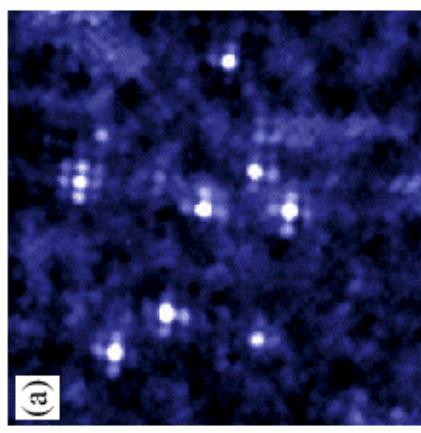
(f) Inhomogeneities

- Disorder is important in underdoped
- Even without interactions, complicated: localization
- Main theoretical tools: impurity averaging, Replica trick
- Instabilities to inhomogeneous ground states:
 - $\mathbf{S}_Q \cdot \mathbf{S}_{Q'} \rho_{-2Q}$
 - $n = 1$ magnetic « anti-stripes »
 - $n = 0.5$ « charged stripes »
- Using impurities as a « diagnostic tool » for superconducting state
 - Complicated : Kondo effect etc...

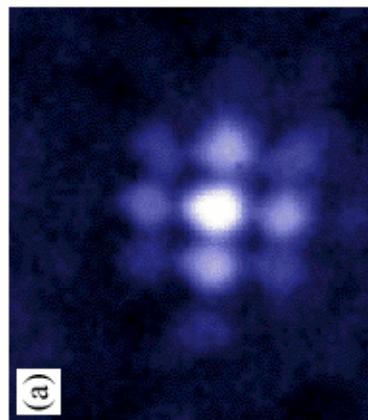


Inhomogeneities

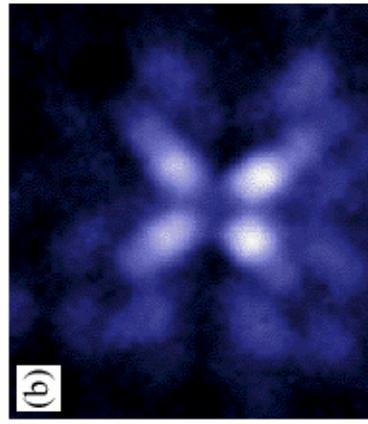
Impurities



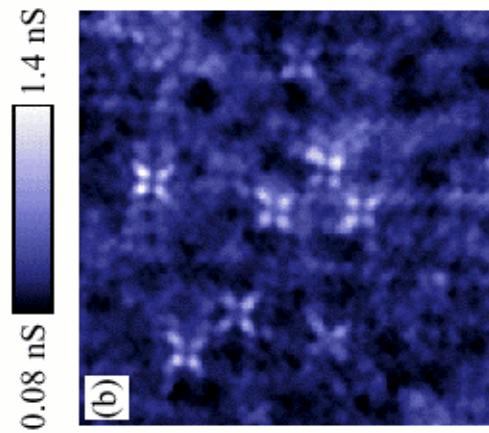
(a)



(b)



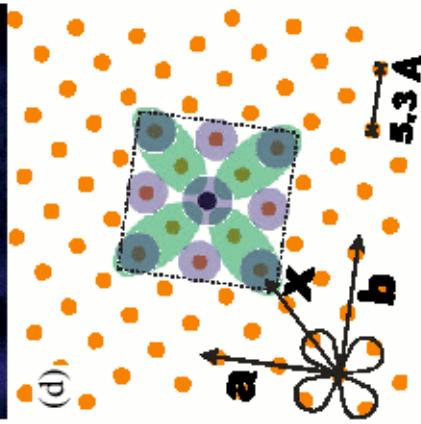
(b)



(b)



(c)



(d)

E.W. Hudson *et al.* cond-mat/0104237

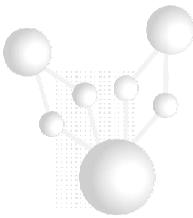
See also : C. Howald, P. Fournier, A. Kapitulnik cond-mat/0101251

(g) Quantum critical points . . .



V. Conclusion

- The pseudogap summarizes anomalous « normal state » properties
 - It is ill-understood
 - Need to understand it to understand the phase diagram and superconductivity.
- It is the motivation for a vast body of work in many directions
- Methods have to be developed at the same time
- Sociology



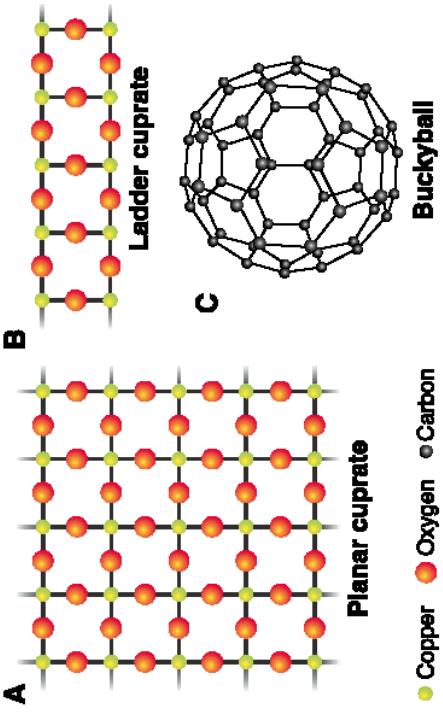


FIG. 1. The structures of superconductors (A) Copper oxide plane, (B) copper oxide ladder, and (C) C_{60} molecule. Ladders of copper and oxygen atoms, as shown in (B), form spontaneously in some compounds.

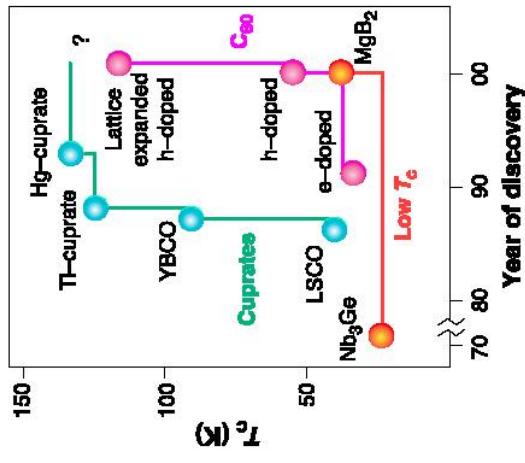
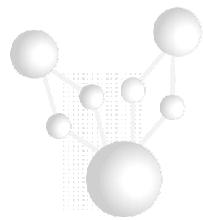


FIG. 2. Head-to-head race, T_c versus year of discovery for some superconducting materials. Orange, representative low- T_c compounds, which held the T_c record before cuprates and fullerenes were discovered. Light blue, representative planar cuprates. Magenta, representative fullerenes, with the highest T_c to date reported in [4].



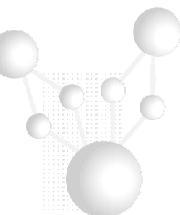
E. Dagotto, cond-mat/0110190

Michel Barrette

Mehdi Bozzo-Rey



David Sénéchal A.-M.T. Alain Veilleux



Liang Chen



Yury Vilk



Steve Allen



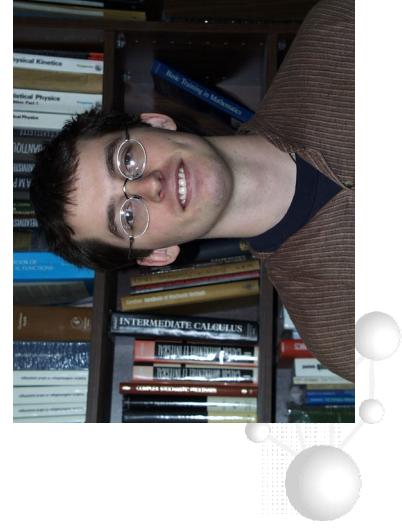
François Lemay

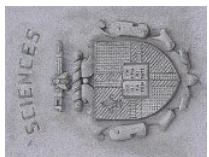


Bumsoo Kyung Samuel Moukouri

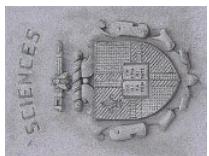


Hugo Touchette





Sébastien Roy Alexandre Blais



Claude Bourbonnais



R. Côté



Jean-Sébastien Landry
A.-M.T.



Bunsoo Kyung



- How can we understand electronic systems that show both localized and extended character?
- Why do both organic and high-temperature superconductors show broken-symmetry states where mean-field-like quasiparticles seem to reappear?
- Why is the condensate fraction in this case smaller than what would be expected from the shape of the would-be Fermi surface in the normal state?
- Are there new elementary excitations that could summarize and explain in a simple way the anomalous properties of these systems?
- Do quantum critical points play an important role in the Physics of these systems?
- Are there new types of broken symmetries?
- How do we build a theoretical approach that can include both strong-coupling and $d = 2$ fluctuation effects?
- What is the origin of d-wave superconductivity in the high-temperature superconductors?

