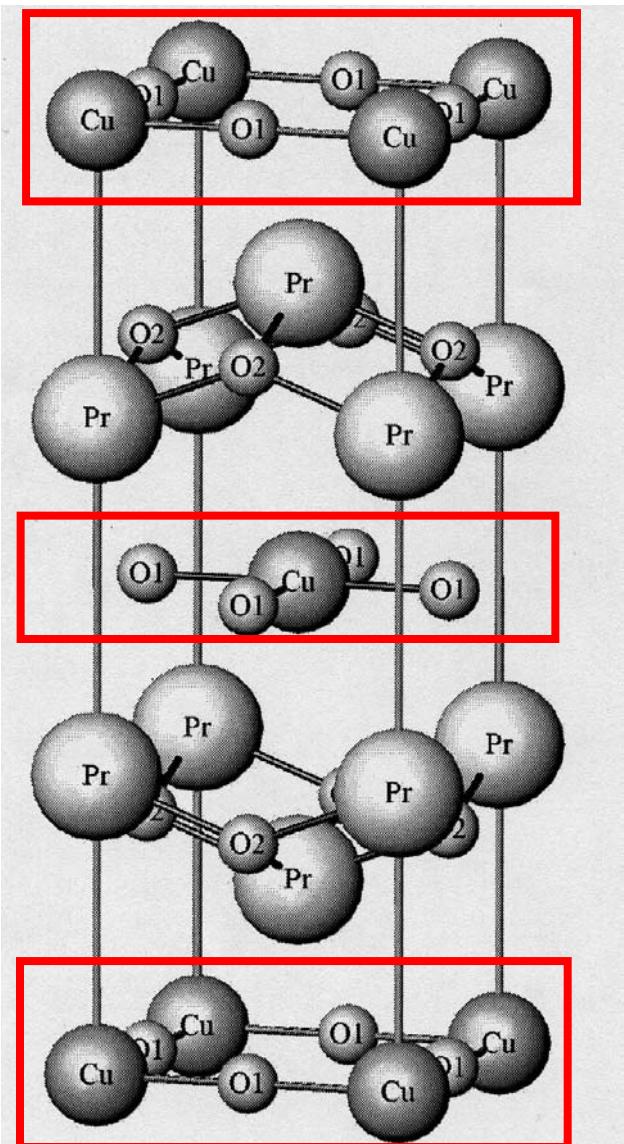


CuO₂ planes



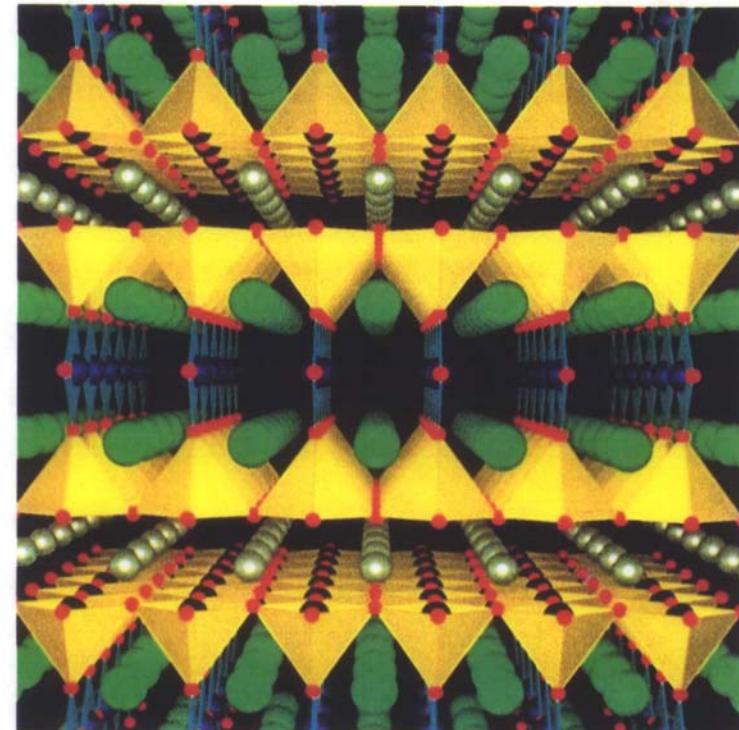
SCIENTIFIC AMERICAN

How nonsense is deleted from genetic messages.

R for economic growth: aggressive use of new technology.

Can particle physics test cosmology?

JUNE 1988
\$3.50



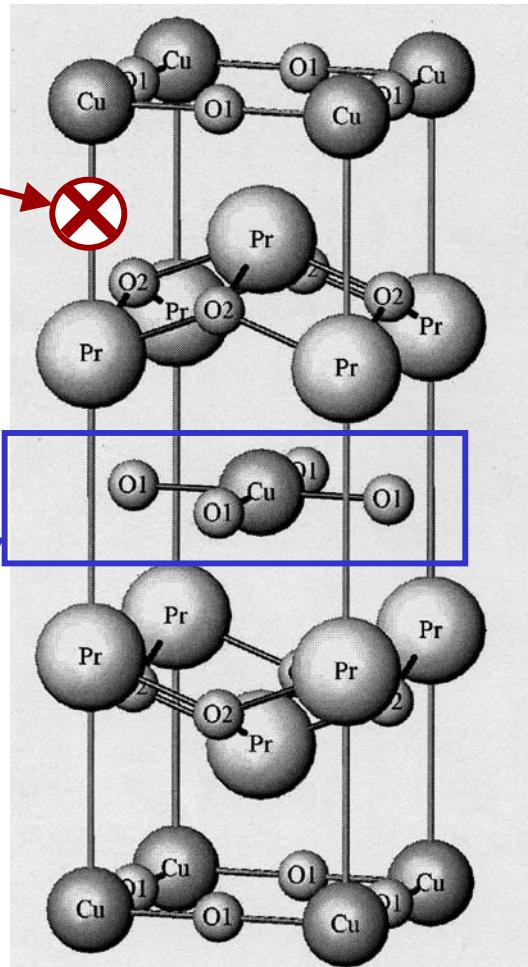
YBa₂Cu₃O_{7-δ}

Different crystal structures

Pr_2CuO_4

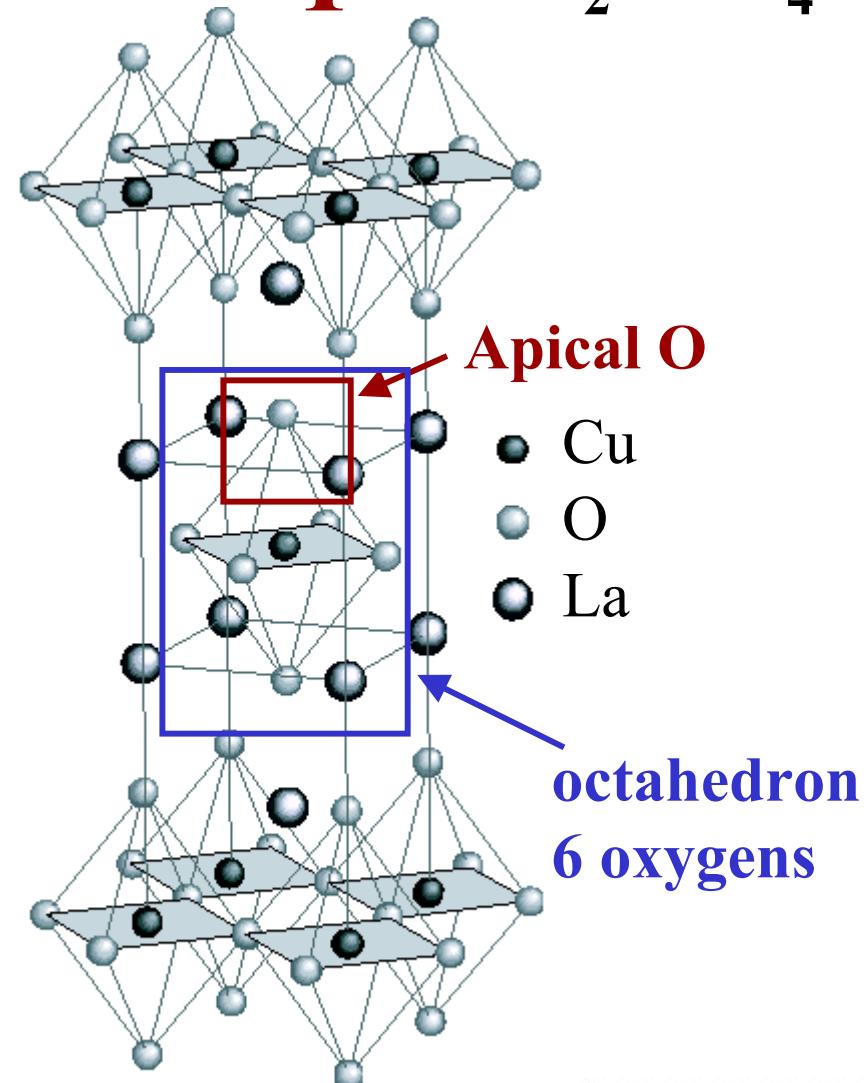
T'

No apical O!



Square
4 oxygens

T La_2CuO_4



Phase diagram

Electron doping \longleftrightarrow Hole doping

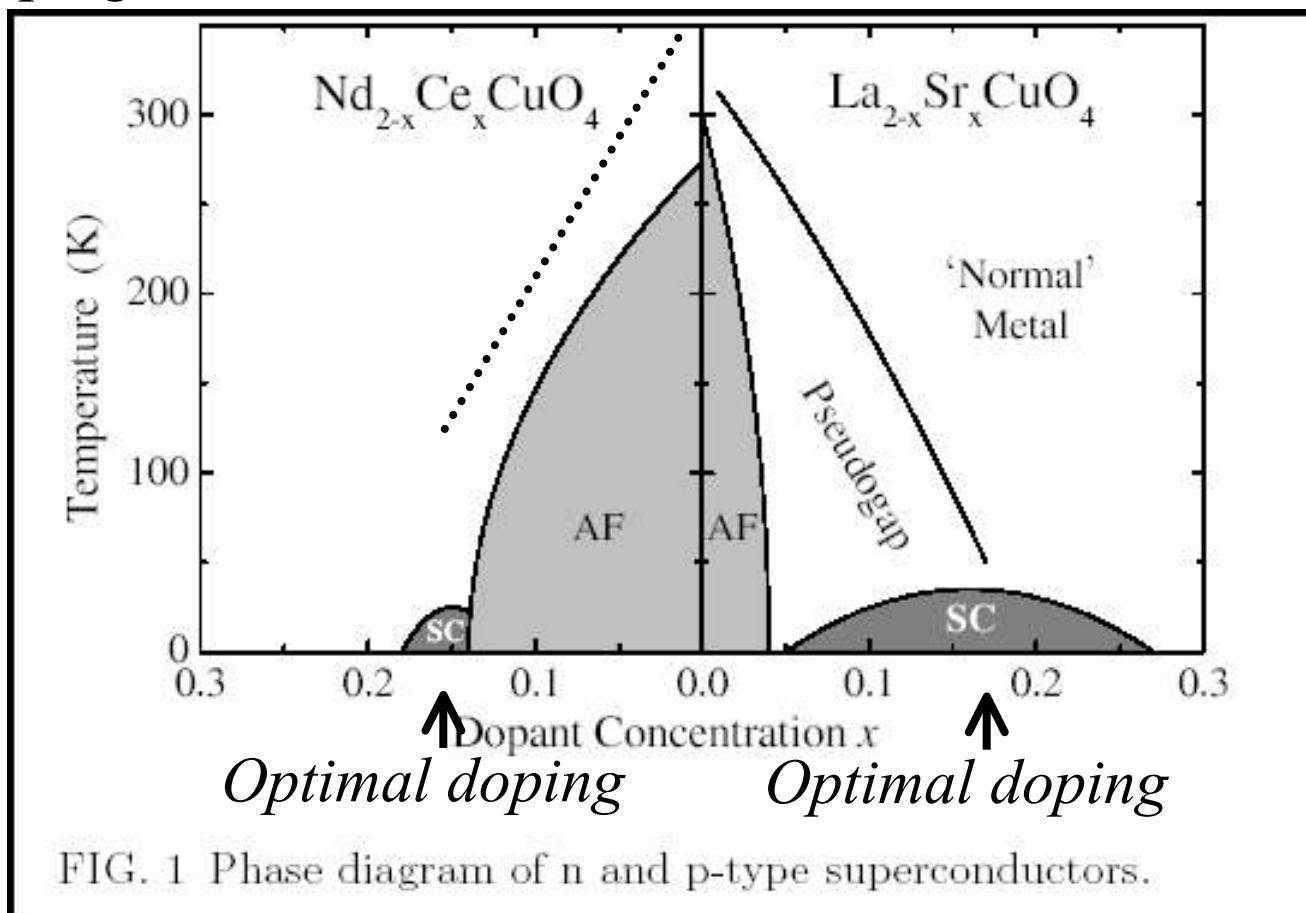
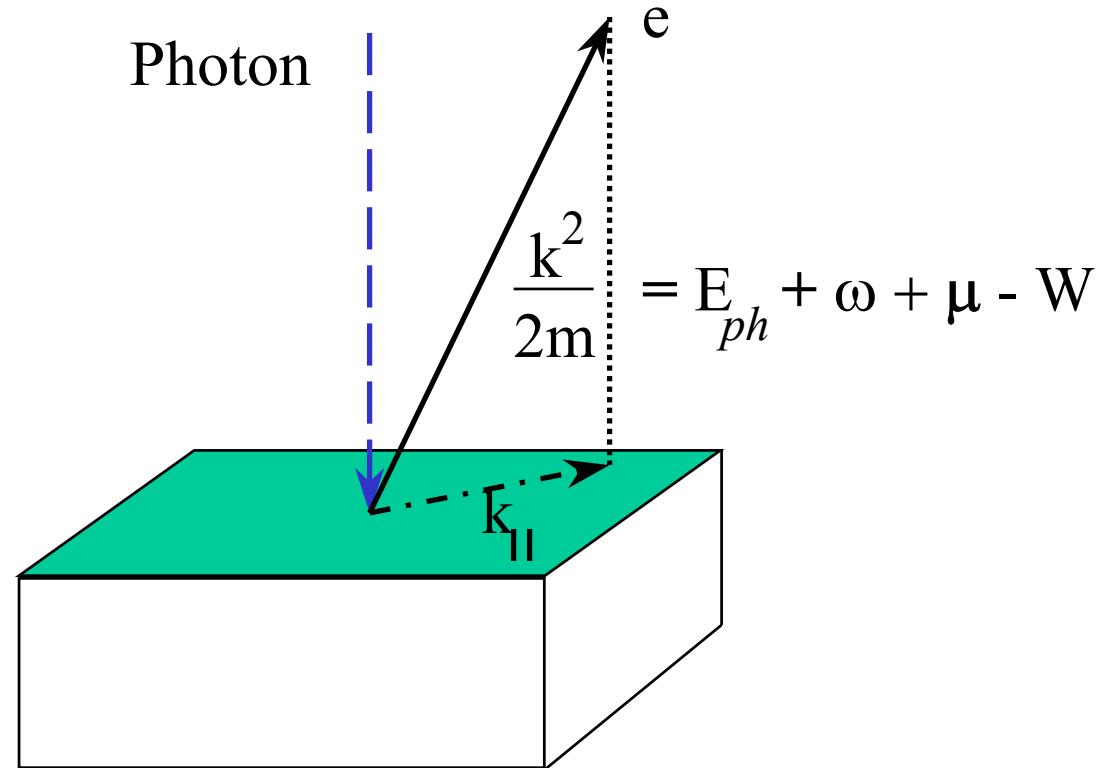


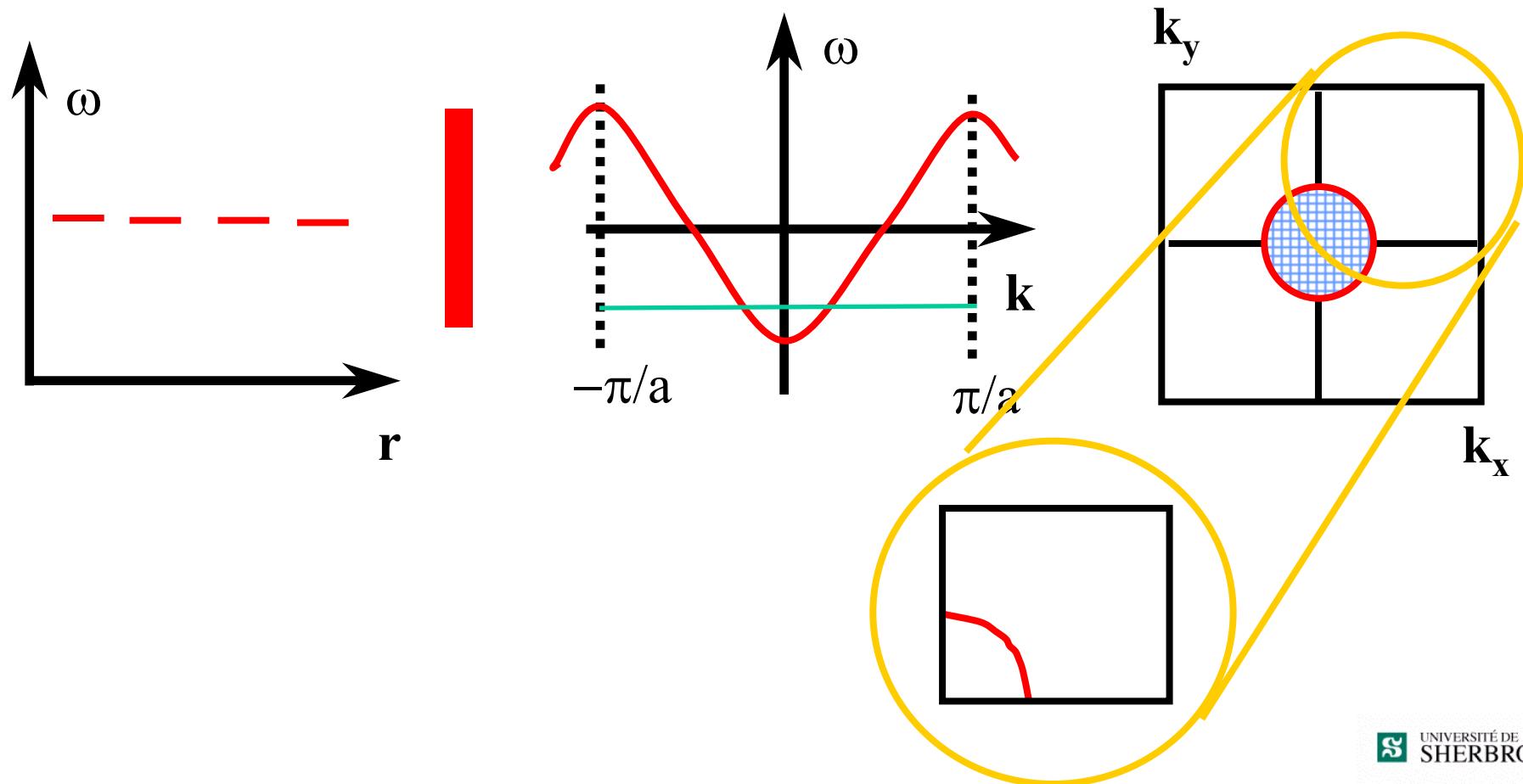
FIG. 1 Phase diagram of n and p-type superconductors.

Electronic states in $d=2$

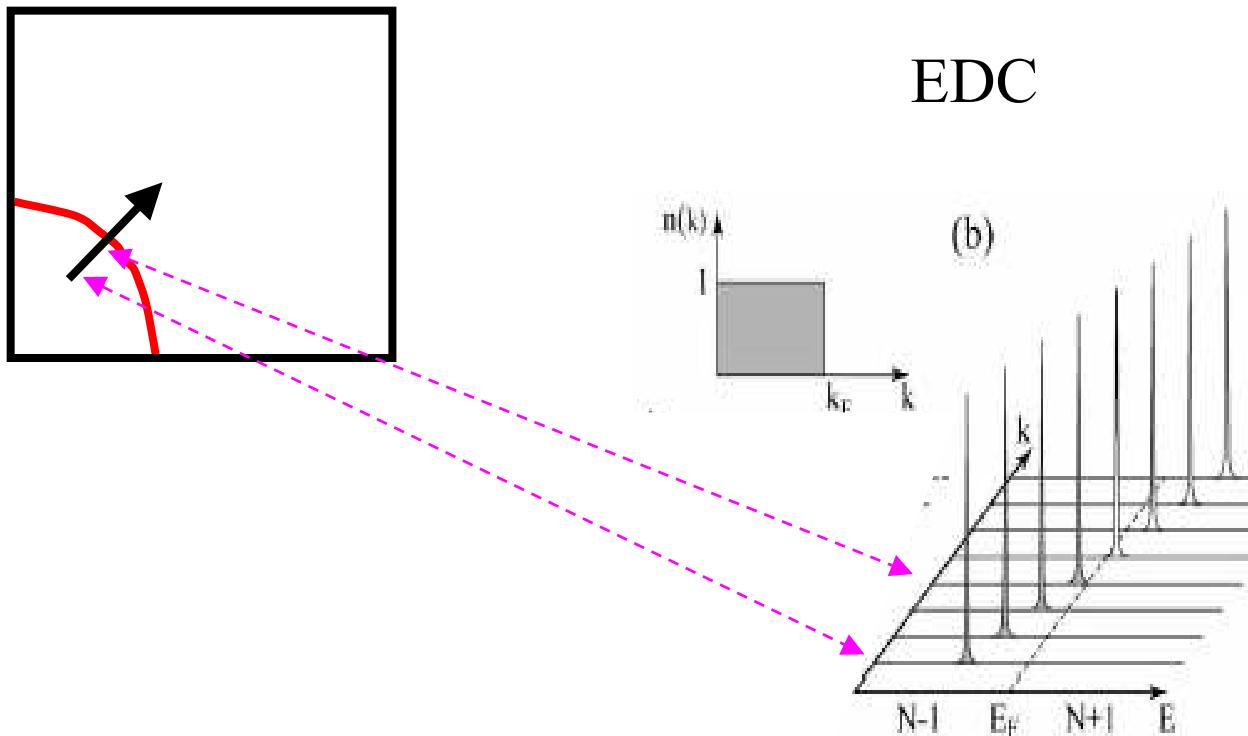
Angle Resolved Photoemission Spectroscopy (ARPES)



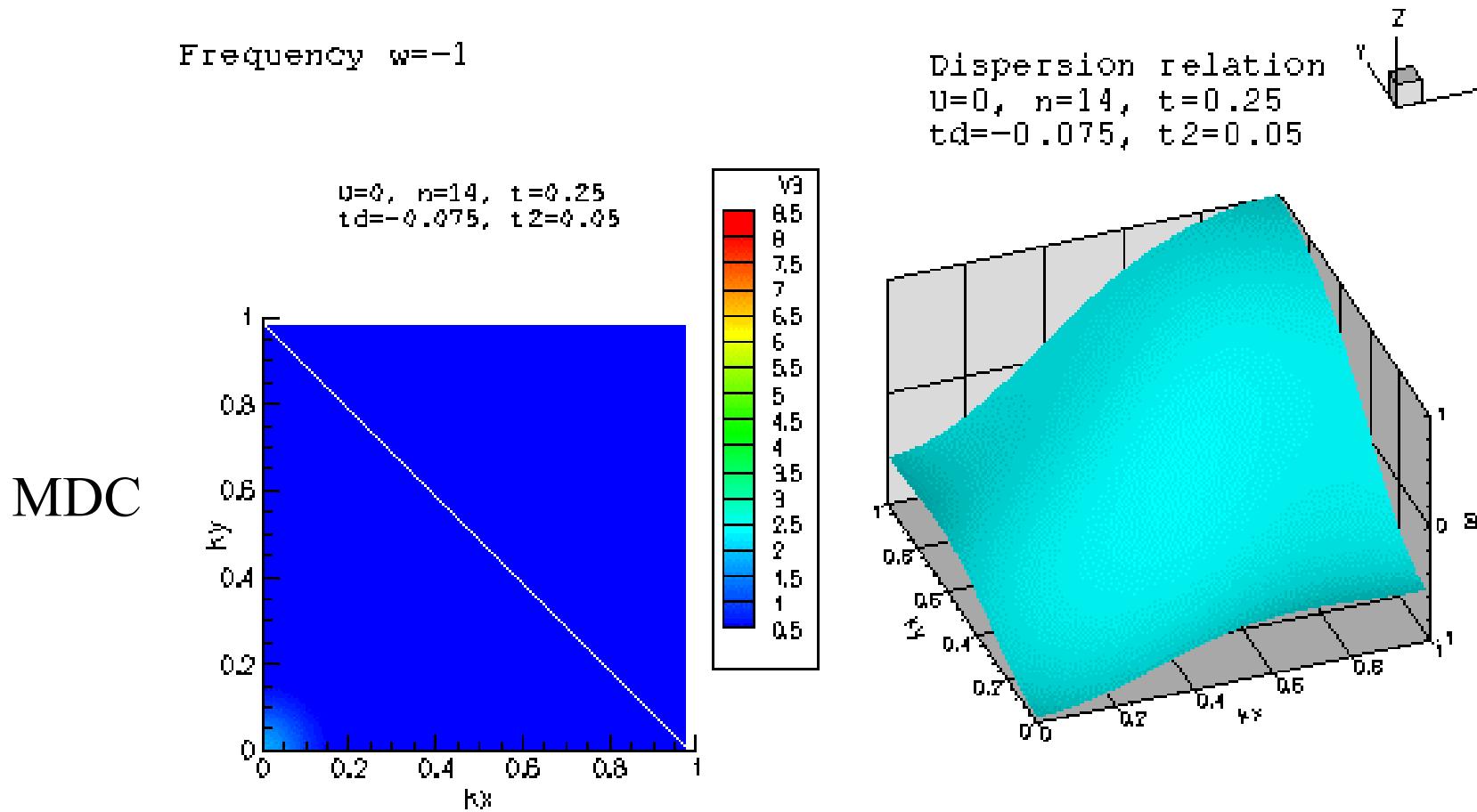
Some basic Solid State Physics



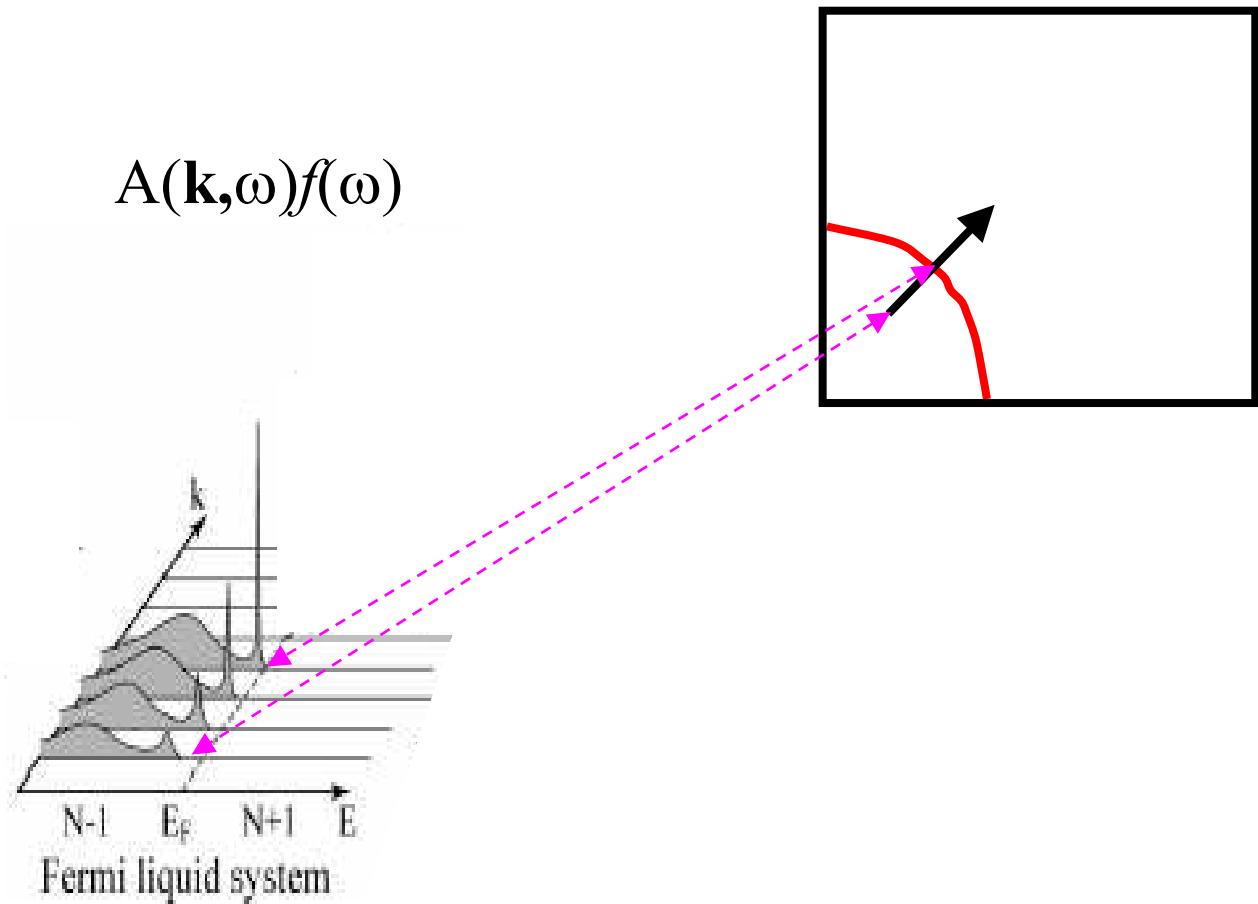
The non-interacting case



Electron-doped, non-interacting



Interacting case: The Fermi liquid



Two ways to destroy a Fermi liquid: hole and electron-doped cuprates.

- I. Introduction
 - Fermi liquid
- II. Experimental results from cuprates and model
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- IV. Weak coupling pseudogap (QMC,TPSC)
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Role of reduction in e-doped

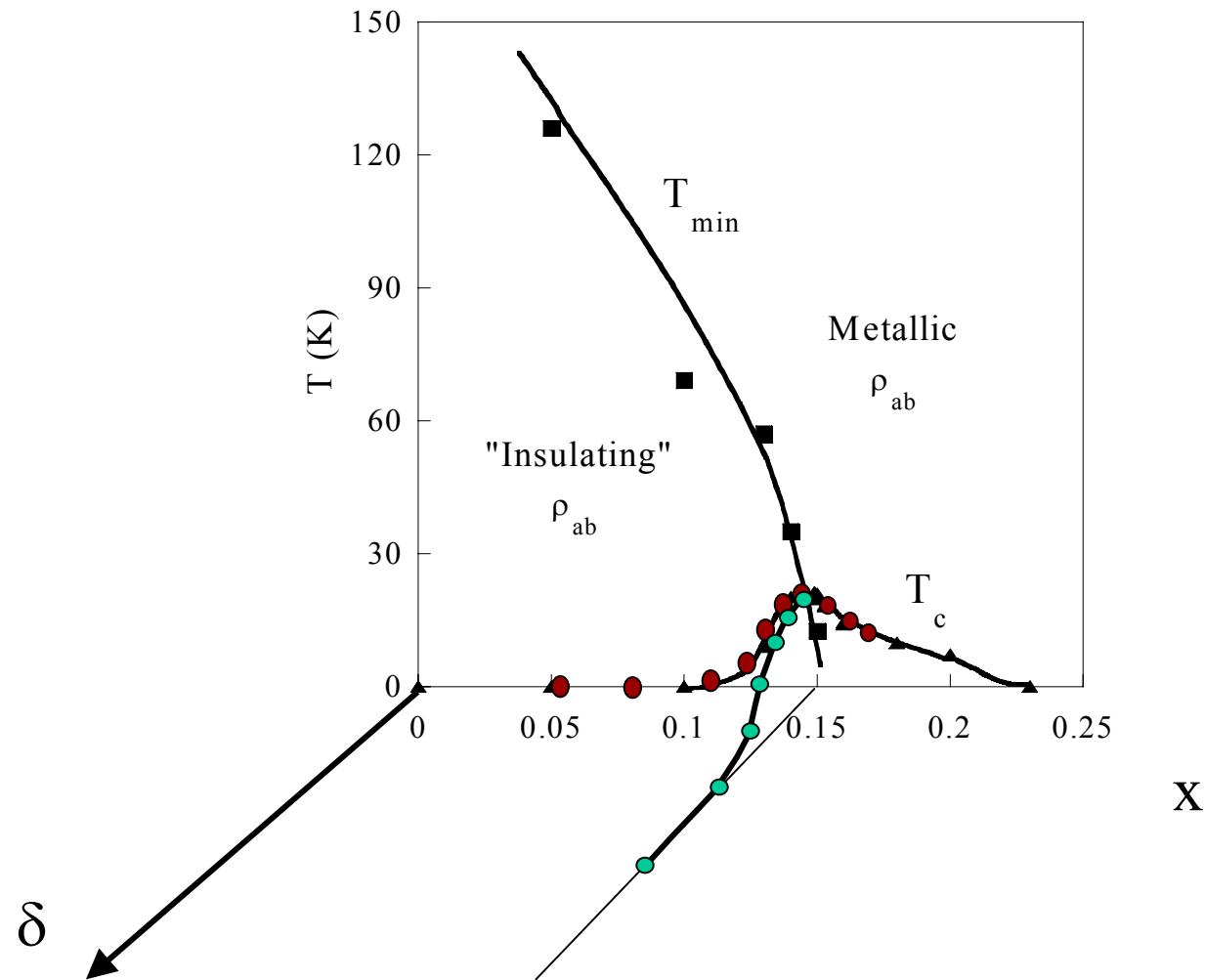
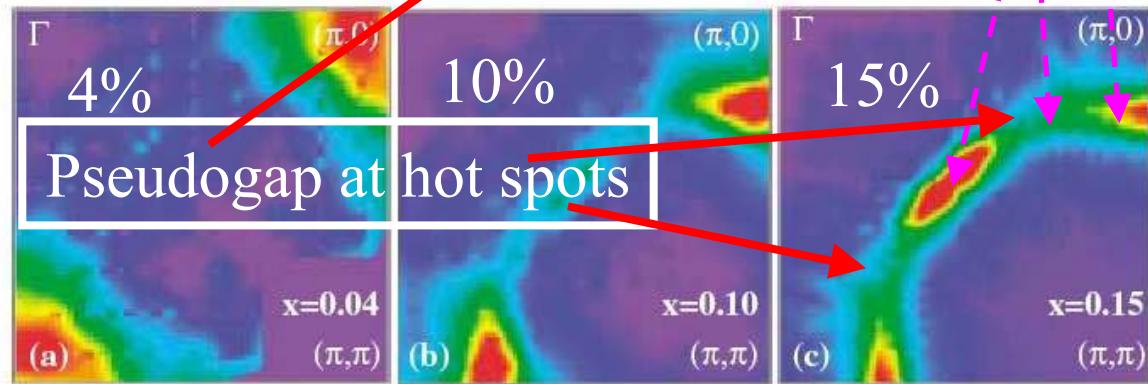
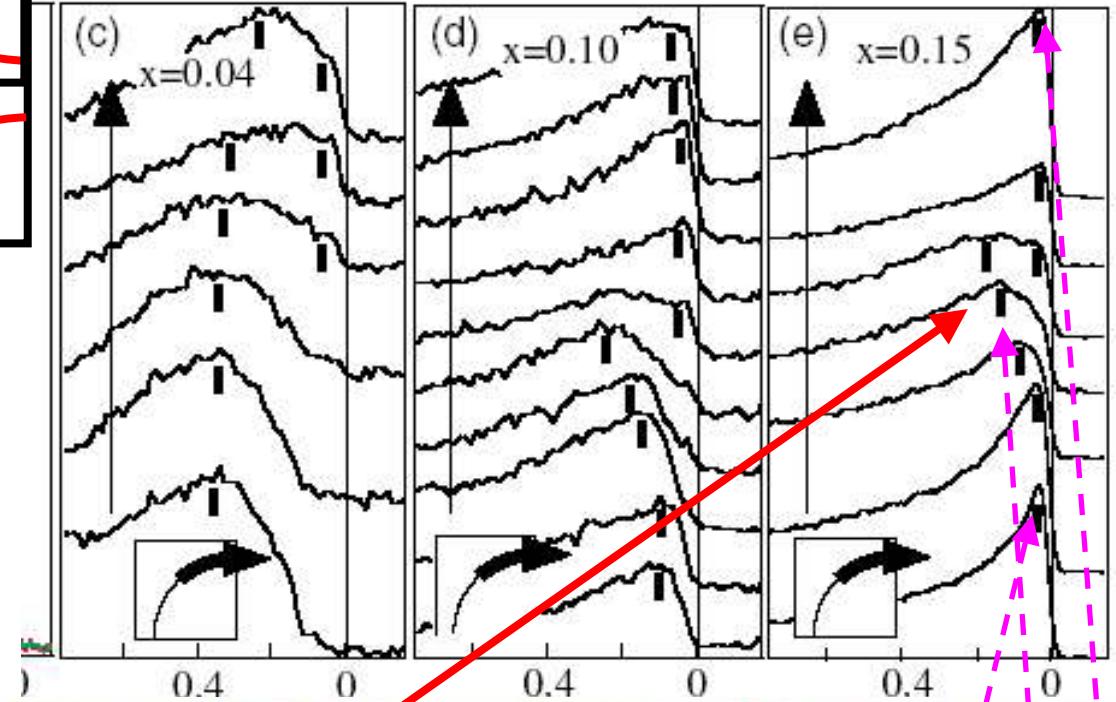
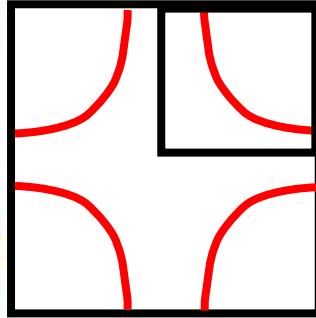
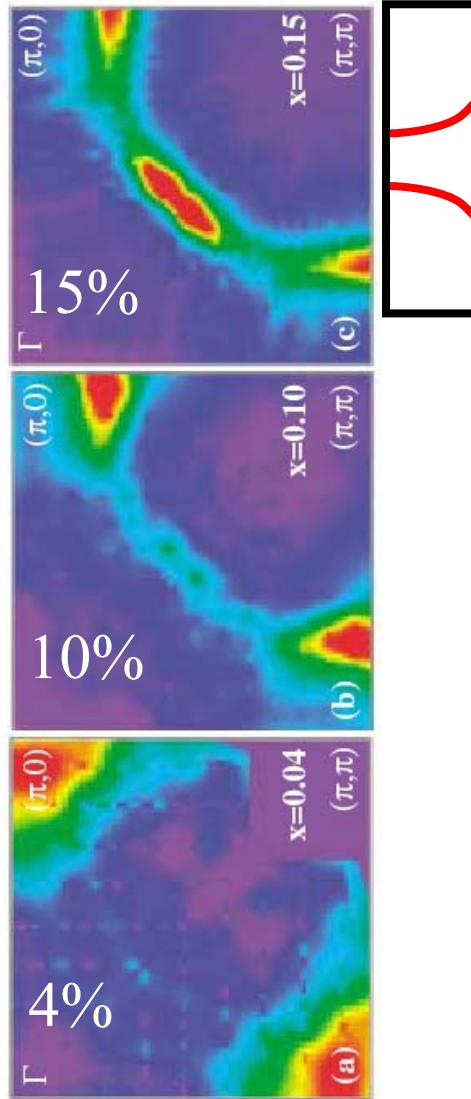


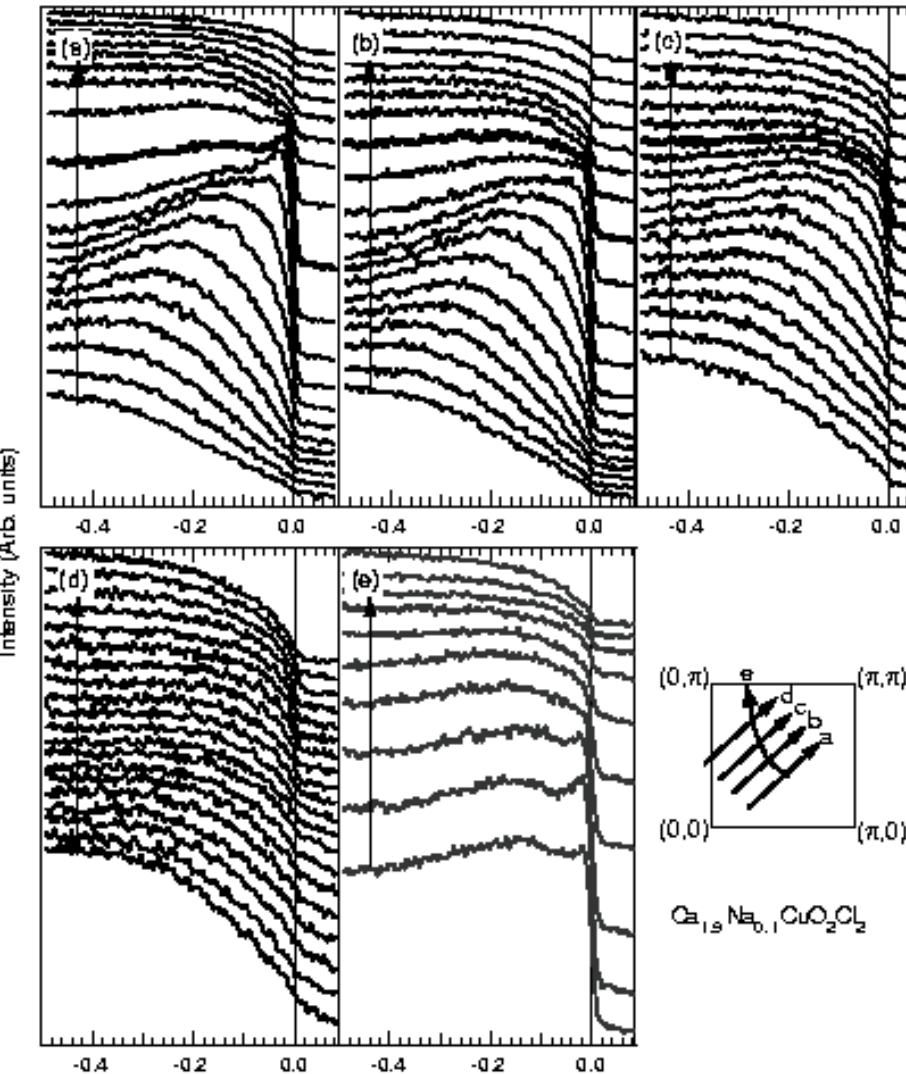
Figure provided by P. Fournier, + PRL 81, 4720 (1998).

Fermi surface, electron-doped case

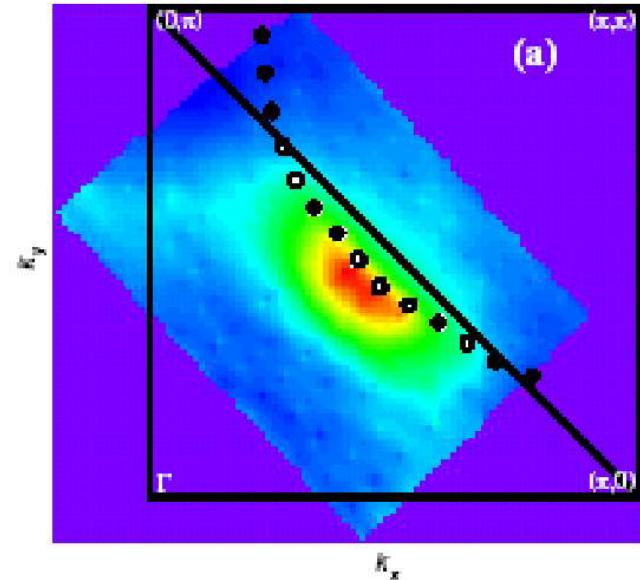
Armitage *et al.* PRL 87, 147003; 88, 257001



Fermi surface, hole-doped case 10%



Hole-doped, 10%



F. Ronning et al. Jan. 2002, $\text{Ca}_{2-x}\text{Na}_x\text{CuO}_2\text{Cl}_2$

The « Hubbard model »

**SCIENTIFIC
AMERICAN**

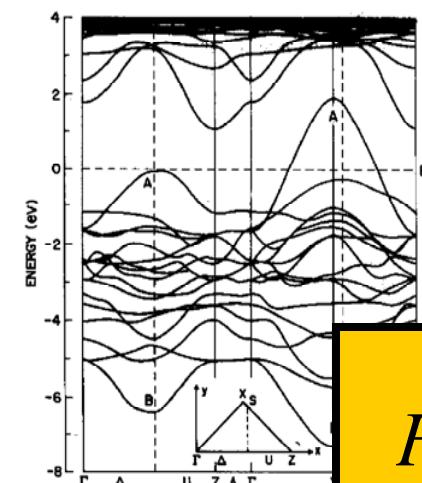
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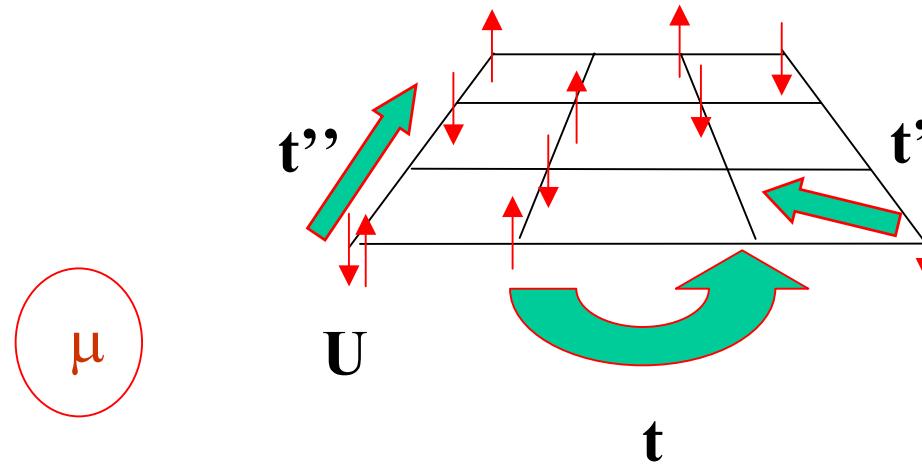


High-Temperature Superconductor belongs to a family of materials that exhibit exotic electronic properties.
 $\gamma \text{Ba}_2\text{Cu}_3\text{O}_{7-\delta}$ 9.2 - 37

LSCO



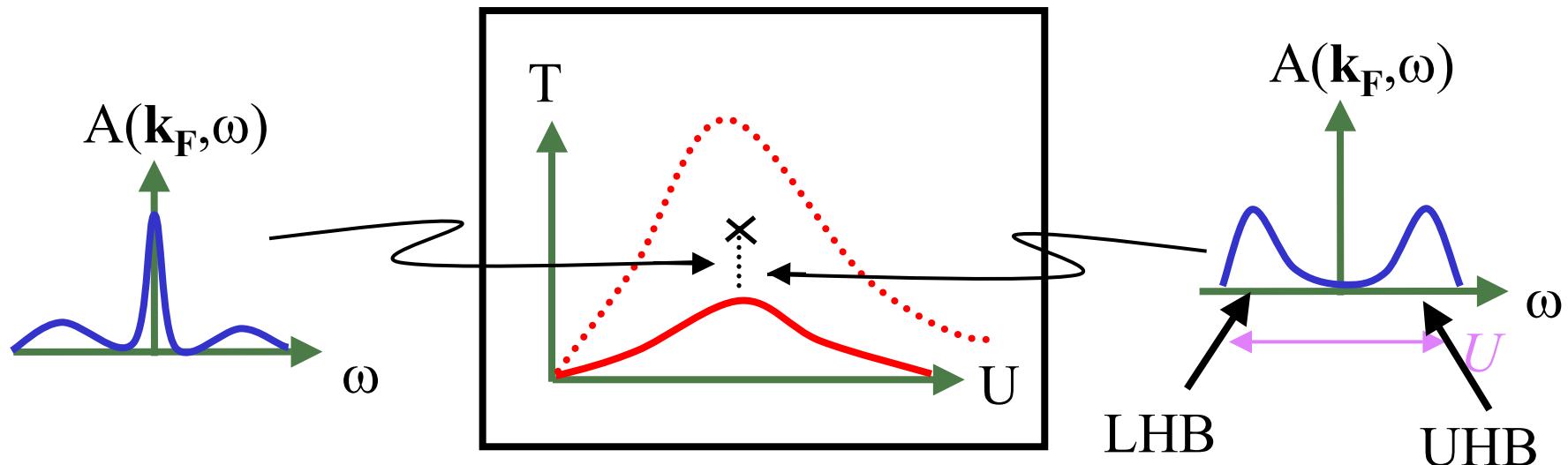
Simplest microscopic model for Cu O planes.



- Size of Hilbert space : 4^N ($N = 16$)
- With $N=16$, It takes 4 GigaBits just to store the states

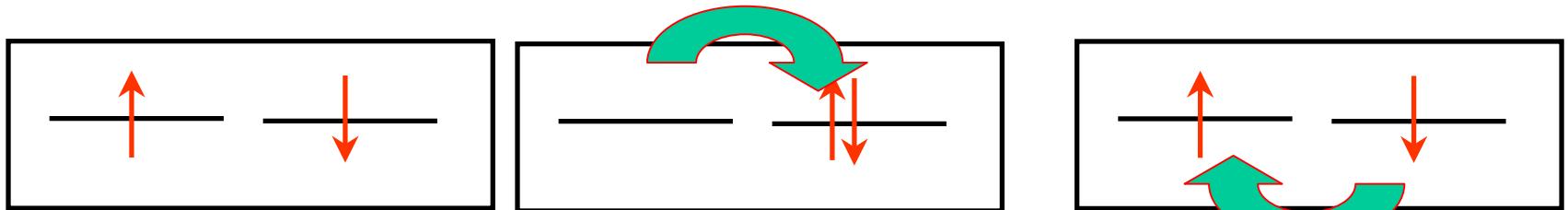
$$H = - \sum_{\langle ij \rangle \sigma} t_{ij} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

Weak vs strong coupling, $n=1$



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

Mott transition



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

Question: quantitative and qualitative

- How do we go from a Mott insulator to a conductor as a function of doping?
- Hot spots and pseudogaps in the Hubbard model (like experiment) ?
- Close to understood in e-doped case.

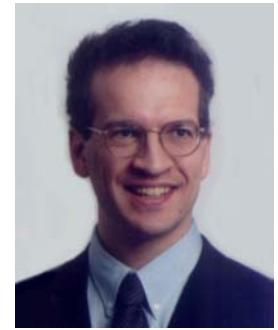
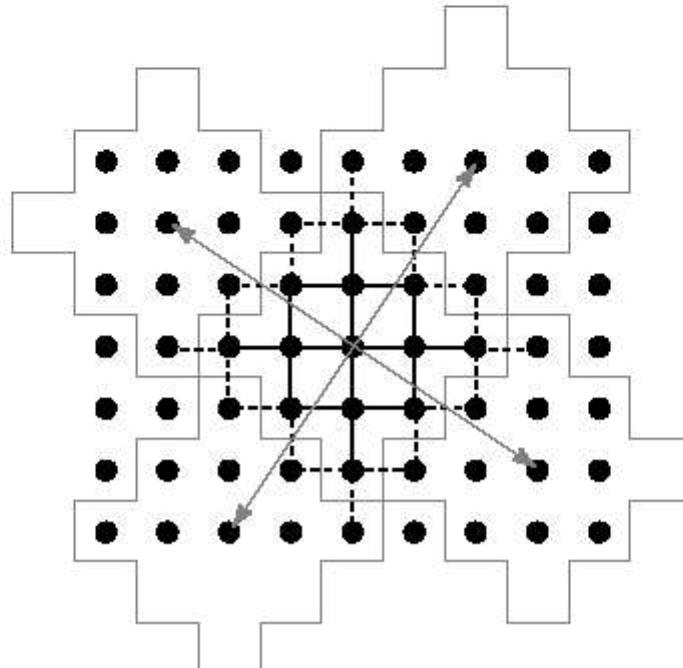
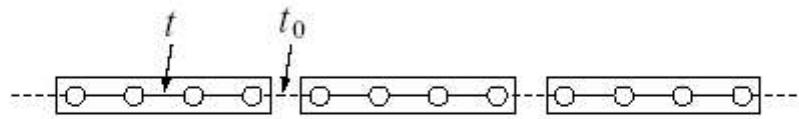
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Cluster perturbation theory (CPT)

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

Vary
cluster
shape and
size

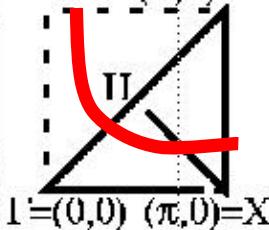


CPT

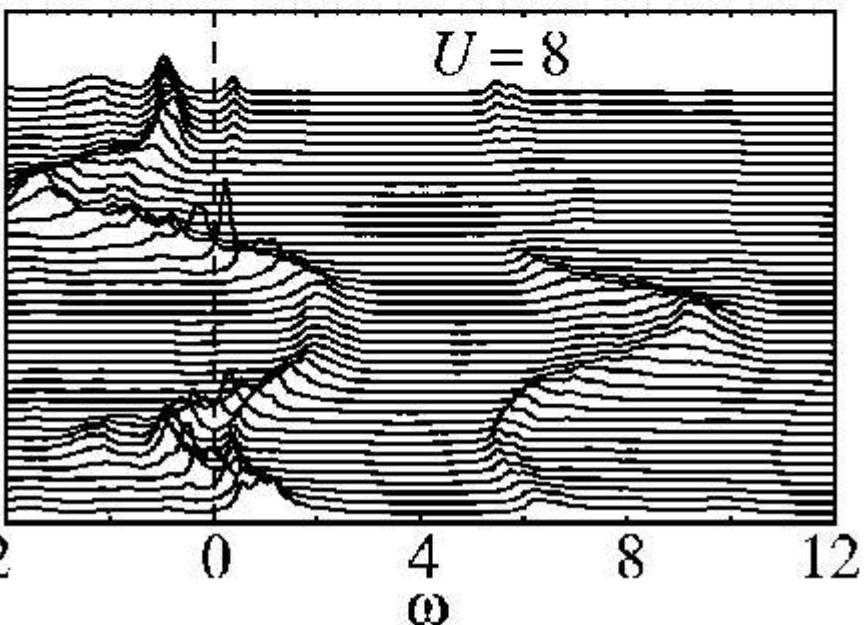
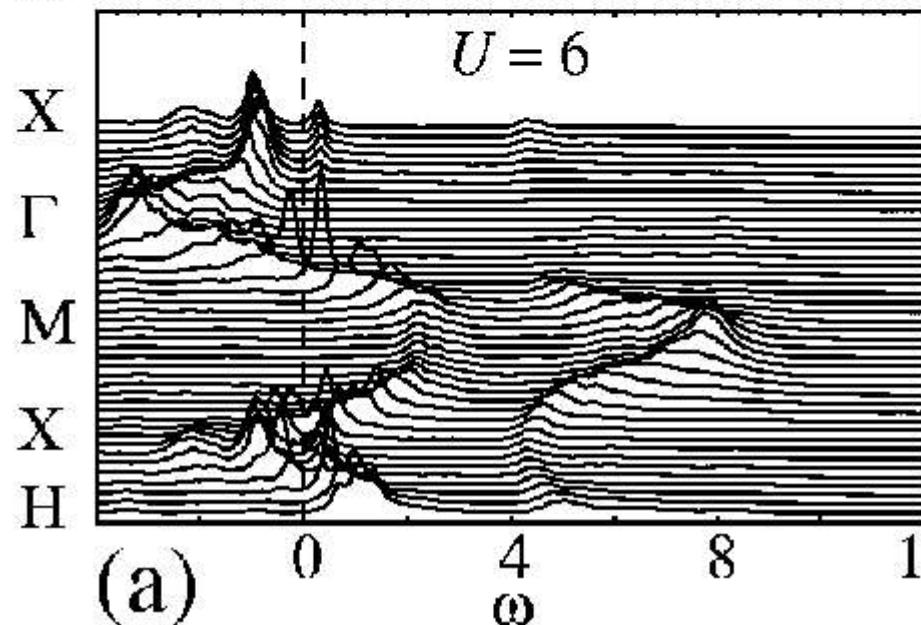
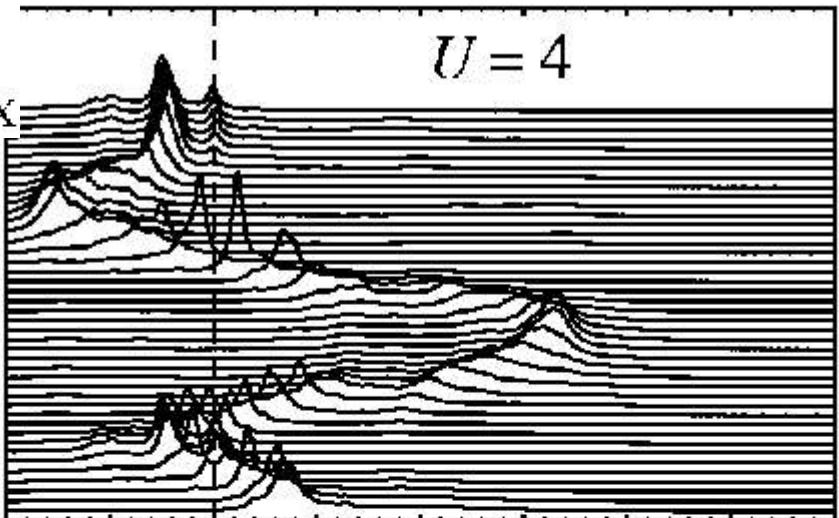
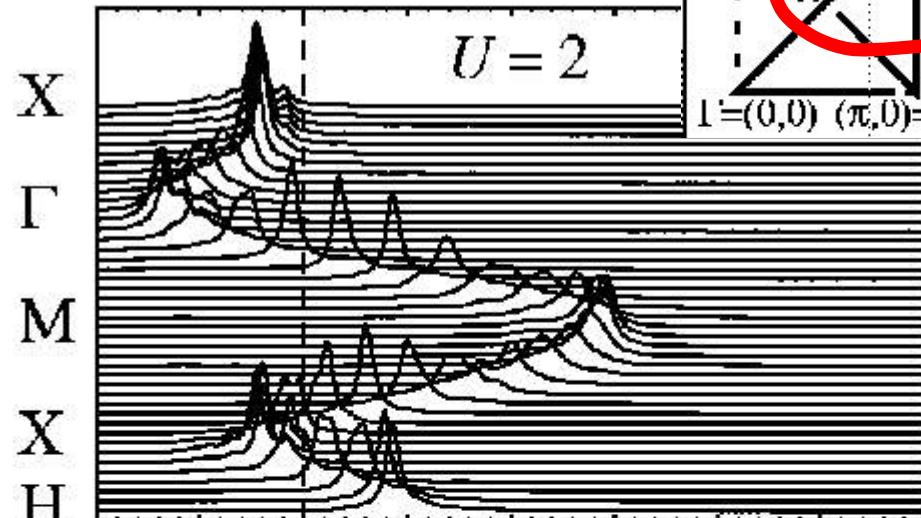
- Wave vector is continuous
 - Underlying cluster 3×4 and 4×4
- Exact for $(t=0, U \text{ finite})$ and $(U=0, t \text{ finite})$
- Finite energy resolution
 - Here about 40 meV (as in experiment).
- Tests:
 - spin-charge separation in $d = 1$.
 - $U=\text{infinity}$ limit.

Hole-doped (17%)

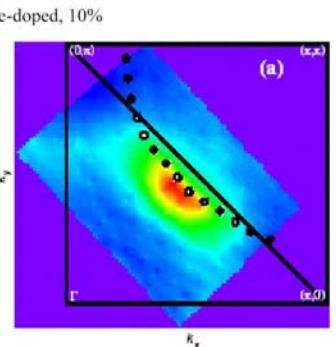
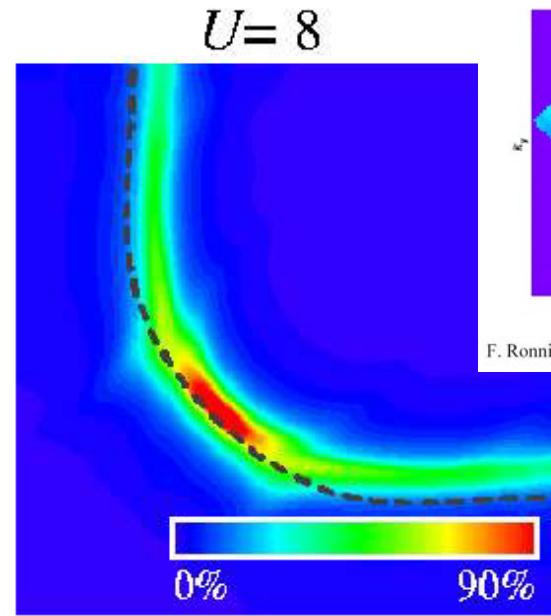
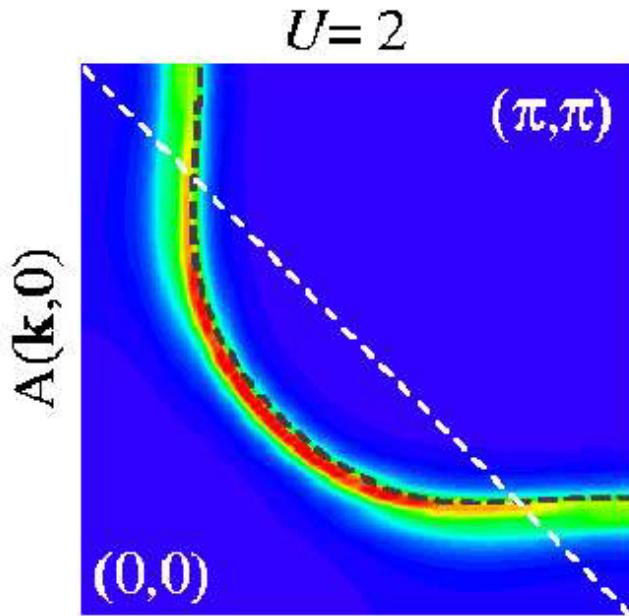
$$t' = -0.3t \quad , \quad t'' = 0.2t$$



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



Hole-doped (17%)

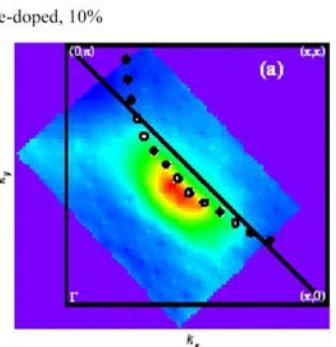
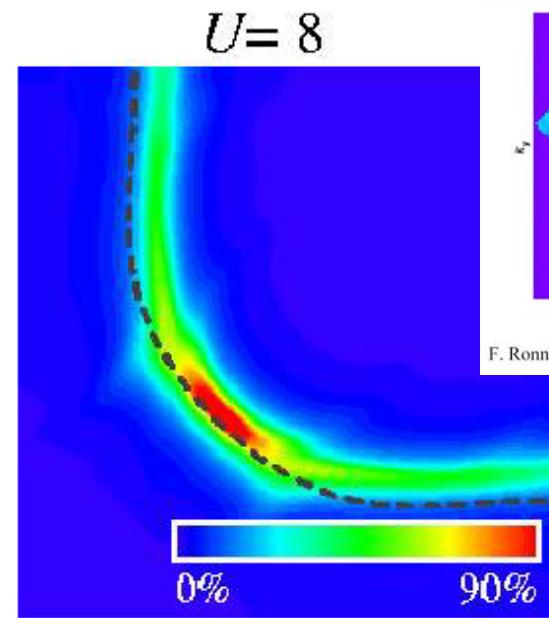
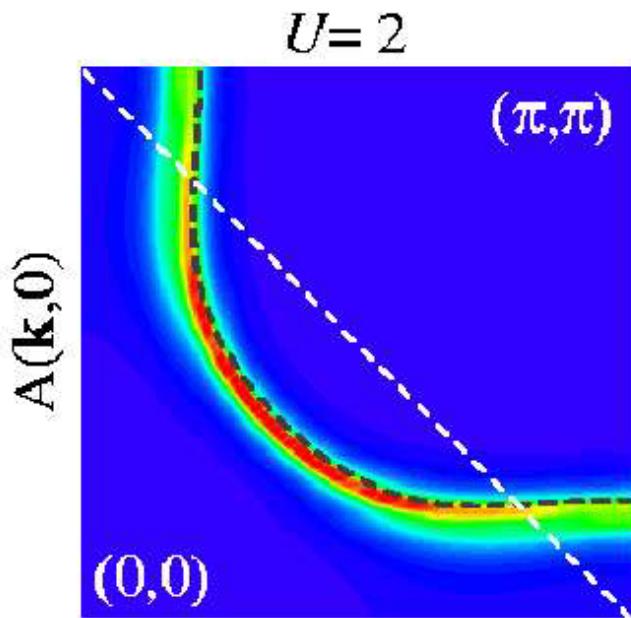


F. Ronning et al. Jan. 2002, $\text{Ca}_{2-x}\text{Na}_x\text{CuO}_2\text{Cl}_2$

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

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

Hole-doped (17%)

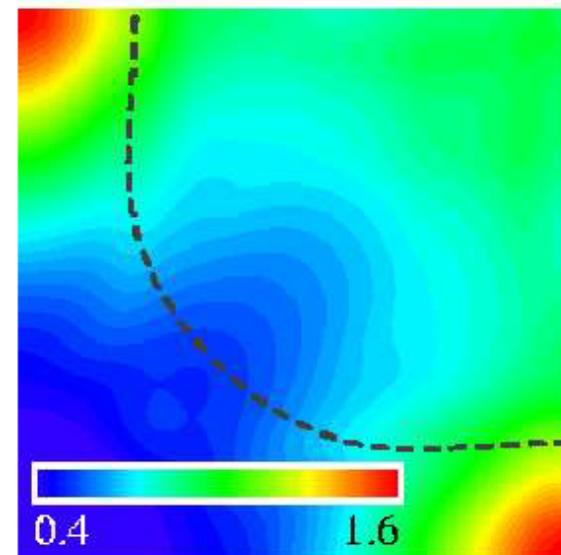


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$$t' = -0.3t$$
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$$\eta = 0.12t$$
$$\eta = 0.4t$$

$\text{Im } \Sigma(\mathbf{k}, 0)$



Sénéchal, AMT, PRL 92, 126401 (2004).

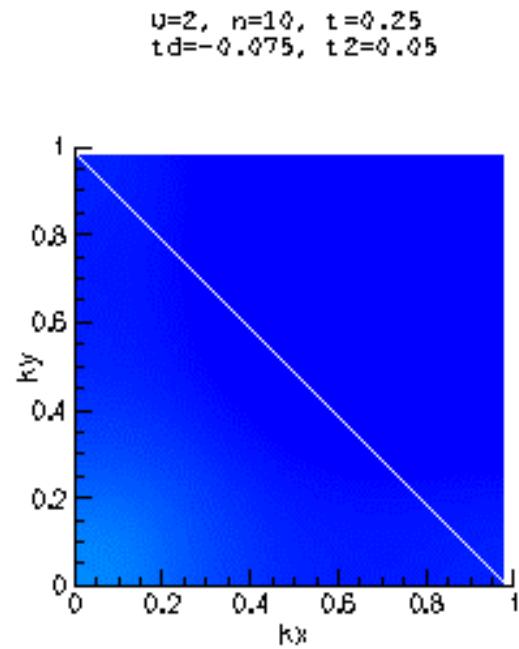
Hole-doped 17%, $U=8t$

$U=8$

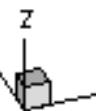
Frequency $\omega=-1$

$U=2, n=10, t=0.25$
 $t_d=-0.075, t_2=0.05$

0% 90%

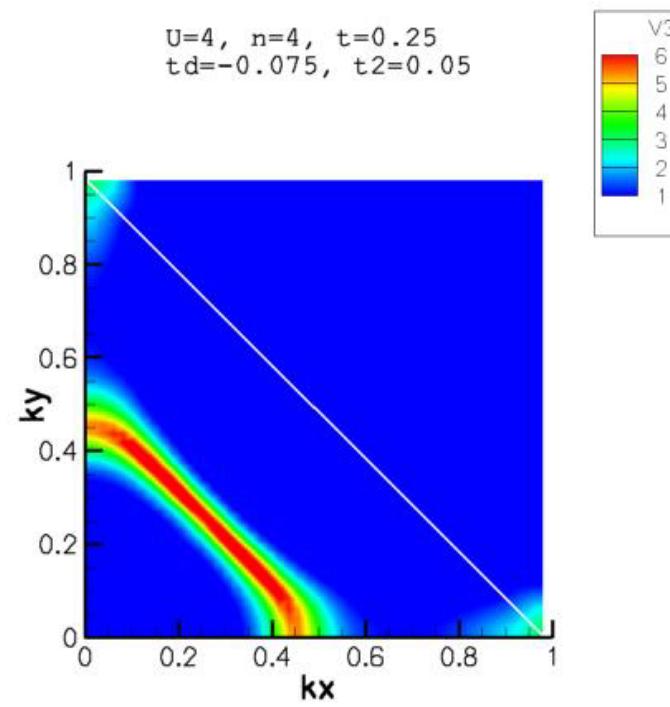


Dispersion relation
 $U=0, n=10, t=0.25$
 $t_d=-0.075, t_2=0.05$

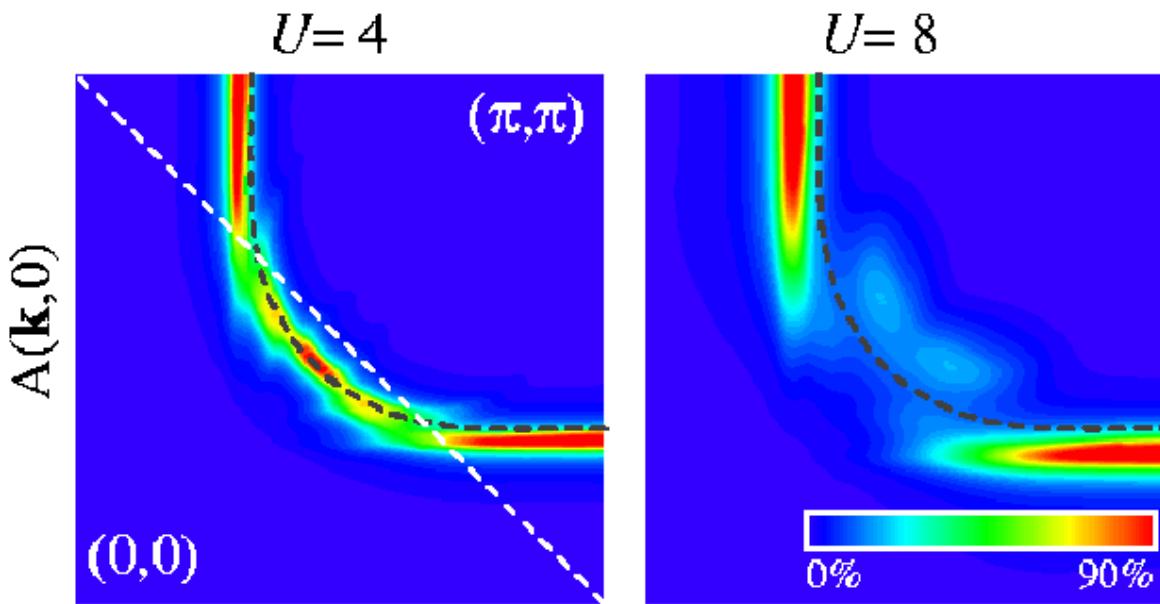


Hole doped, 75%, $U = 16 t$

Frequency $w=6.245e-17$



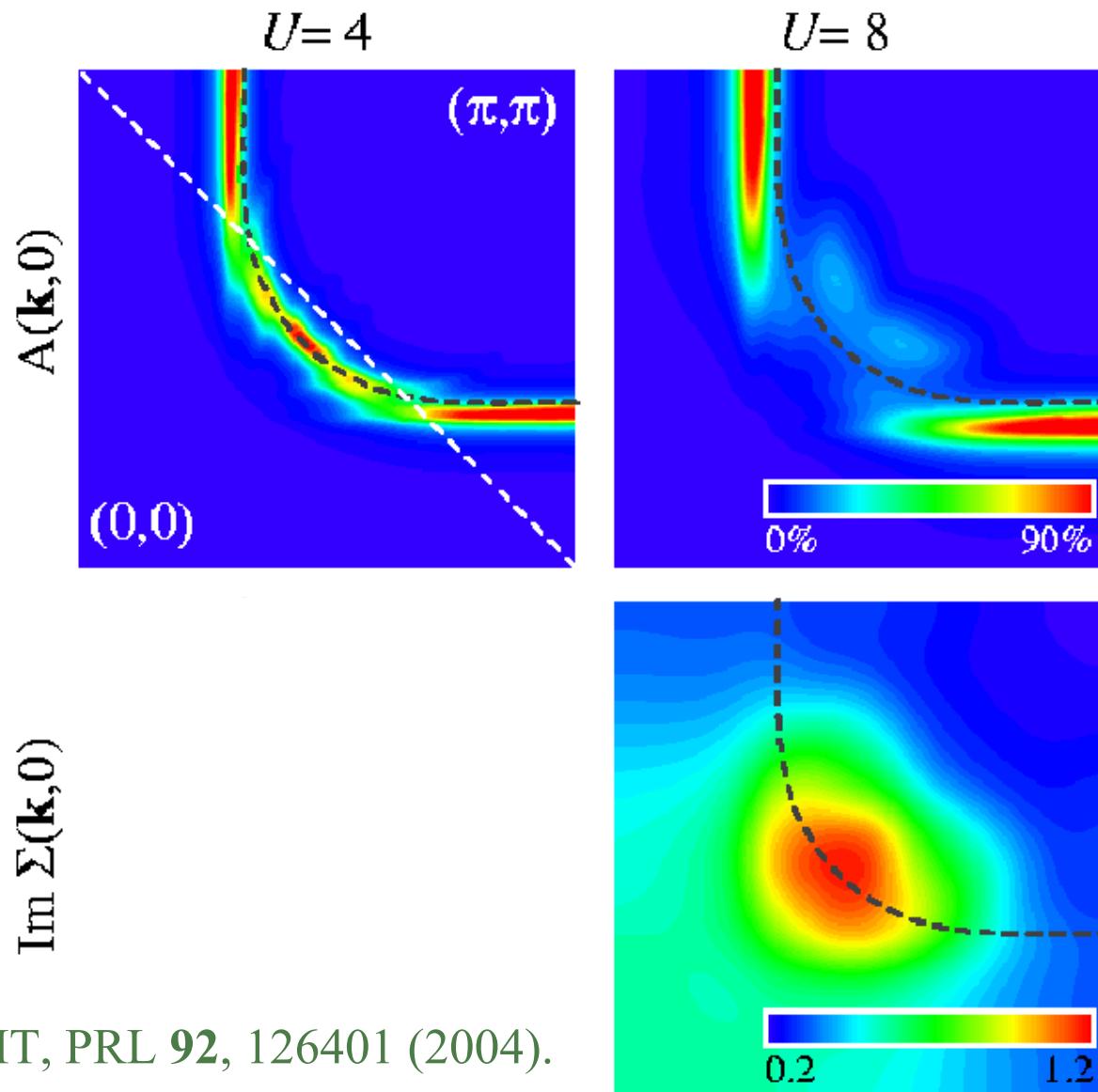
Electron-doped (17%)



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

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

Electron-doped (17%)

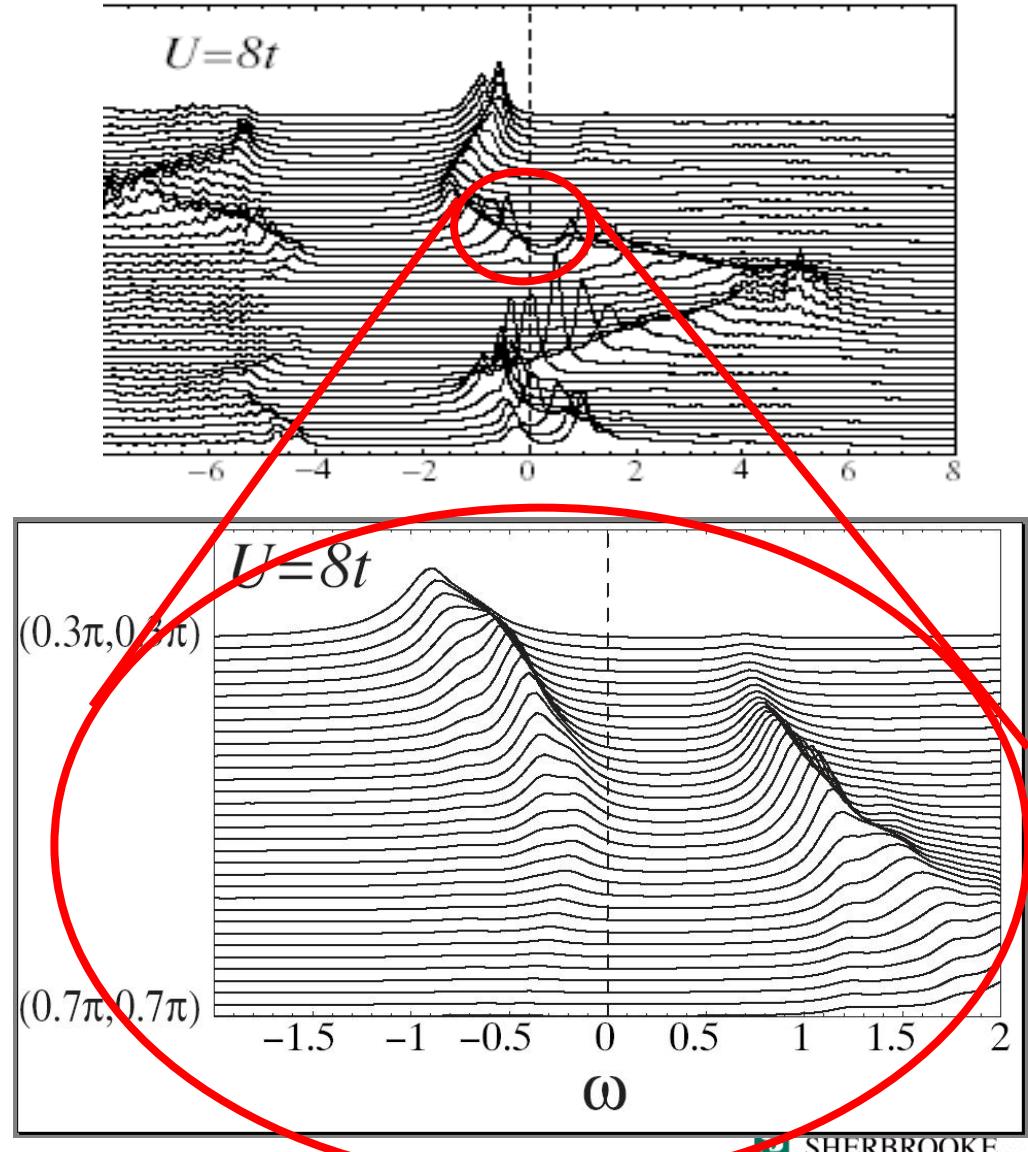
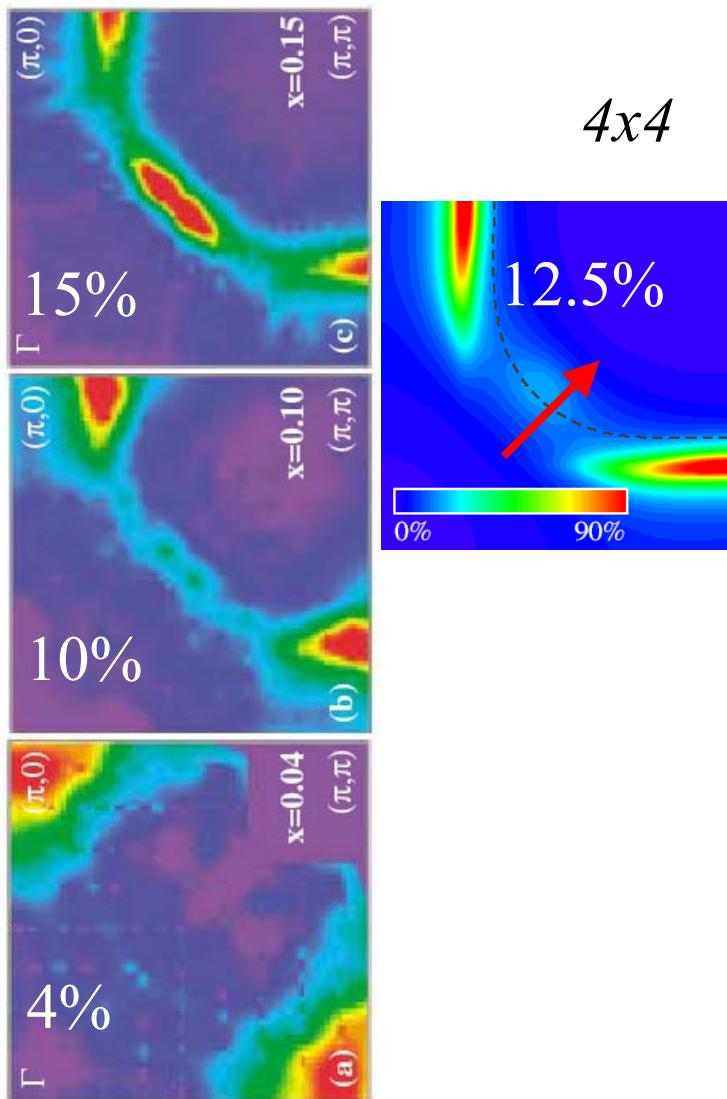


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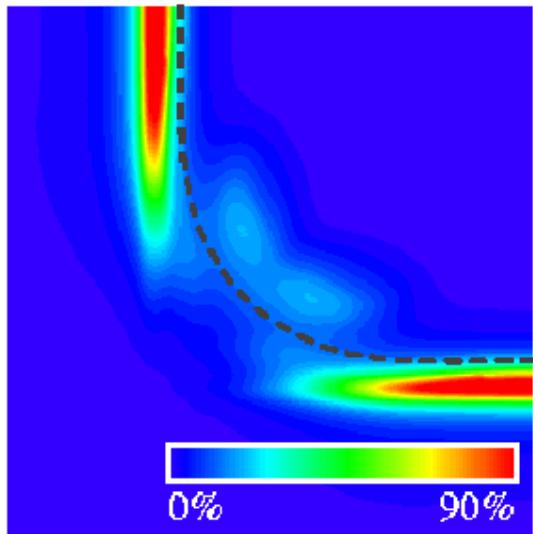
Sénéchal, AMT, PRL **92**, 126401 (2004).

Electron-doped 12.5%, $U=8t$

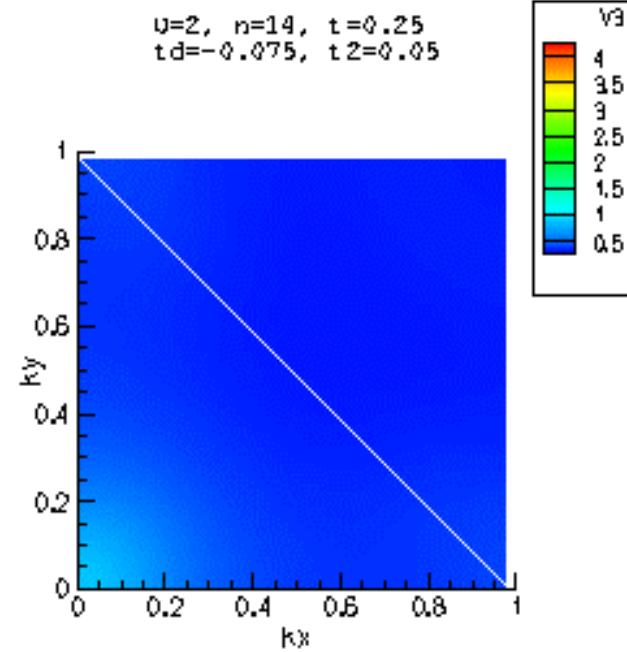


Electron-doped, 17%, $U=8t$

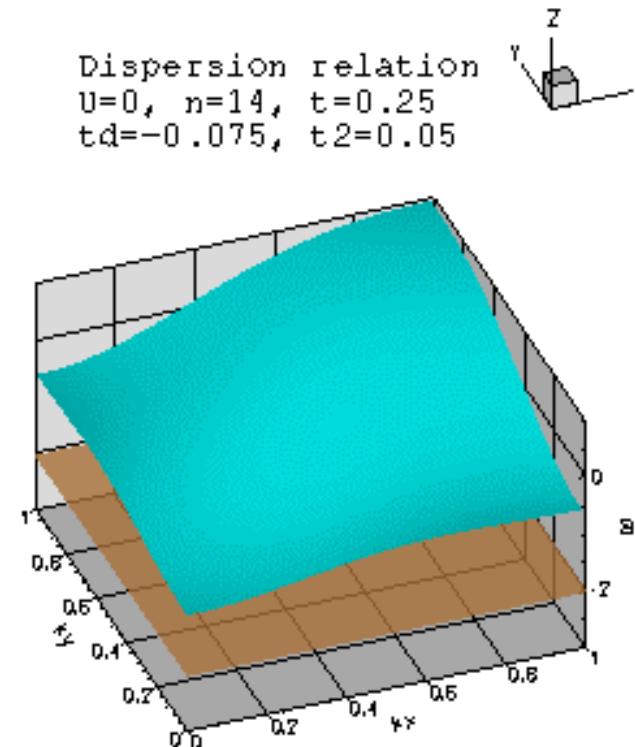
$U=8$



Frequency $\omega=-2$

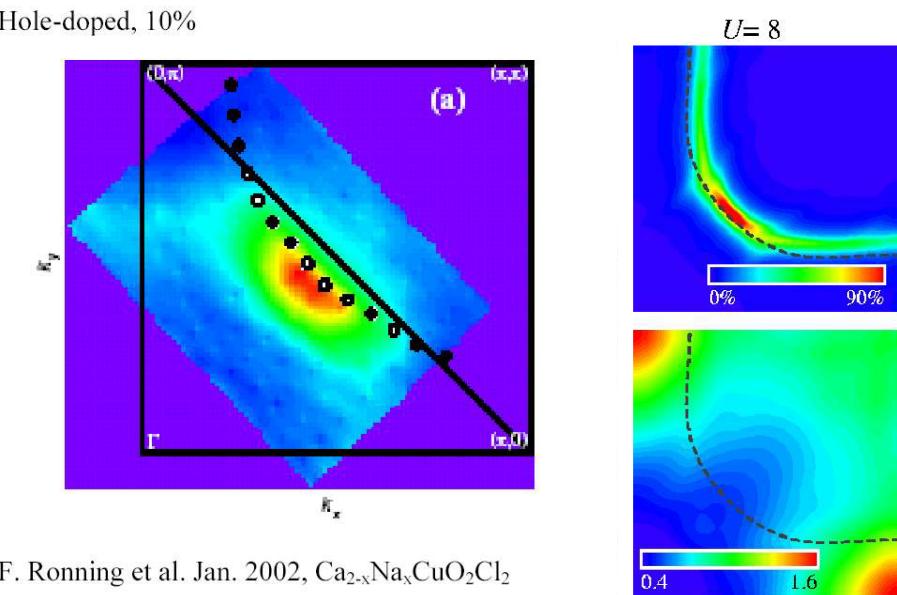


Dispersion relation
 $U=0$, $n=14$, $t=0.25$
 $t_d=-0.075$, $t_2=0.05$



Strong coupling pseudogap ($U > 8t$)

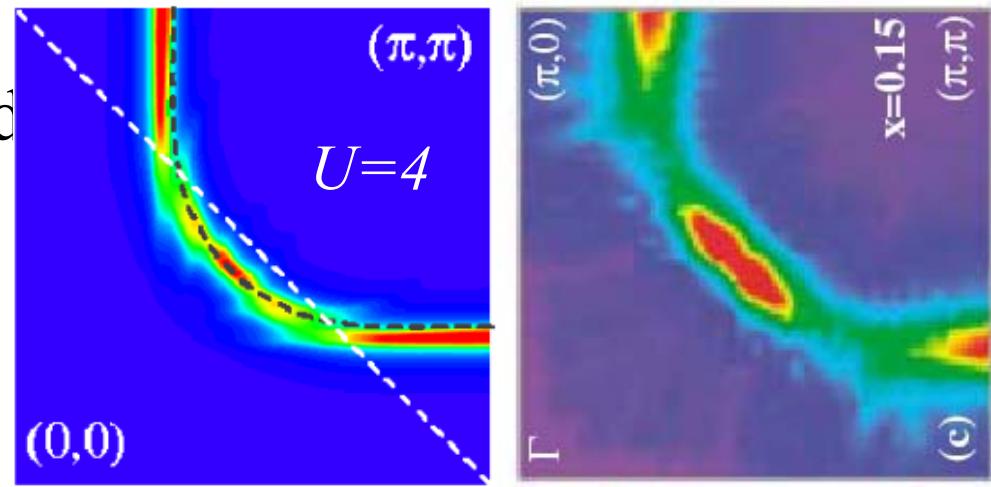
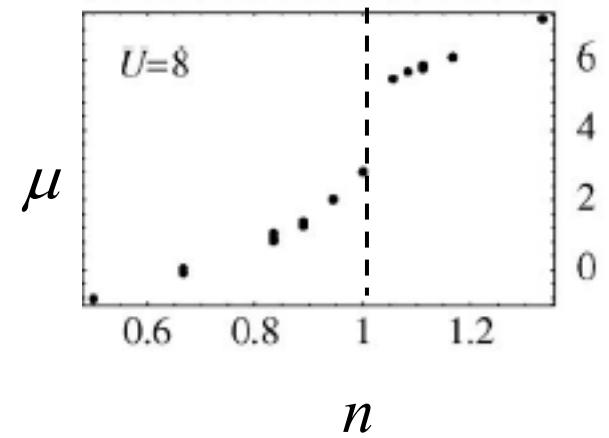
- Mott gap local (all k) not tied to $\omega=0$.
- Pseudogap tied to $\omega=0$ and only in regions nearly connected by (π,π) . (e and h),
- Pseudogap is independent of cluster shape (and size) in CPT.
- Not caused by AFM LRO
 - No LRO, few lattice spacings.
 - Not very sensitive to t'
 - Scales like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



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
 $U(n) \sim d\mu/dn$

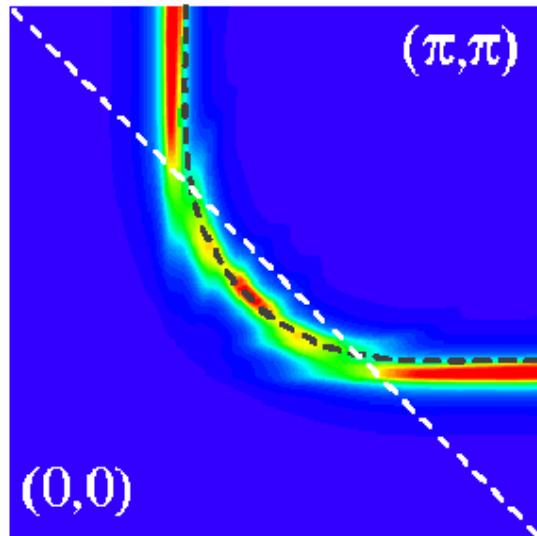


Sénéchal, AMT, PRL **92**, 126401 (2004).

Electron-doped, 17%, $U=4t$

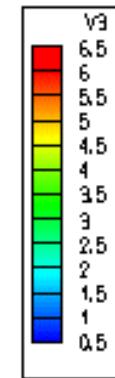
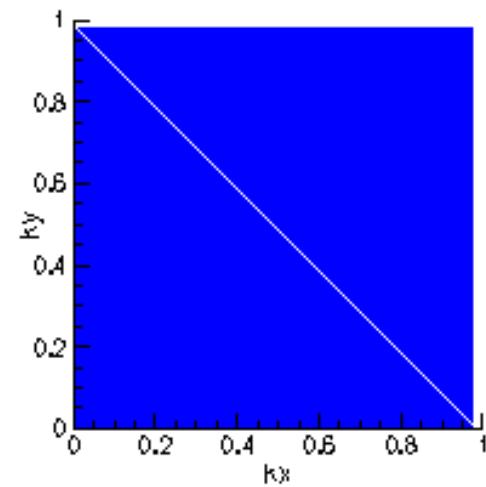
$U=4$

$A(\mathbf{k}, 0)$

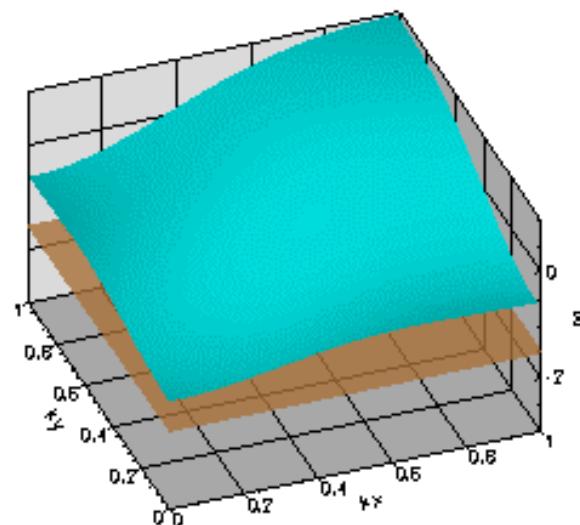
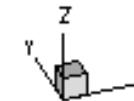


Frequency $w=-1.5$

$U=1, n=14, t=0.25$
 $t_d=-0.075, t_2=0.05$



Dispersion relation
 $U=0, n=14, t=0.25$
 $t_d=-0.075, t_2=0.05$



Electron-doped cuprates : where theory and experiment meet

- I. Introduction
 - Fermi liquid
- II. Experimental results from cuprates and model
- III. Strong and weak coupling pseudogap (CPT)
- **IV. Weak coupling pseudogap (QMC,TPSC)**
- V. d-wave superconductivity
- VI. Conclusion

Theory difficult even at weak to intermediate coupling!

- RPA
 - Mermin-Wagner
 - Pauli ~~X~~
- Moryia
 - Adjustable parameters: c and U_{eff}
- FLEX
 - No pseudogap
 - Pauli ~~X~~

Two-Particle Self-Consistent Approach ($U < W$)

- How it works

- General philosophy
 - Drop diagrams
 - Impose constraints and sum rules and ask to satisfy them.
 - Pauli principle
 - Conservation laws
 - Local moment and local density sum-rules
- Get for free:
 - Mermin-Wagner theorem
 - Kanamori-Brückner screening

Vilk, AMT J. Phys. I France, 7, 1309 (1997); Allen et al.in *Theoretical methods for strongly correlated electrons* also cond-mat/0110130

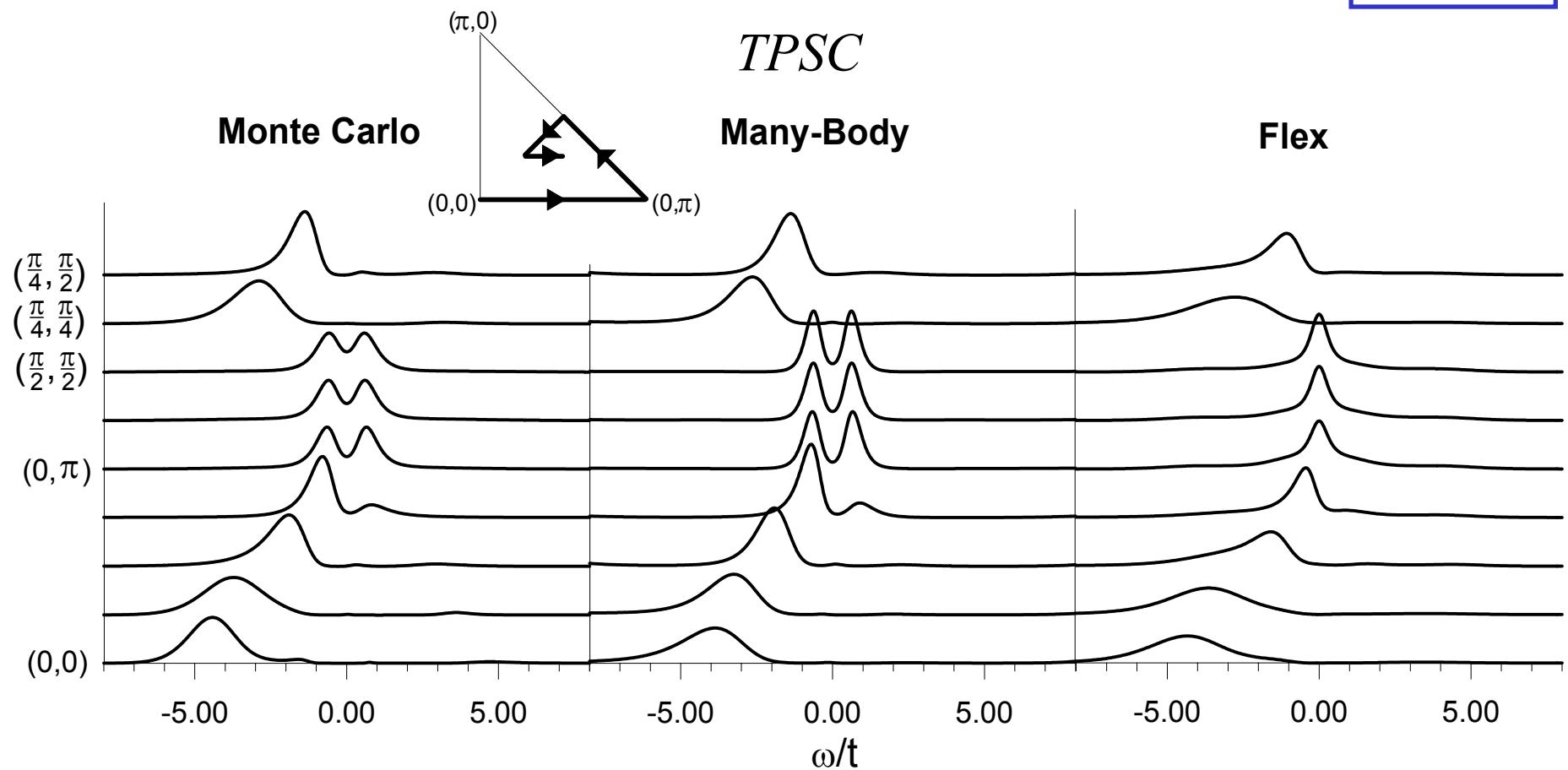
(Mahan, third edition)

Quantum Monte Carlo

- **Use as benchmark for TPSC**
- Advantages
 - Sizes much larger than exact diagonalizations
 - As accurate as needed
- Disadvantages
 - 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).

TPSC approach: two steps

I: Two-particle self consistency

1. Functional derivative formalism (conservation laws)

(a) analog of the Bethe-Salpeter equation:

$$\chi_{sp} = \frac{\delta G}{\delta \phi} = GG + GU_{sp}\chi_{sp}G$$

(b) spin vertex: $U_{sp} = \frac{\delta \Sigma_\uparrow}{\delta G_\downarrow} - \frac{\delta \Sigma_\uparrow}{\delta G_\uparrow}$

(c) self-energy:

$$\Sigma_\sigma(1, \bar{1}; \{\phi\}) G_\sigma(\bar{1}, 2; \{\phi\}) = -U \langle c_{-\sigma}^\dagger(1^+) c_{-\sigma}(1) c_\sigma(1) c_\sigma^\dagger(2) \rangle_\phi$$

$\approx A_{\{\phi\}} G_{-\sigma}^{(1)}(1, 1^+; \{\phi\}) G_\sigma^{(1)}(1, 2; \{\phi\})$

2. Factorization

TPSC...

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

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

3. The F.D. theorem and Pauli principle

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

II: Improved self-energy

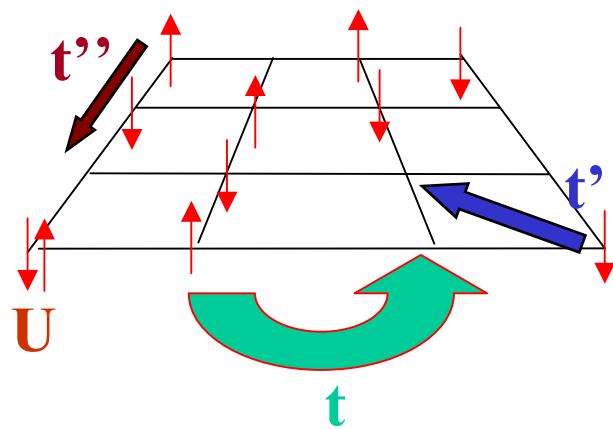
Insert the first step results

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

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

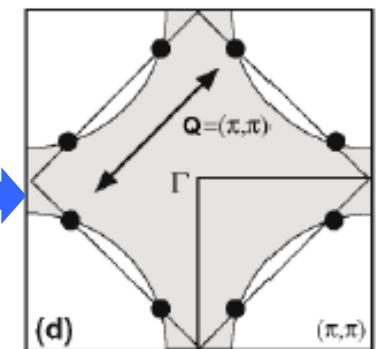
The 2D Hubbard model

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



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

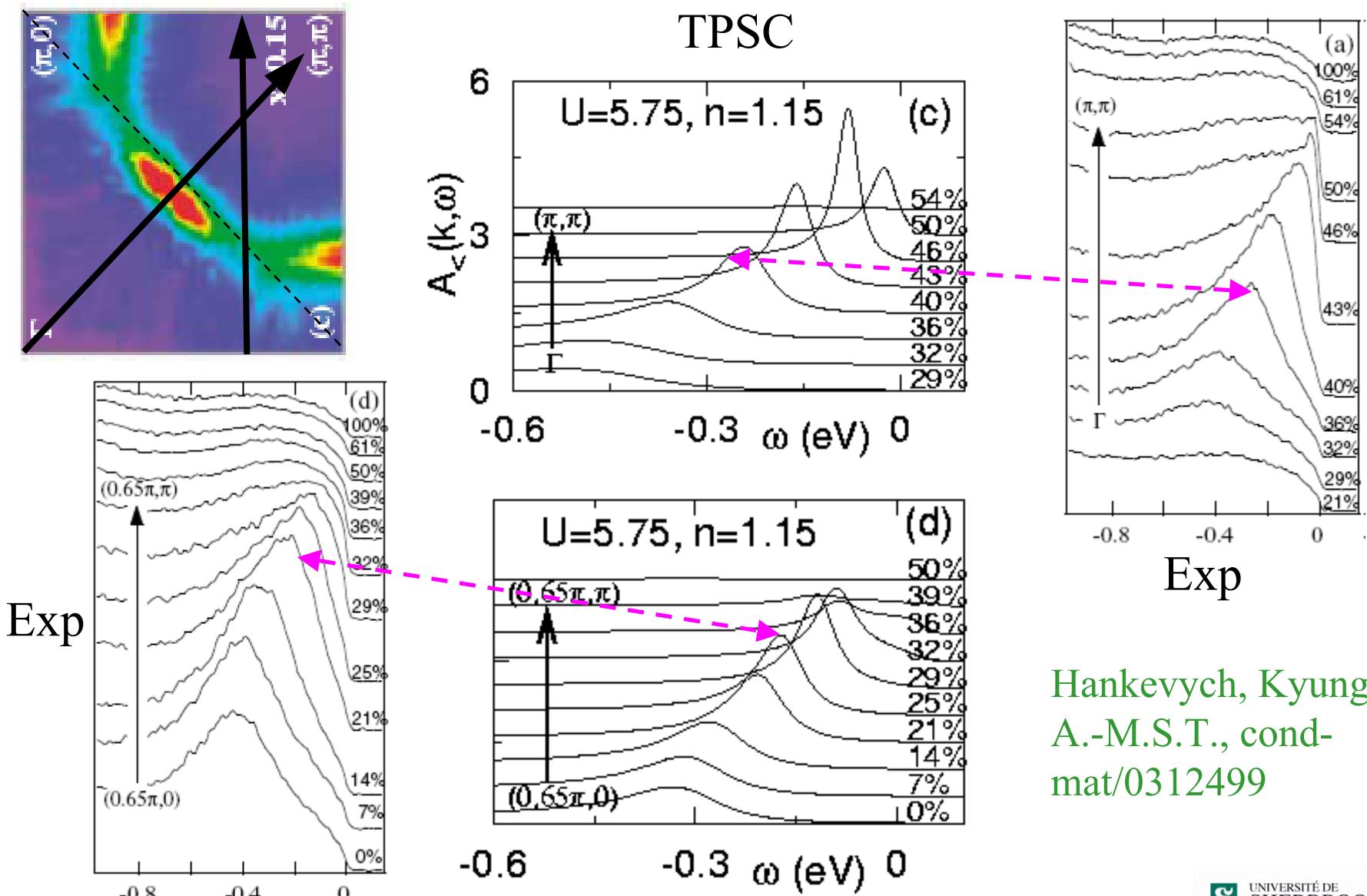
fixed



Weak coupling $U < 8t$

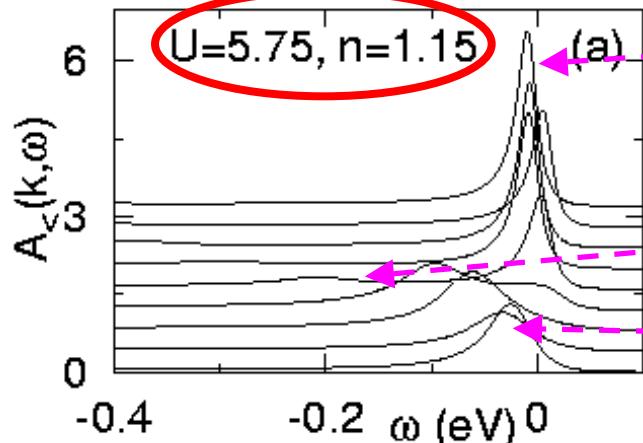
$n = 1 + x$ – electron filling

15% doped case: EDCs in two directions



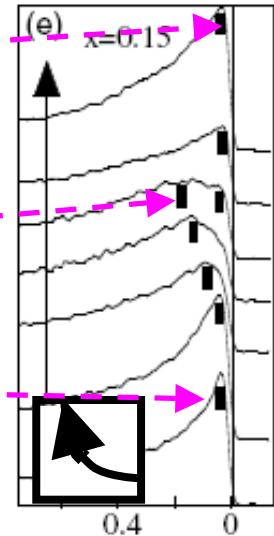
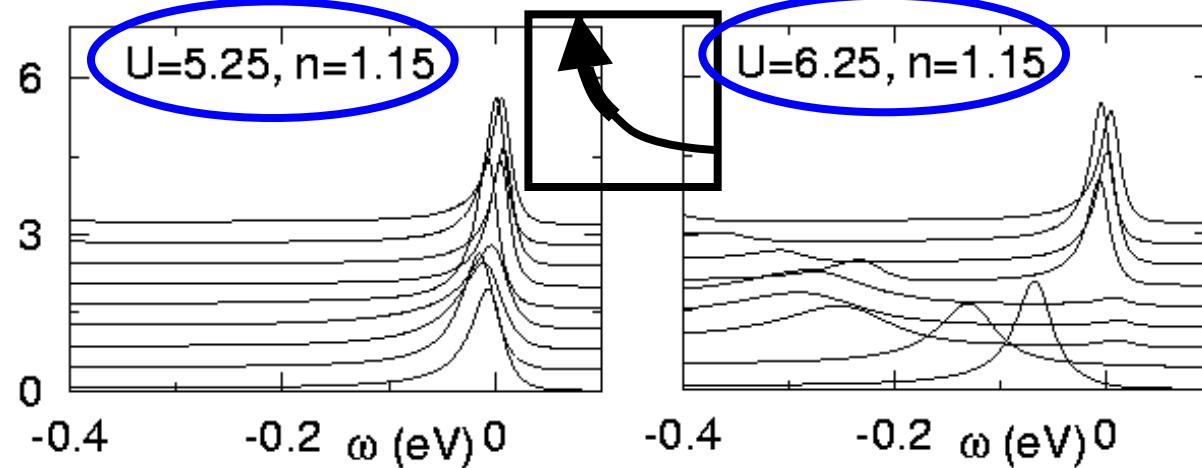
Hankevych, Kyung,
A.-M.S.T., cond-
mat/0312499

15% doping: EDCs along the Fermi surface TPSC

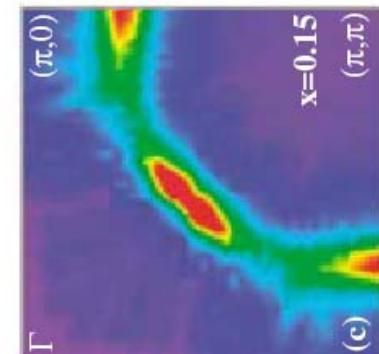


$$U_{min} < U < U_{max}$$

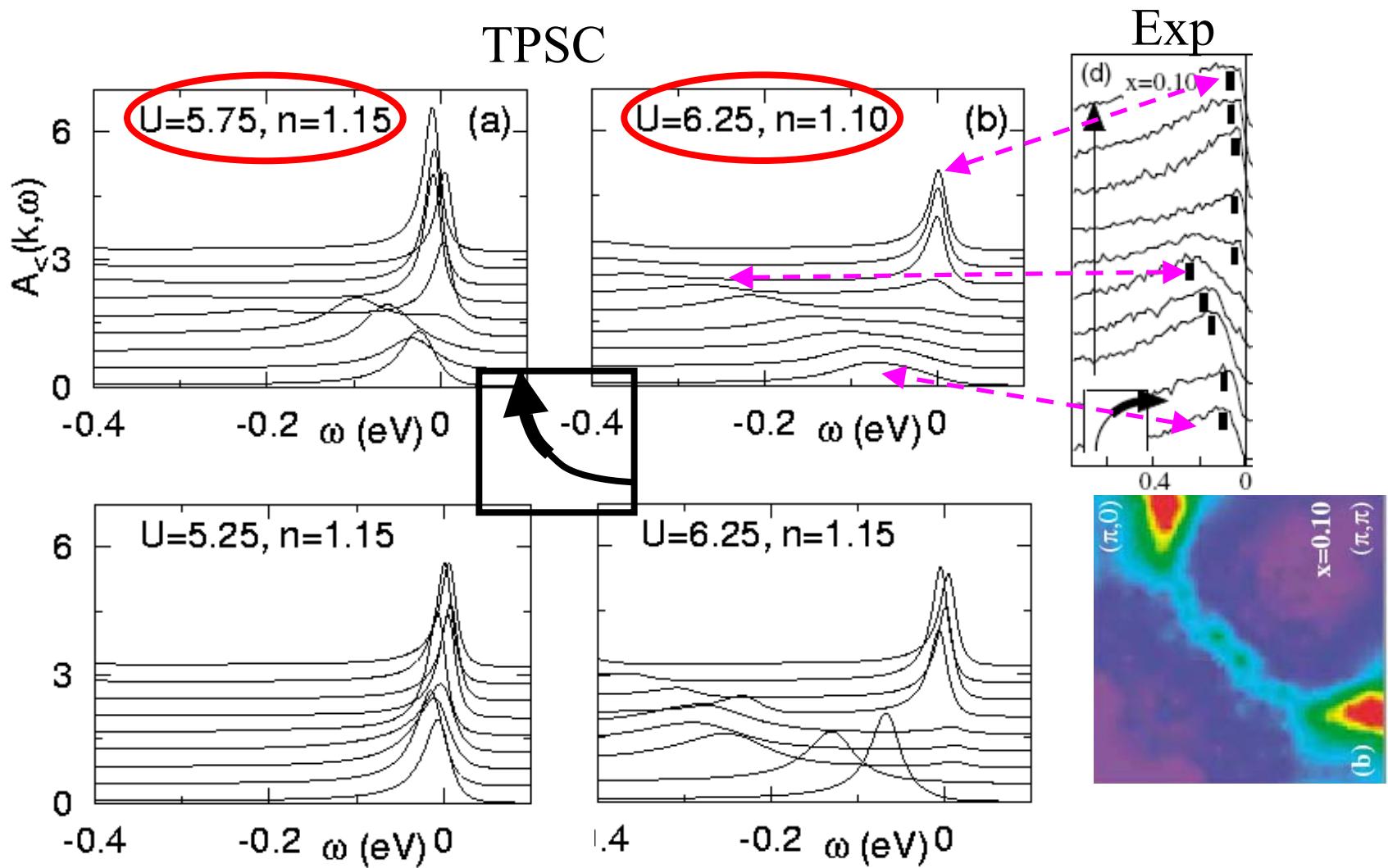
U_{max} also from CPT



Exp

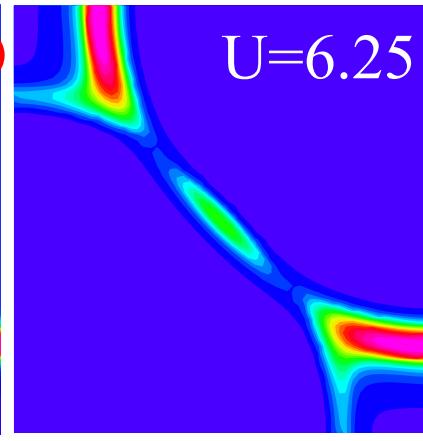
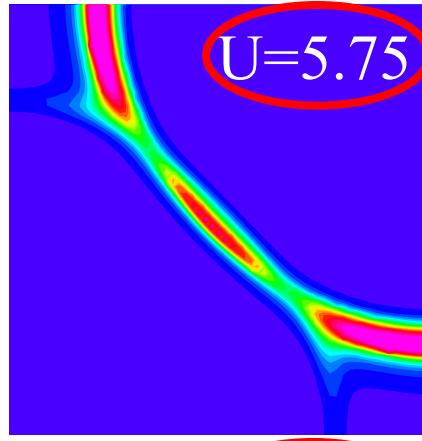
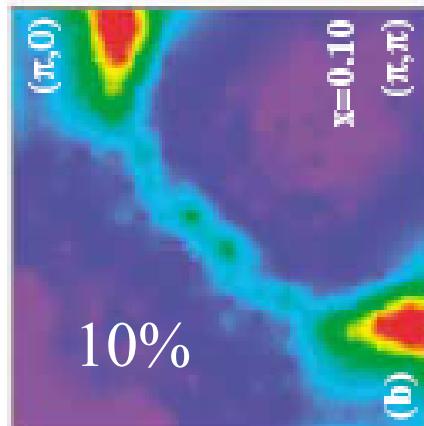
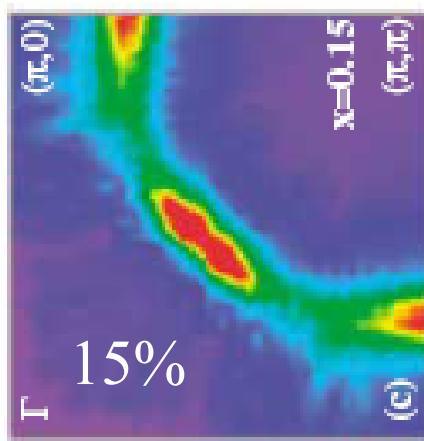


EDCs along the Fermi surface TPSC



Fermi surface plots

Hubbard repulsion U has to...

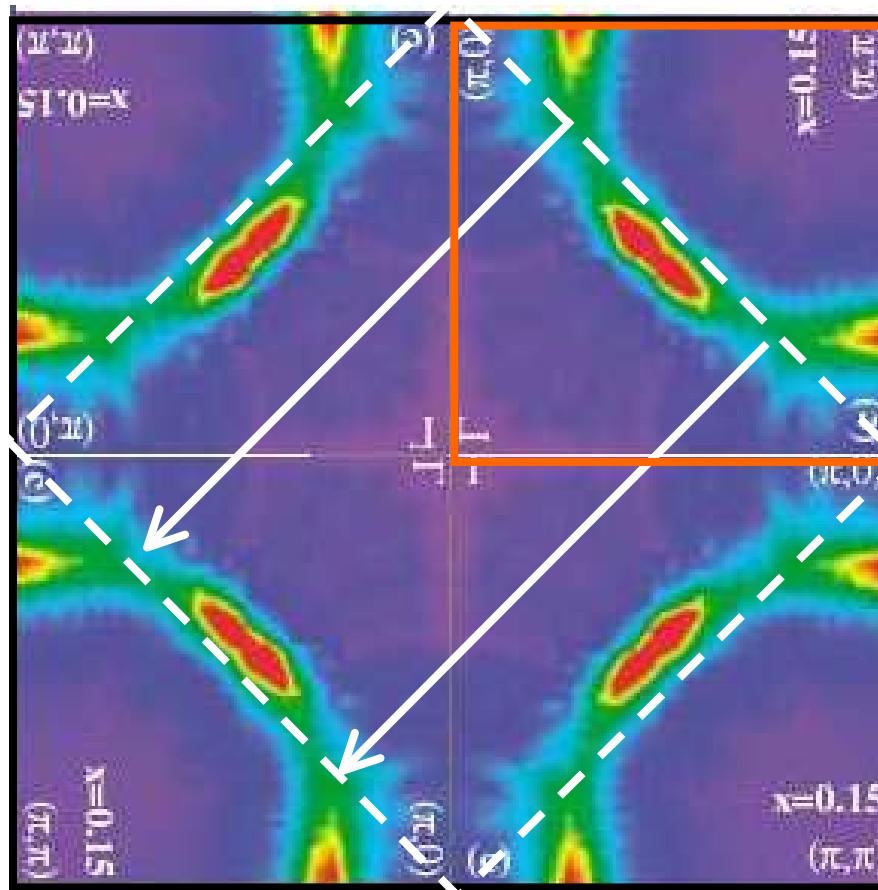


be not too large

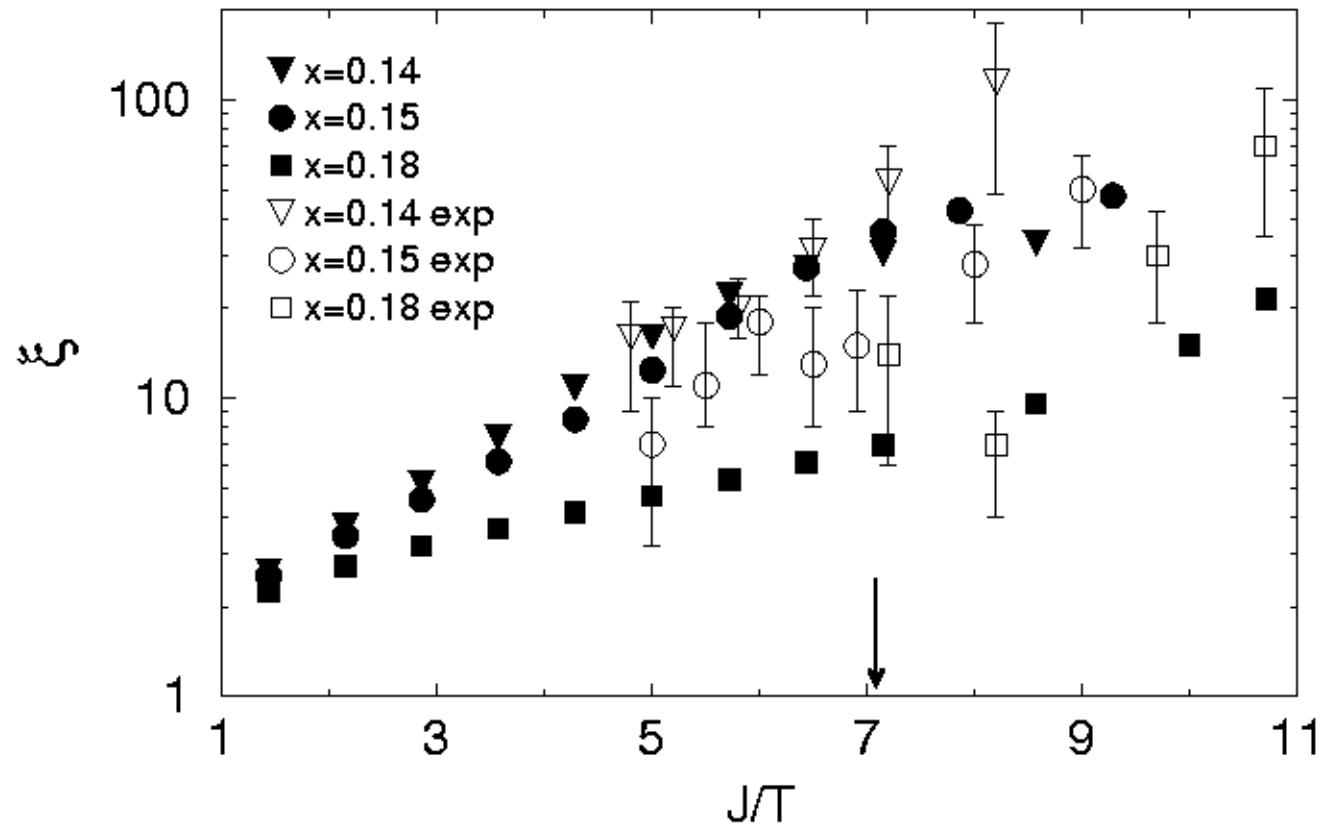


increase for
smaller doping

Hot spots from AFM quasi-static scattering



AFM correlation length (neutron)



Hankevych, Kyung, A.-M.S.T., cond-mat/0312499

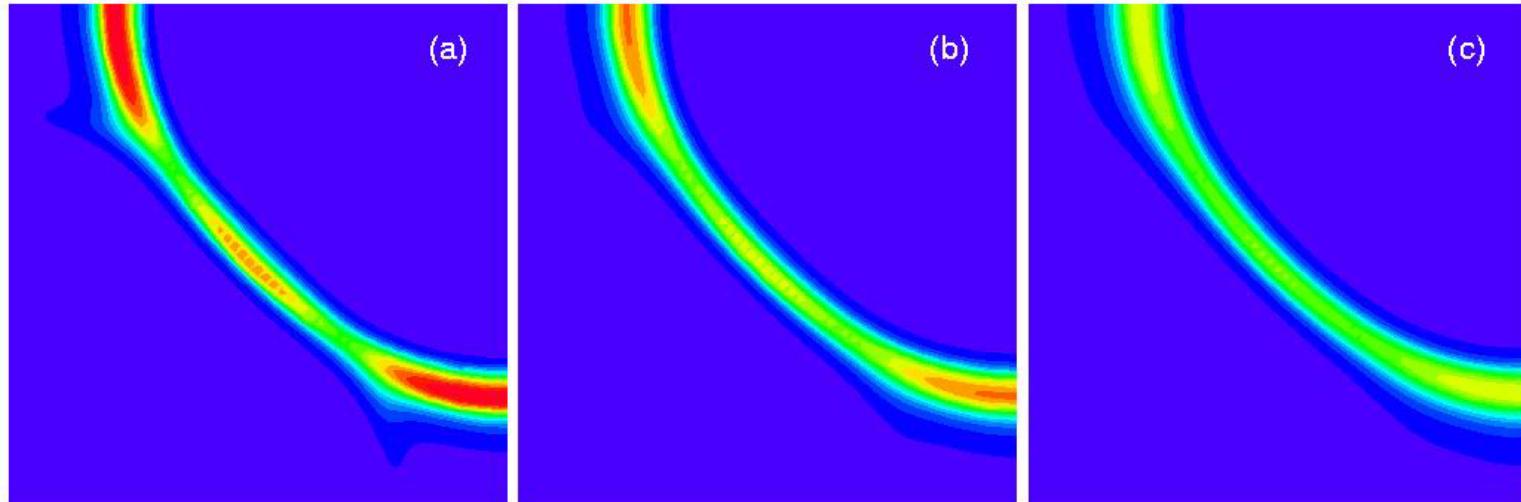
Expt: P. K. Mang et al., cond-mat/0307093, Matsuda (1992).

Temperature dependence of ARPES

$\beta = 15$

$\beta = 10$

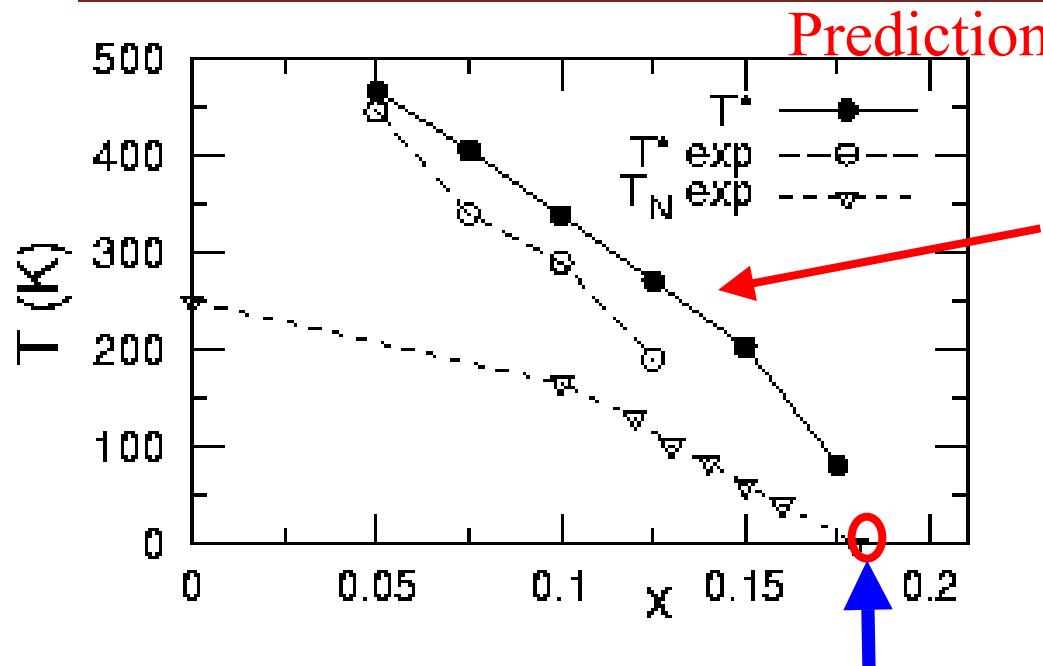
$\beta = 7.5$



$U=5.75,$
 $t'=-0.175, t''=0.05,$
 $n = 1.15$

Kyung, Hankevych, AMT, cond-mat/0312499

Pseudogap temperature and QCP



Prediction QCP
may be masked by 3D transitions

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

Prediction \downarrow
supports further AFM
fluctuations origin of PG

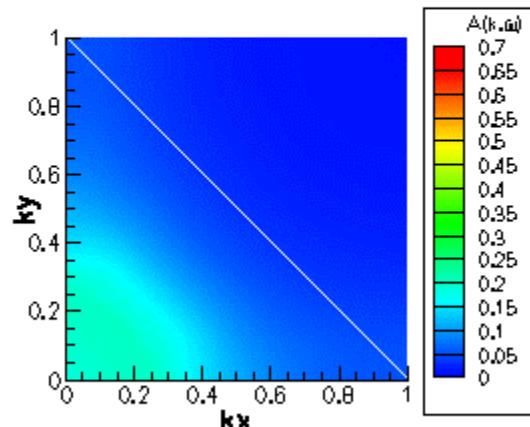
ARPES to do:
when does PG disappear
with increasing T

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

Electron doped, 15% low $T=0.05t$

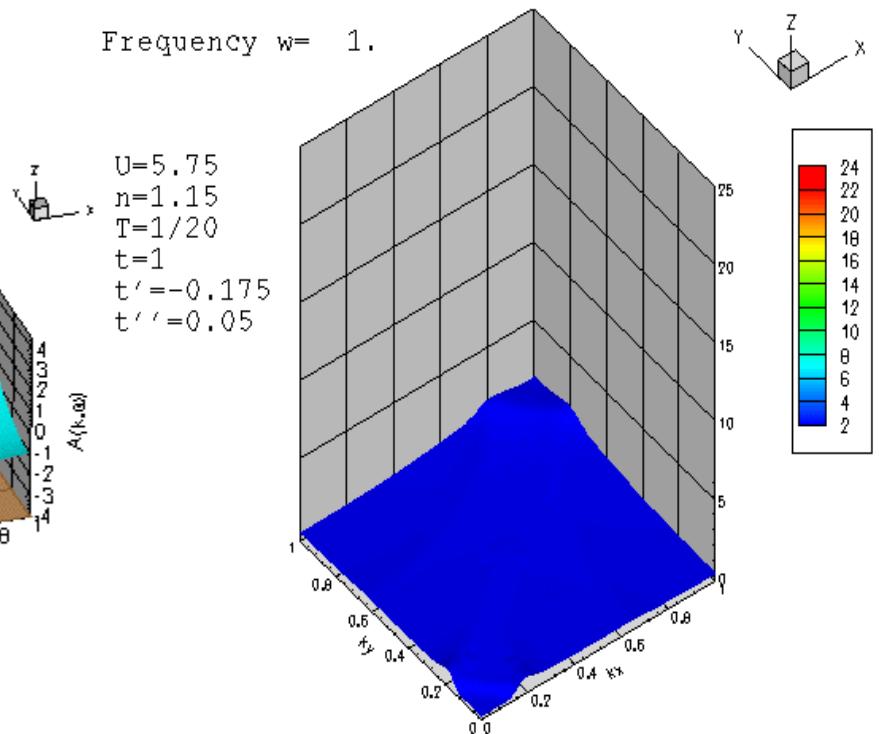
Frequency $w = -4$.

$U=5.75$, $n=1.15$, $T=1/20$
 $t=1$, $t'=-0.175$, $t''=0.05$



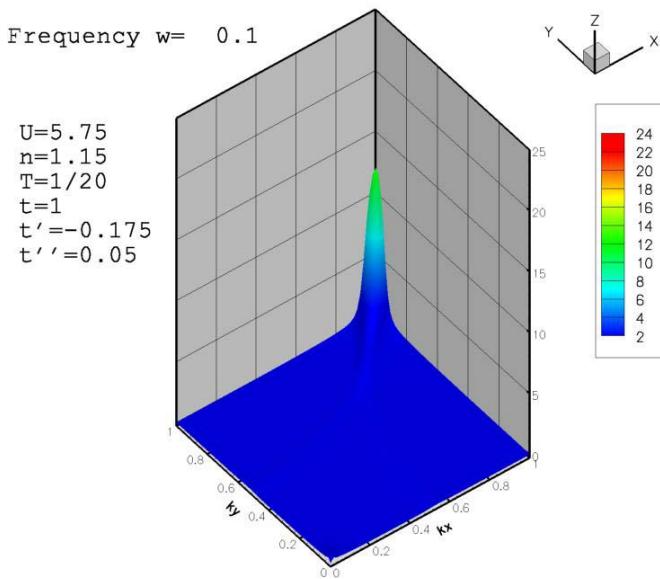
Frequency $w = 1$.

$U=5.75$
 $n=1.15$
 $T=1/20$
 $t=1$
 $t'=-0.175$
 $t''=0.05$

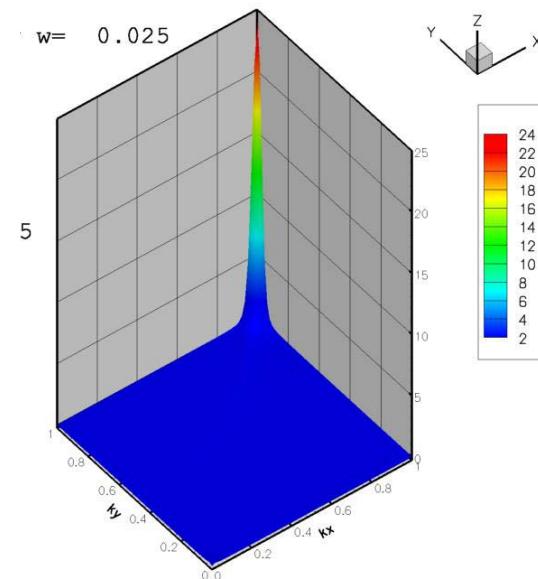


Electron doped 15% low $T=0.05t$

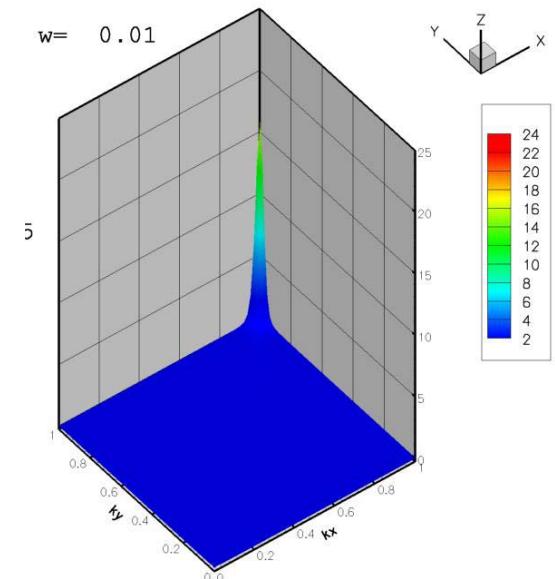
$\omega = 0.1t$



$\omega = 0.02t$



$\omega = 0.01t$

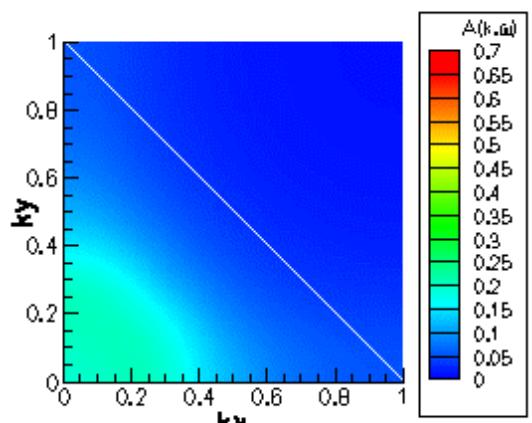


Prediction: $\hbar \omega_{sf} \ll k_B T$ in pseudogap begins at $T > T^*$

Electron doped, 15%, high $T=0.2t$

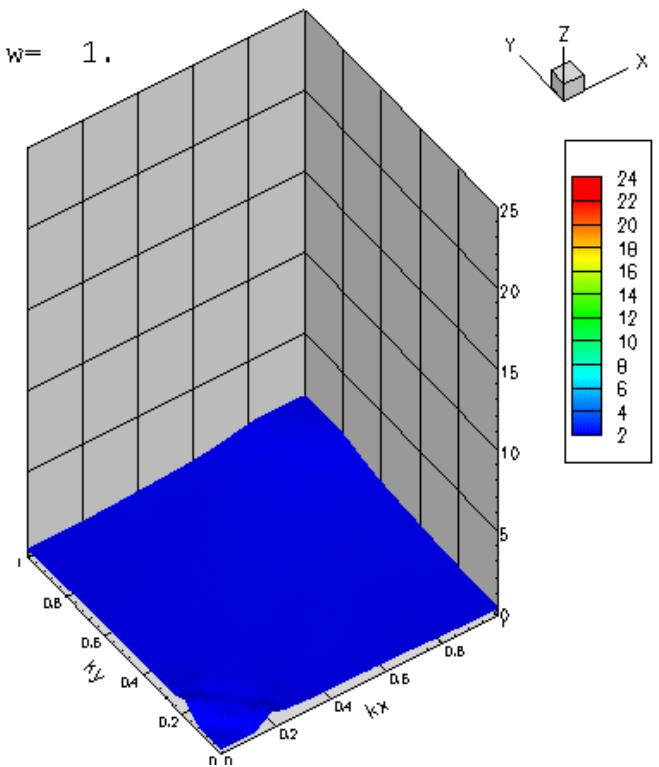
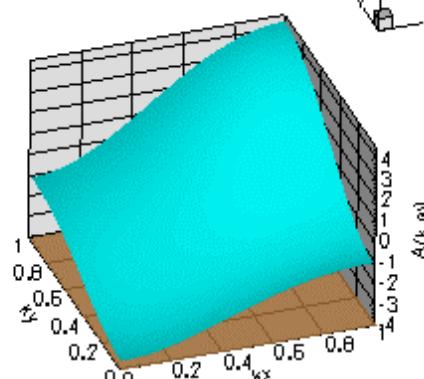
Frequency $\omega = -4$.

$U=5.75$, $n=1.15$, $T=1/5$
 $t=1$, $t'=-0.175$, $t''=0.05$



Frequency $\omega = 1$.

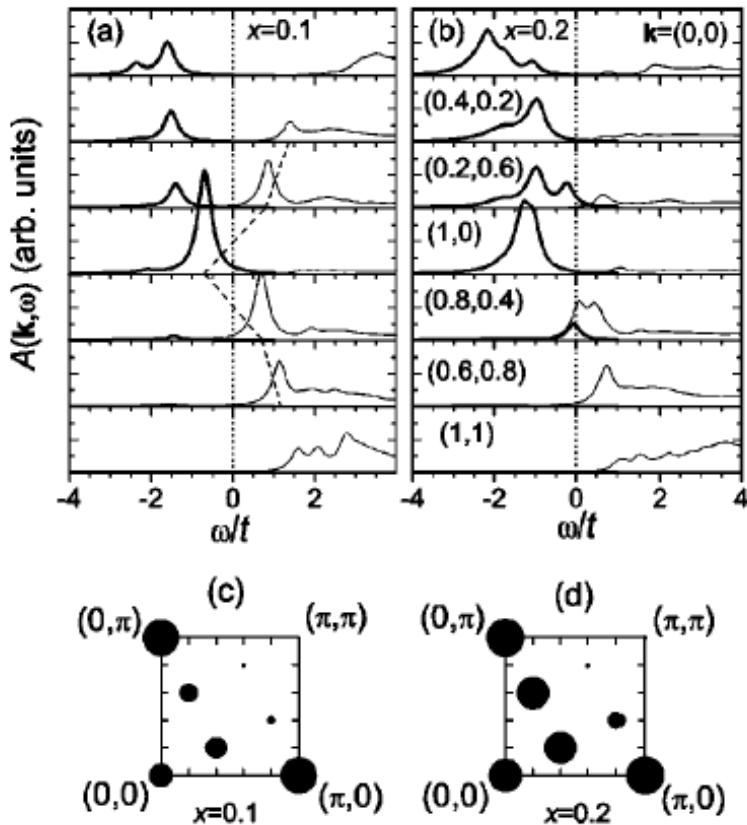
$U=5.75$
 $n=1.15$
 $T=1/5$
 $t=1$
 $t'=-0.175$
 $t''=0.05$



Precursor of SDW state (dynamic symmetry breaking)

- A.P. Kampf and J.R. Schrieffer, Phys. Rev. B **42**, 7967 (1990)
- 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., cond-mat/0312499
- R. S. Markiewicz, cond-mat/0308469.

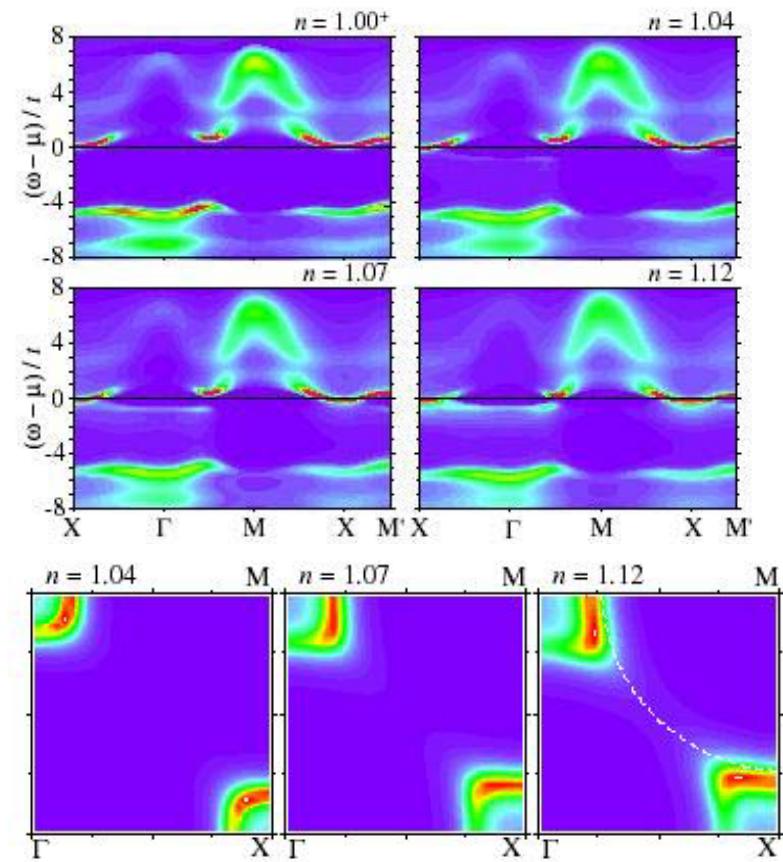
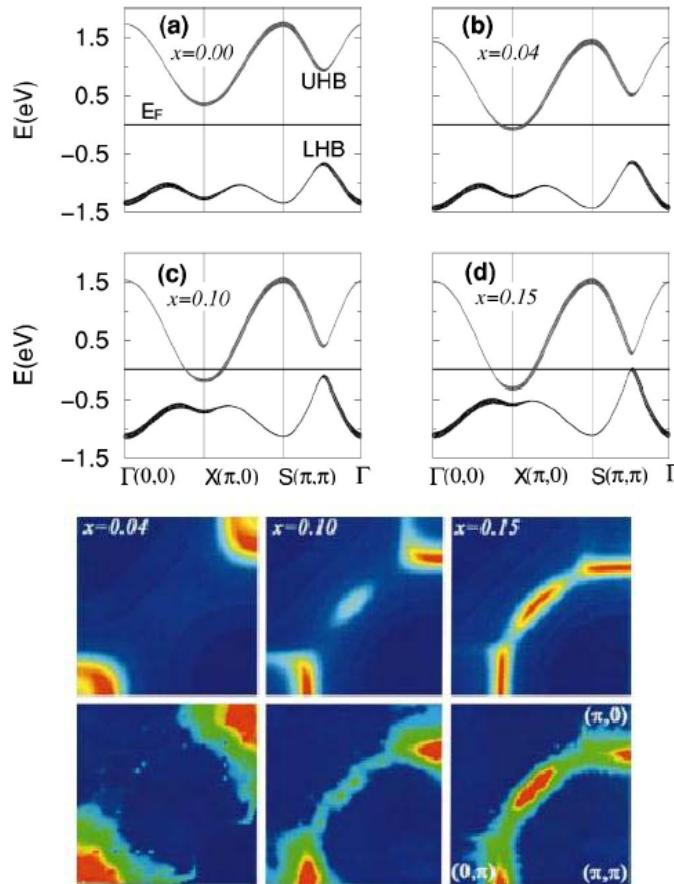
Exact diagonalization for t - t' - t'' - J model



- Absence of $\omega=0$ excitations near $(\pi/2, \pi/2)$ at optimal doping
- Small lattice size
- **Not applicable near optimal doping since no LHB**

T.Tohyama *et al.*, PRB **64**, 212505 (2001)

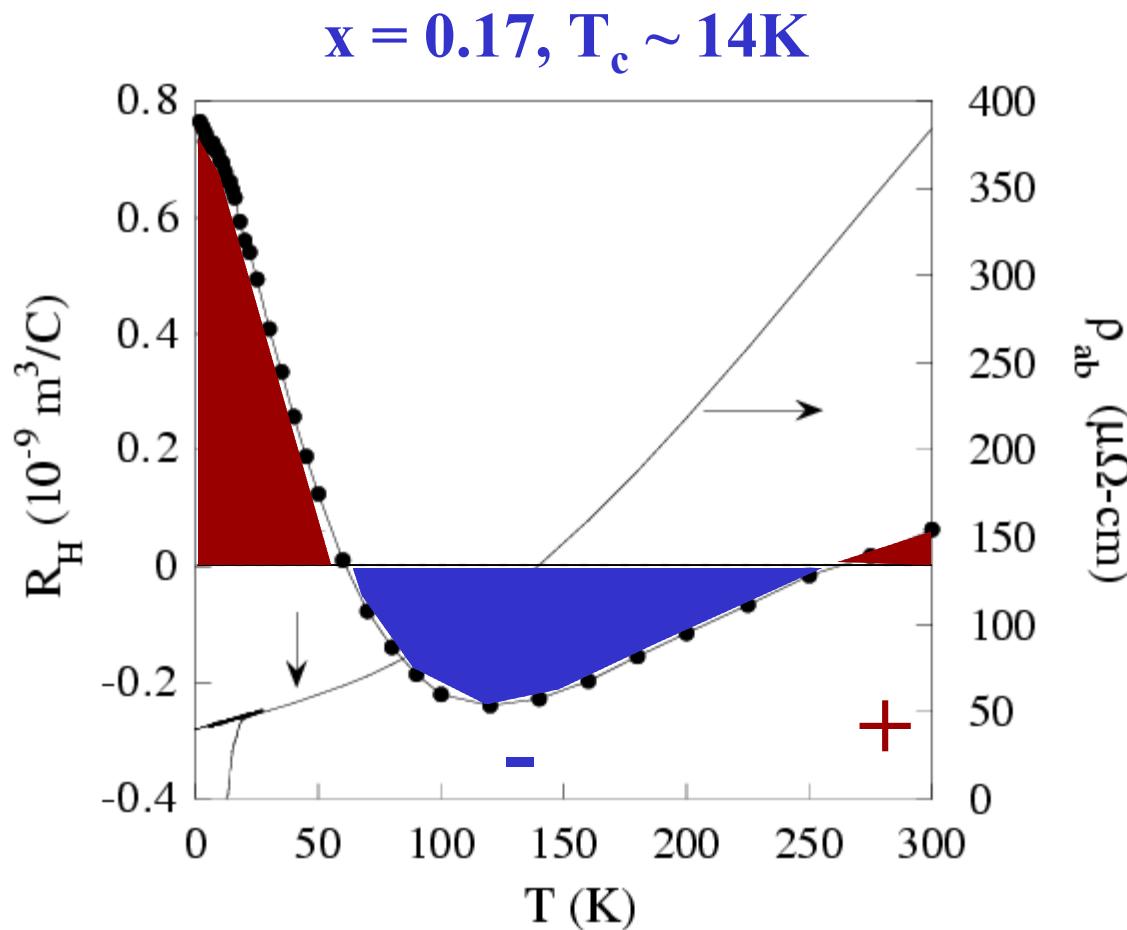
Contrast



Kusko, Markiewicz, Bansil, PRB 2002,

Kusunose, Rice, Phys. Rev. Lett. (2003).

Reduction introduces holes...



P. Fournier et al., Phys. Rev. Lett. **81**, 4720 (1998).

VI- Conclusion

- One model, weak and strong coupling
- Strong-coupling pseudogap
 - h- or (e- very underdoped)
 - CPT (+ DCA + Phillips + ...) Like Mott, short-range effect (but not zero range). Scales like t .
- Weak-coupling pseudogap
 - Electron-doped high Tc in this regime near optimal n .
 - ARPES and neutron scattering are explained in detail by Hubbard model solved within TPSC
 - Only Hubbard parameters (no mode-coupling, U_{eff} etc.)
 - Remarkable (best?) agreement with experiment in high-Tc.

Perspectives

- $\hbar\omega_{sf} \ll k_B T$ in pseudogap begins at $T > T^*$
- $T^*(\delta)$ predicted for ARPES
- In EDC will appear when $\xi/\xi_{\text{th}} \sim 1$ (precursor effect) in ARPES.
- No hot spots beyond QCP
- Speculation: going smoothly to strong coupling?
 $\xi_{\text{th}} \rightarrow a$
- More studies of e-doped cuprates (great samples)

Liang Chen Yury Vilk



Steve Allen



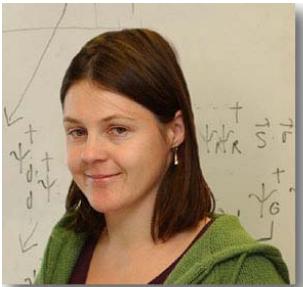
François Lemay

Samuel Moukouri



David Poulin Hugo Touchette J.-S. Landry M. Boissonnault





K. LeHur



C. Bourronnais



R. Côté



D. Sénéchal

Alexis Gagné-Lebrun

A-M.T. Alexandre Blais Vasyl Hankevych



Sébastien Roy

Sarma Kanchala

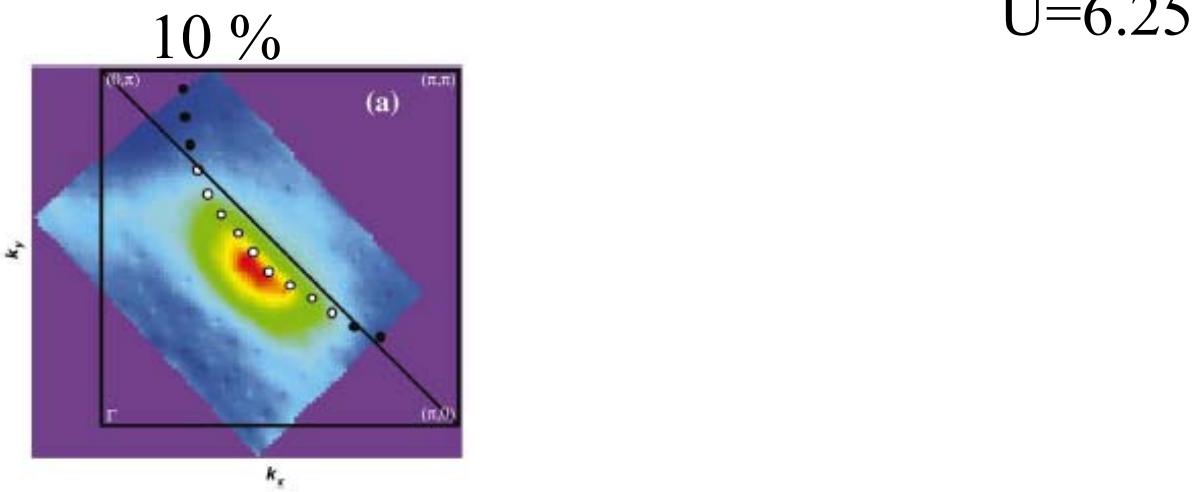
Bumsoo Kyung

Maxim Mar'enko

C'est fini... .

enfin

Hole-doped systems: Fermi surface plot



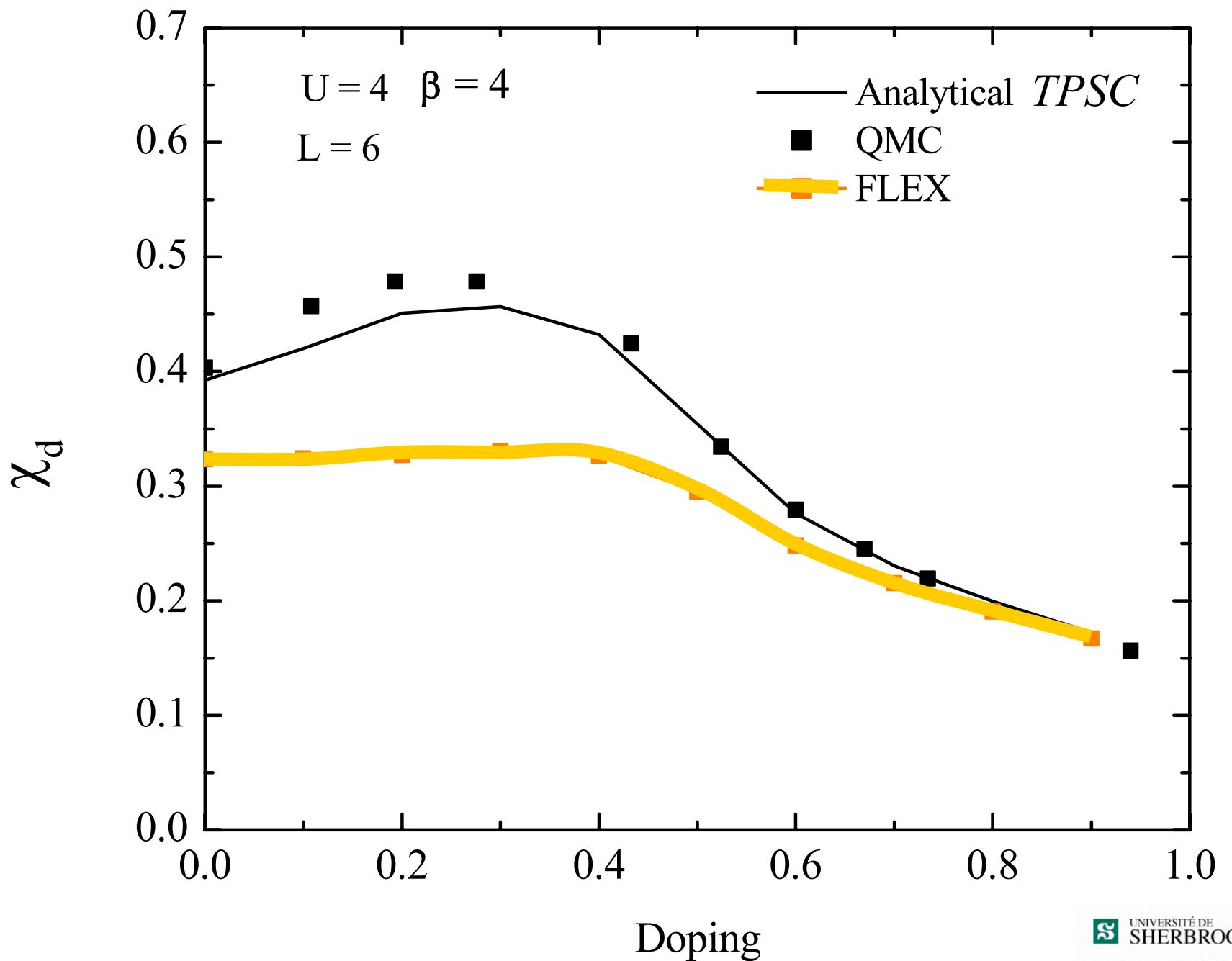
Ronning et al., PRB **67**, 165101 (2003)

Quantitative for electron-doped, qualitative for hole-doped.
Essential differences with e-doped:

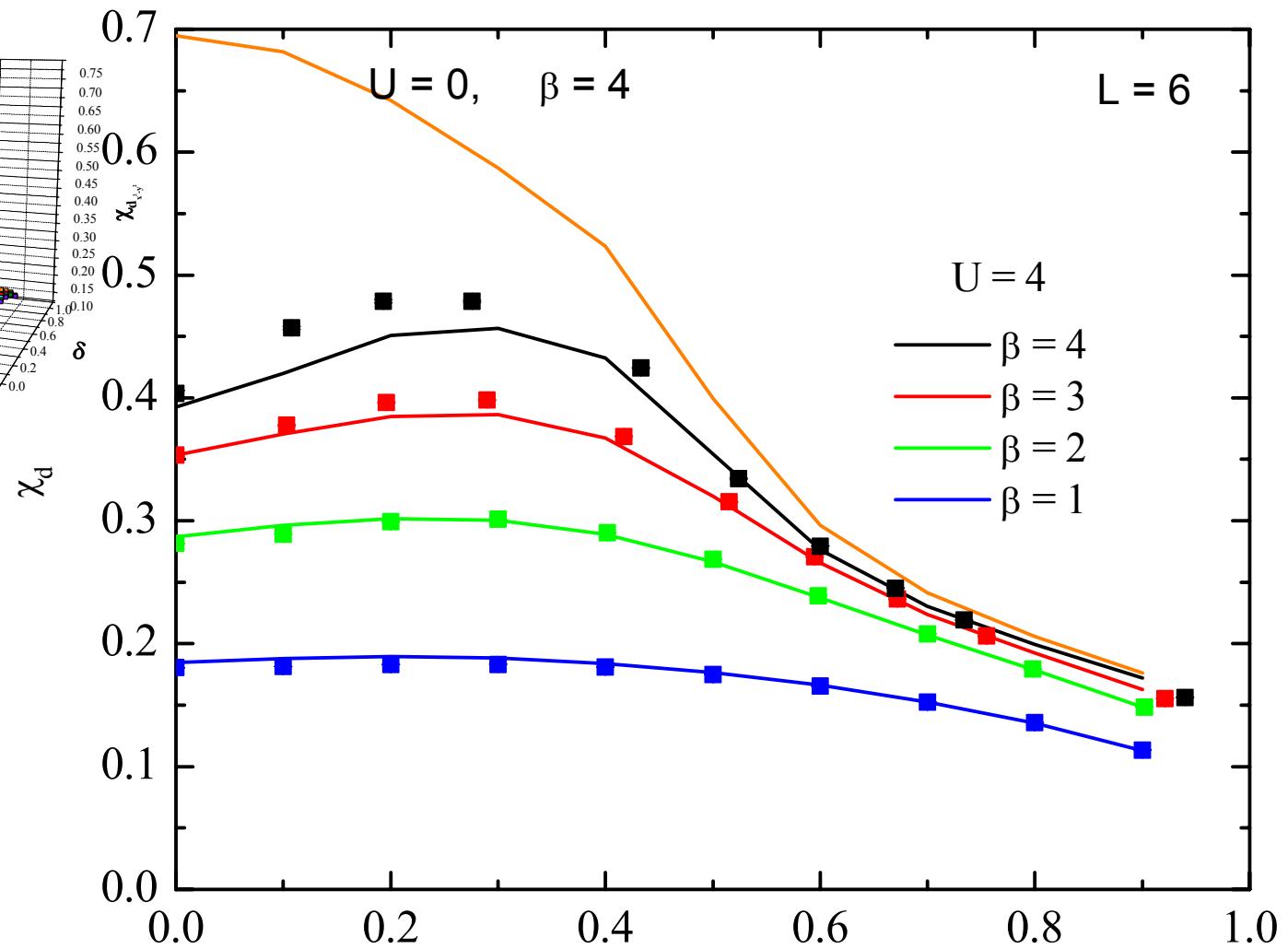
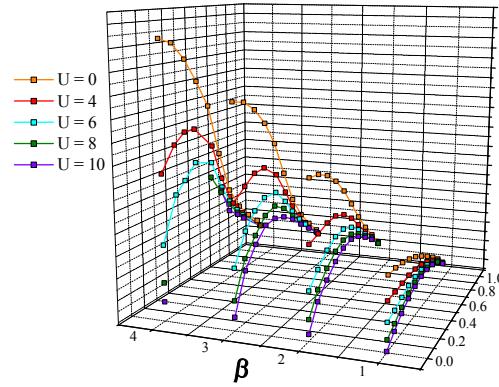
- AFM correlation length is much smaller
- Smaller region for nodal quasiparticles

Short range mechanisms (Mott,...) may come into play

Hankevych, Kyung, A.-M.S.T., 0312499



$d_{x^2-y^2}$ -wave susceptibility for 6×6 lattice



$$\chi_d = \frac{\delta G}{\delta \eta} =$$

+

$$\frac{\delta G}{\delta \eta} = GG \left(1 + \frac{\delta \Sigma}{\delta \eta} \right)$$

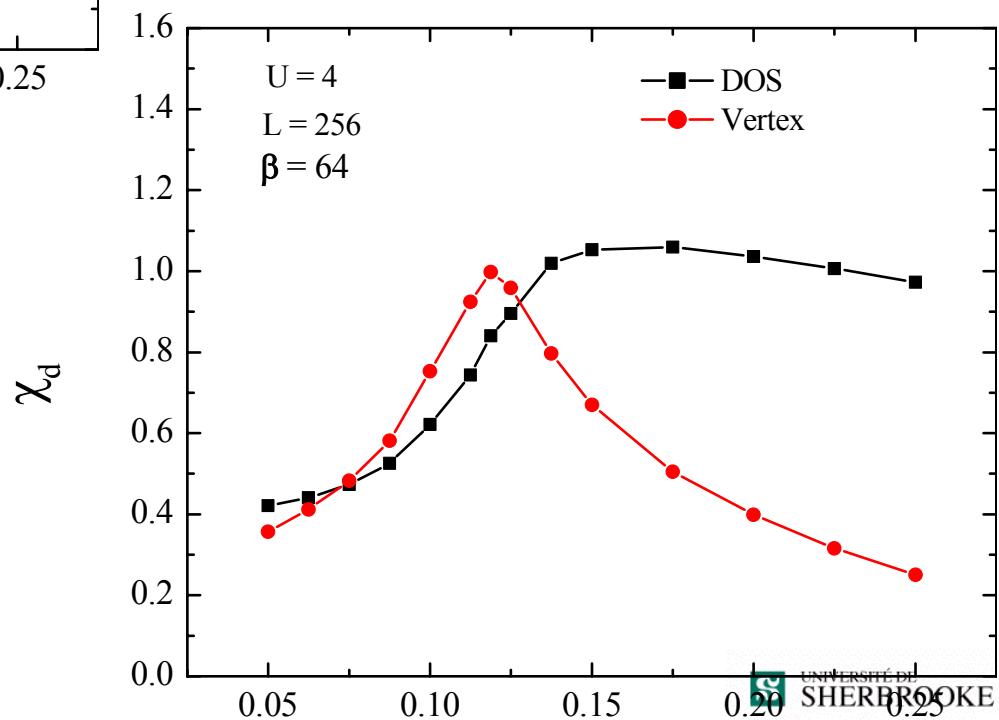
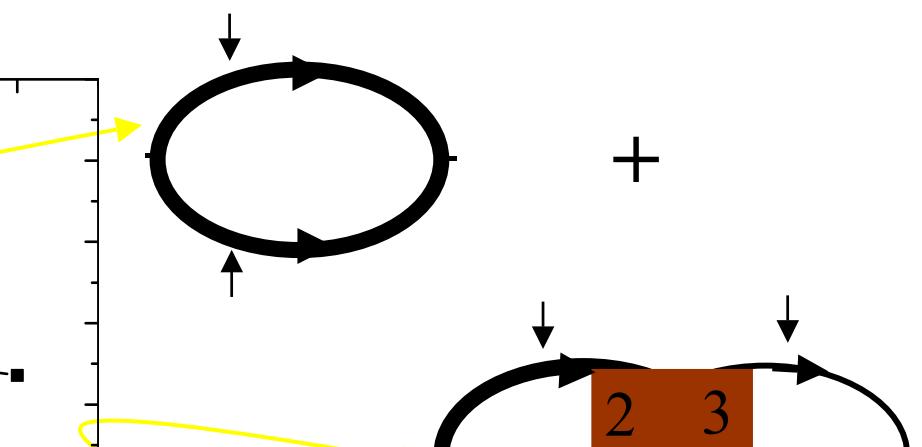
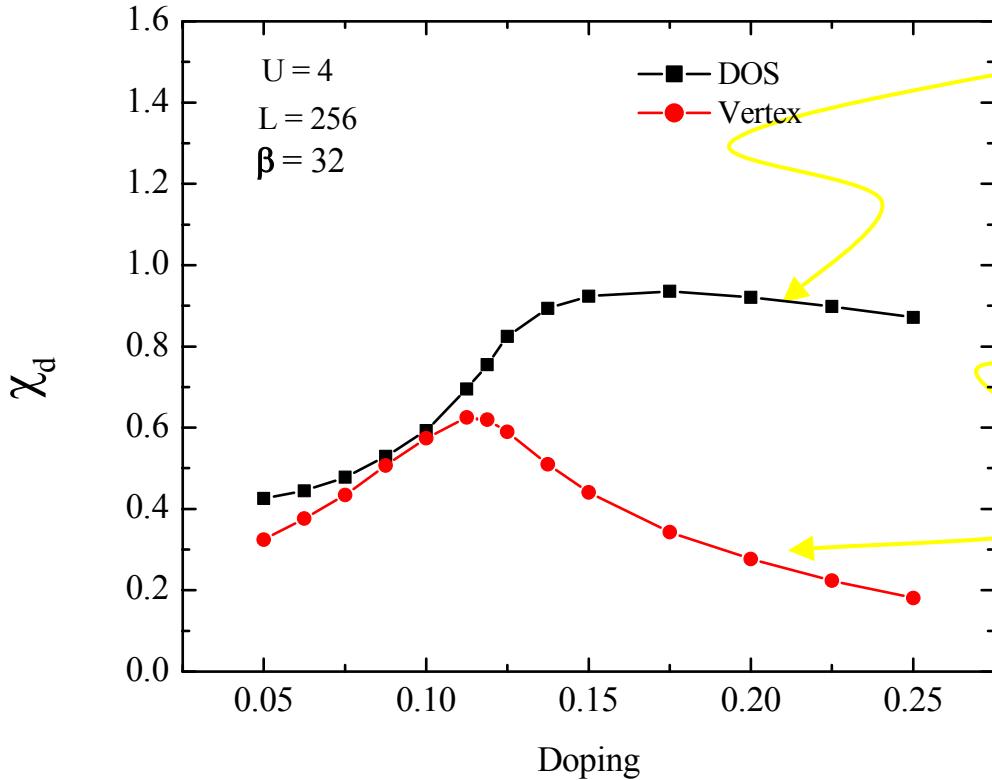
$$G = \frac{1}{G_0^{-1} - \eta - \Sigma}$$

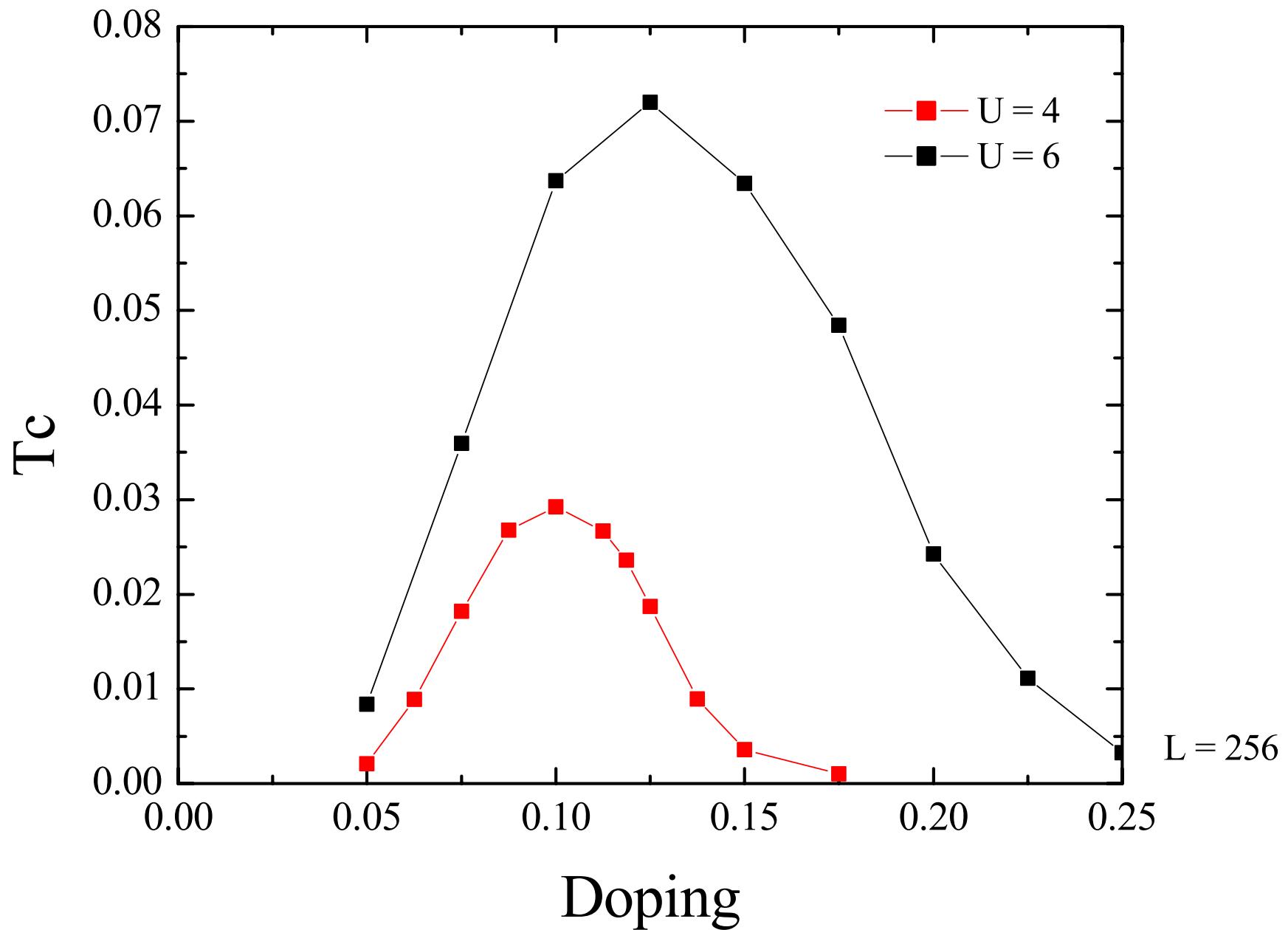
$$\chi_d = \frac{\delta G}{\delta \eta} \sim$$

+

$$\chi_s^\perp =$$

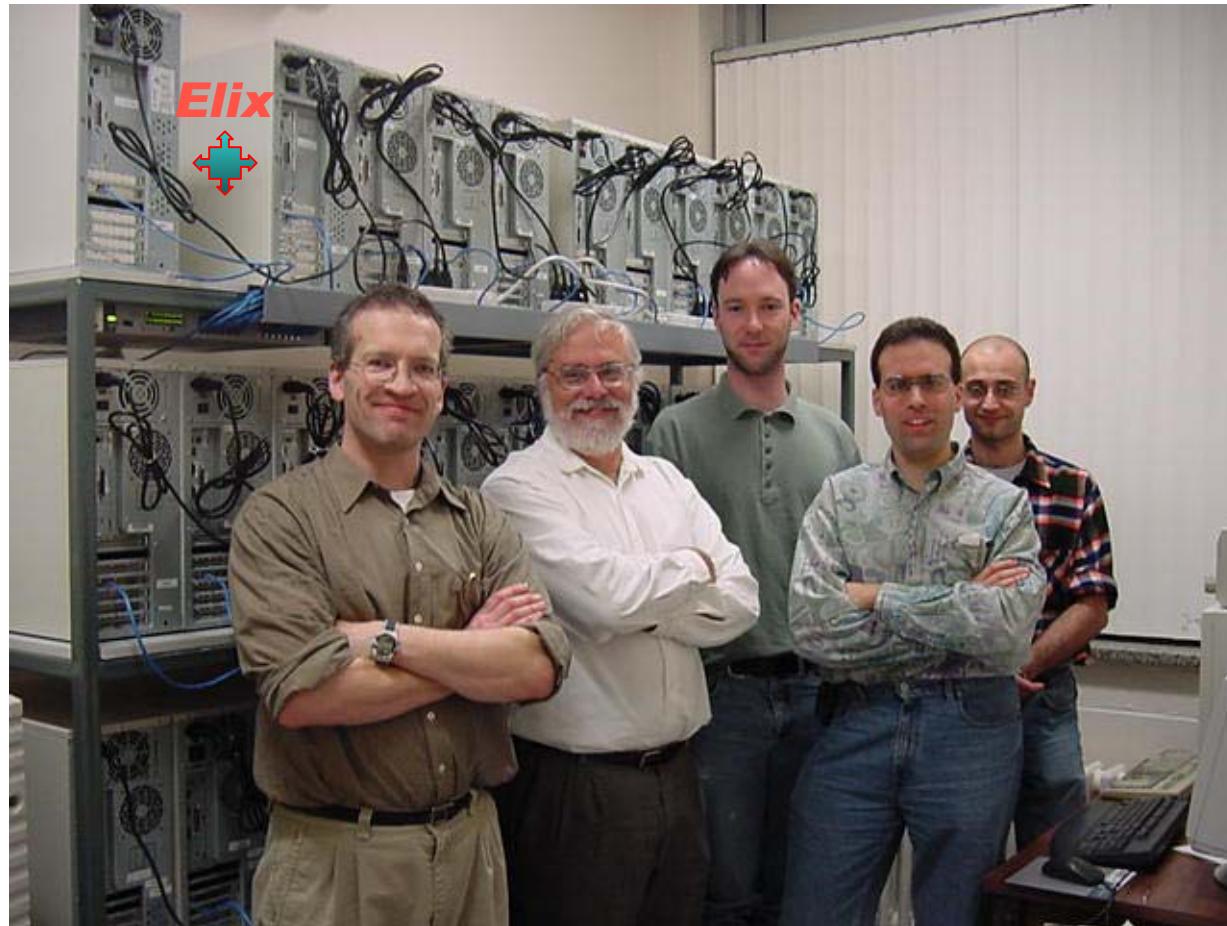
+





Michel Barrette

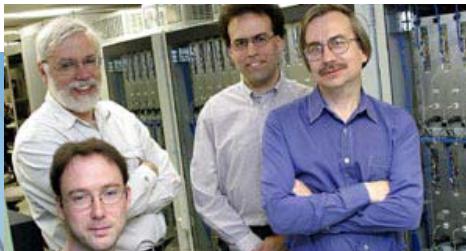
Mehdi Bozzo-Rey



David Sénéchal

A.-M.T.

Alain Veilleux



Un noeud d'Elix2

Carol Gauthier,
analyste en Calcul
du CCS en plein
machinage d'un
noeud d'Elix2



Elix2 vu de profil



De gauche à droite: Alain Veilleux, Michel Barrette, Jean-Phillipe Turcotte, Carol Gauthier, Patrick Vachon et le 1er noeud d'Elix

Equipe du CCS devant Elix2. Al'arrière: Patrick Vachon, Minh-Nghia Nguyen, David Lauzon, Michel Barrette, Mehdi Bozzo-Rey, Simon Lessard, Alain Veilleux. A l'avant: Patrice Albaret, Karl Gaven-Venet, Benoît des Ligneris, Francis Giraldeau. Etait absent de la photo: Jean-Philippe Turcotte, Carol Gauthier, Xavier Barnabé Thériault et Mathieu Lutfy

