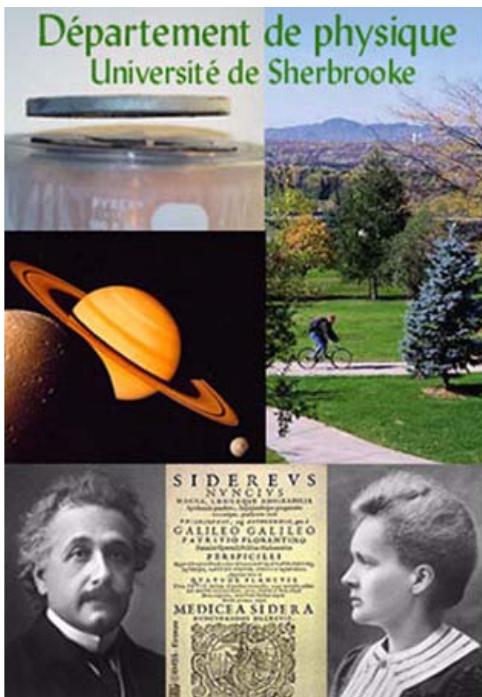


# André-Marie Tremblay



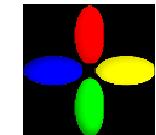
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## REGROUPEMENT QUÉBÉCOIS SUR LES MATÉRIAUX DE POINTE



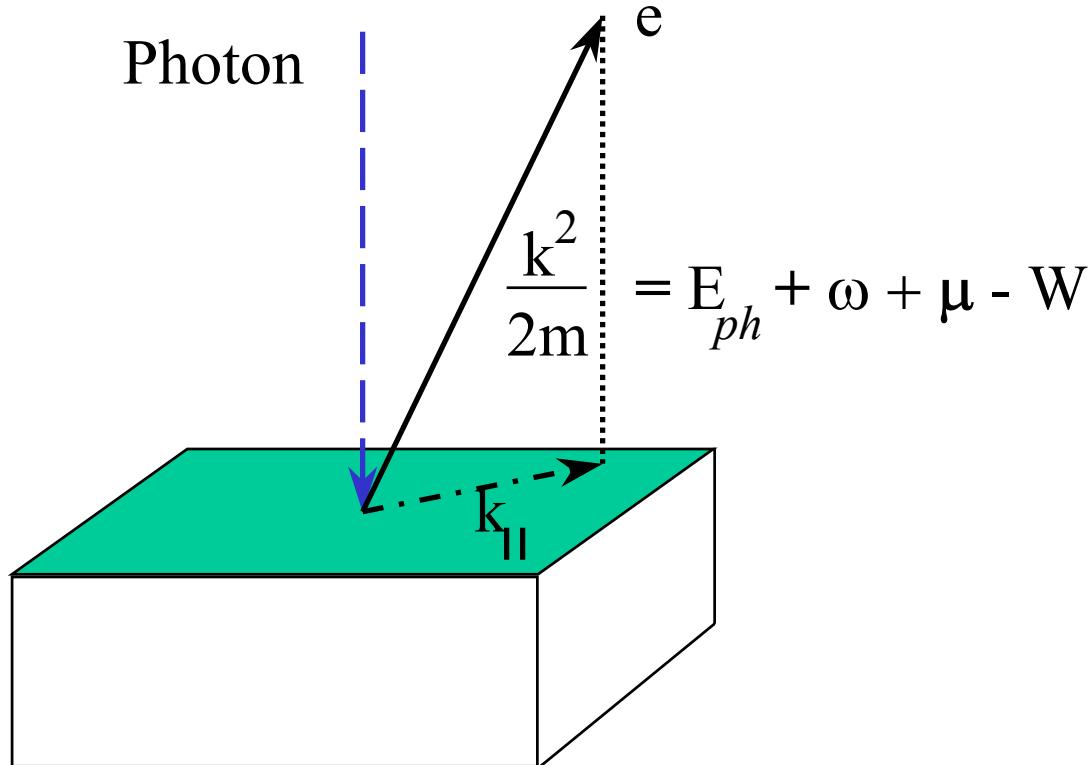
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## Sponsors:

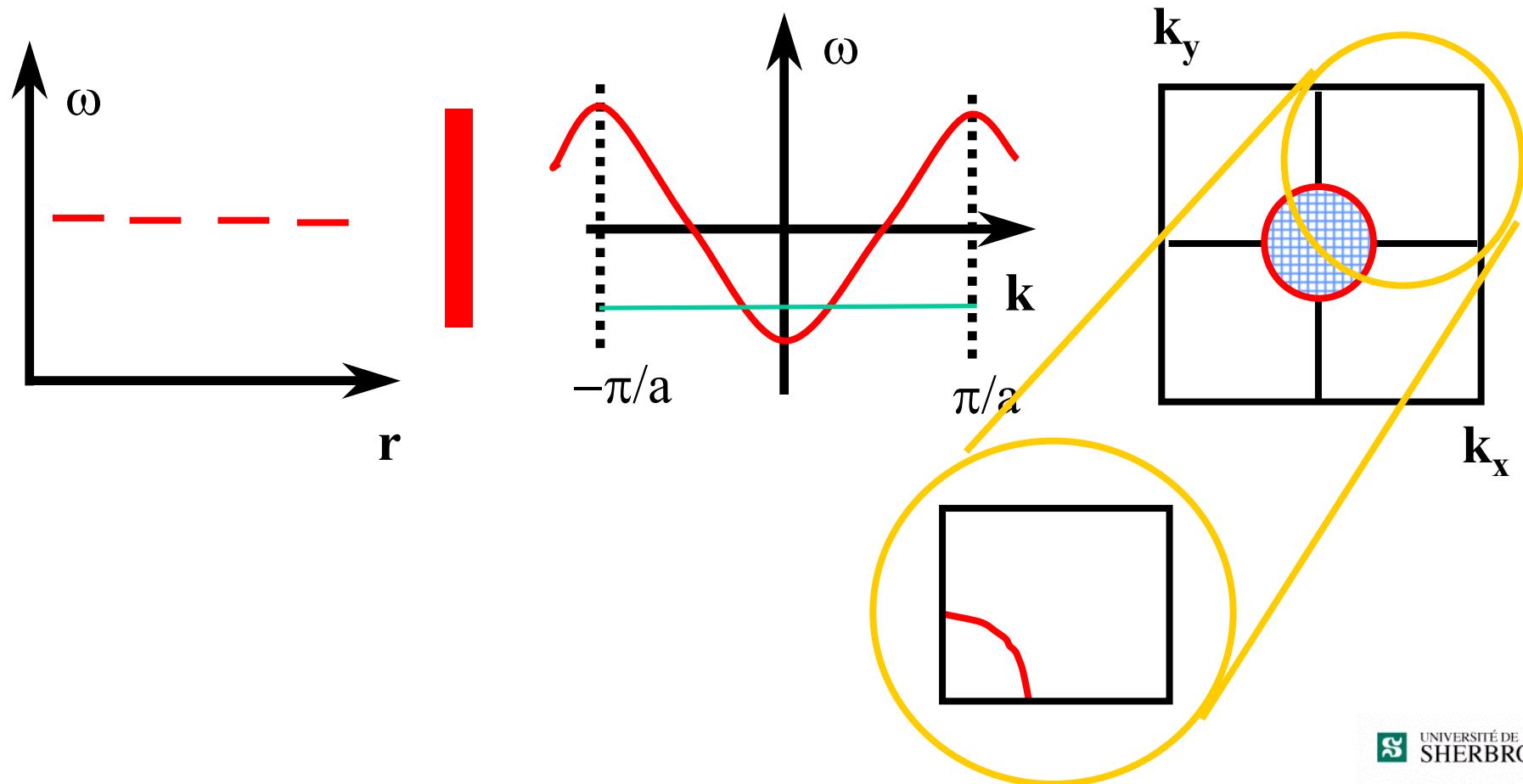


# Measuring electronic states in $d=2$

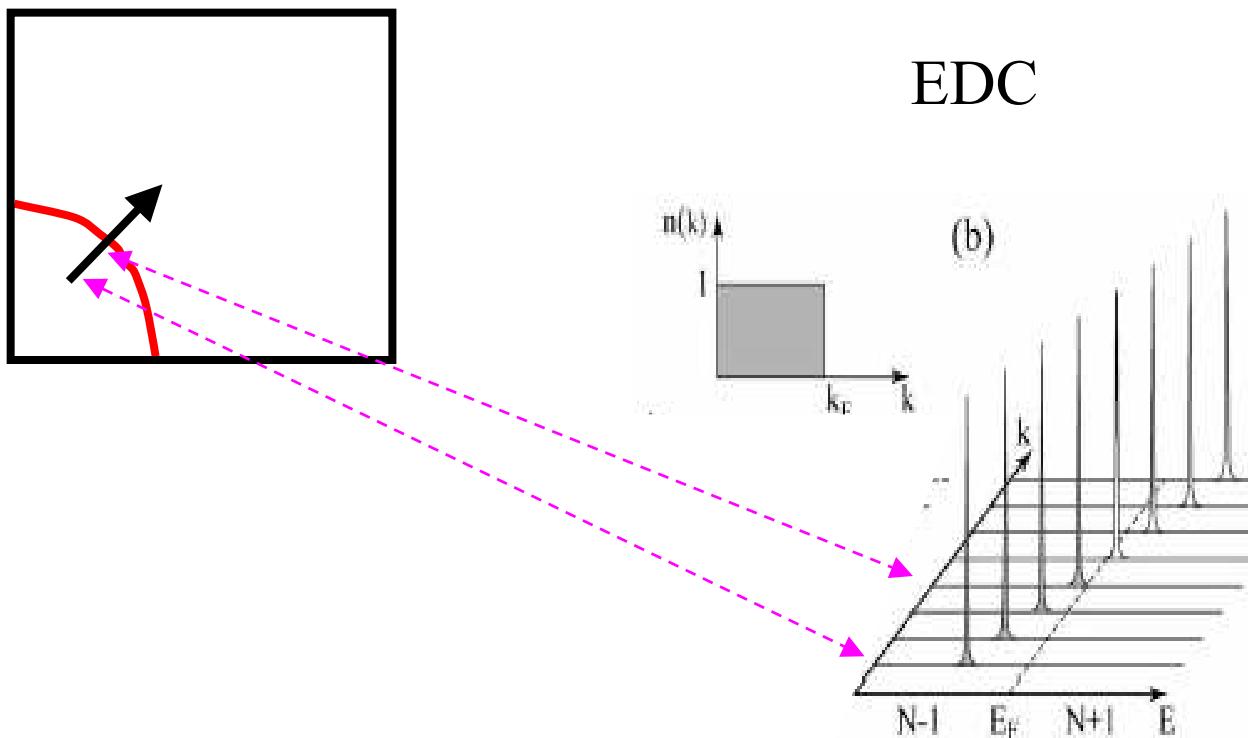
## Angle Resolved Photoemission Spectroscopy (ARPES)



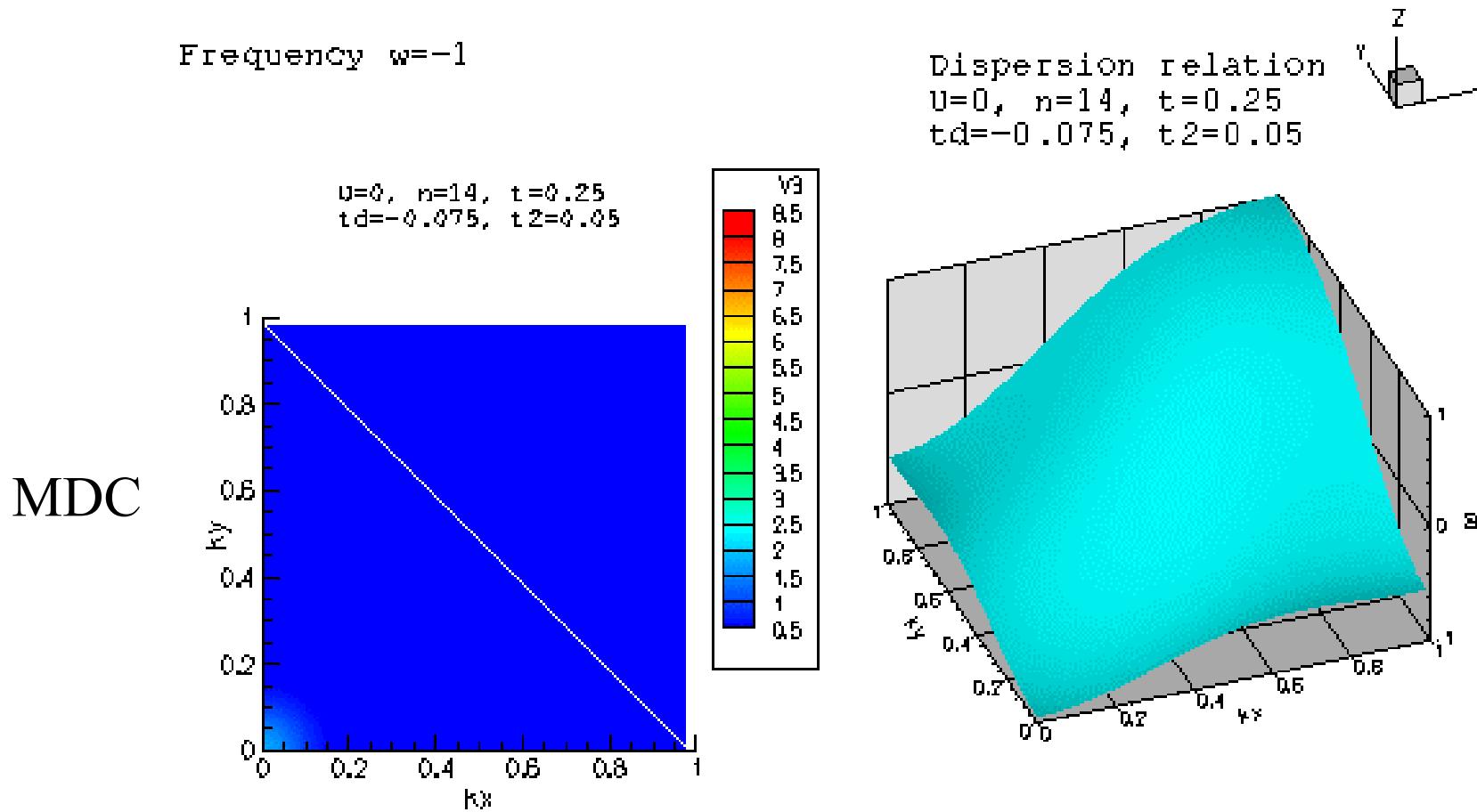
# Some basic Solid State Physics



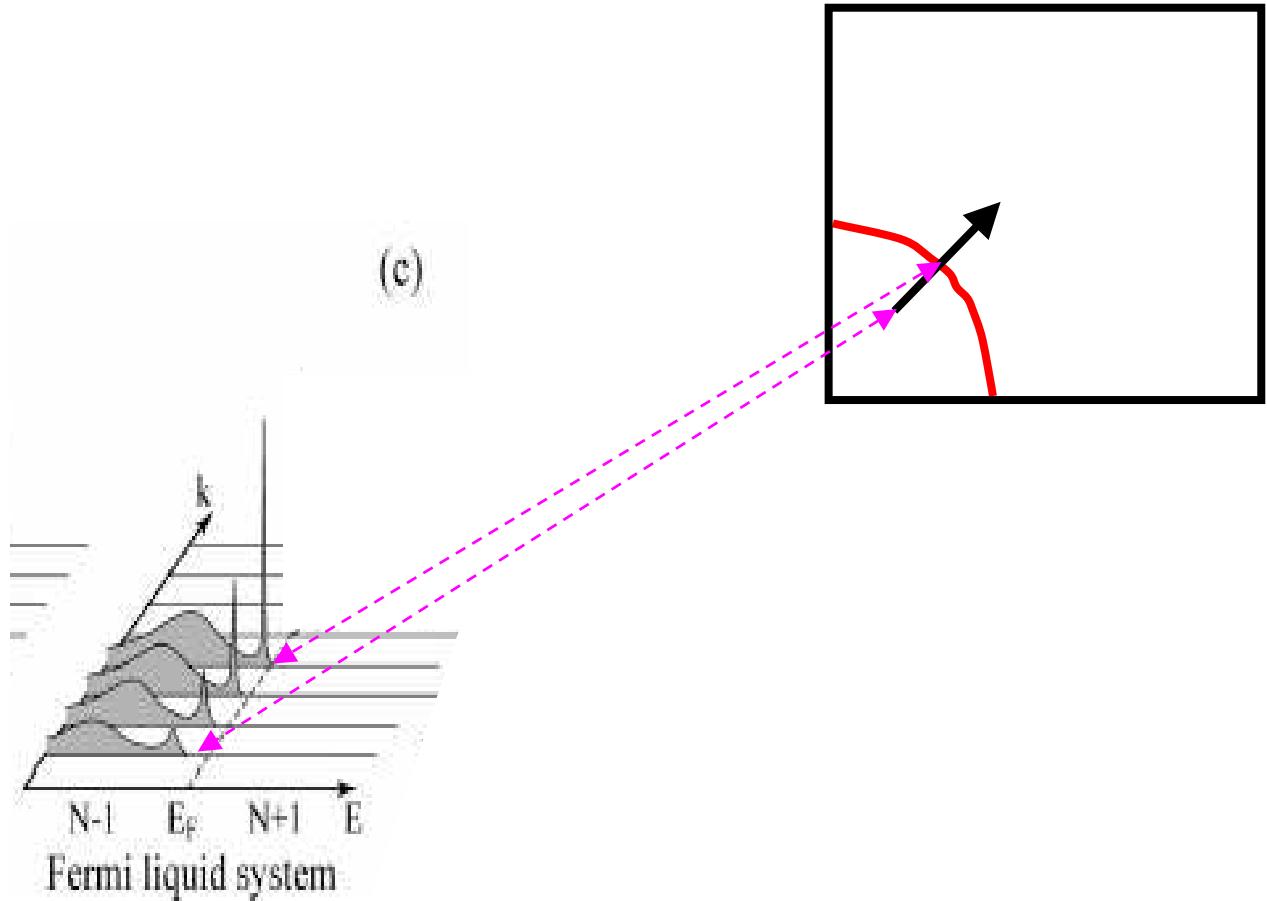
# The non-interacting case



# Electron-doped, non-interacting



# Interacting case: The Fermi liquid



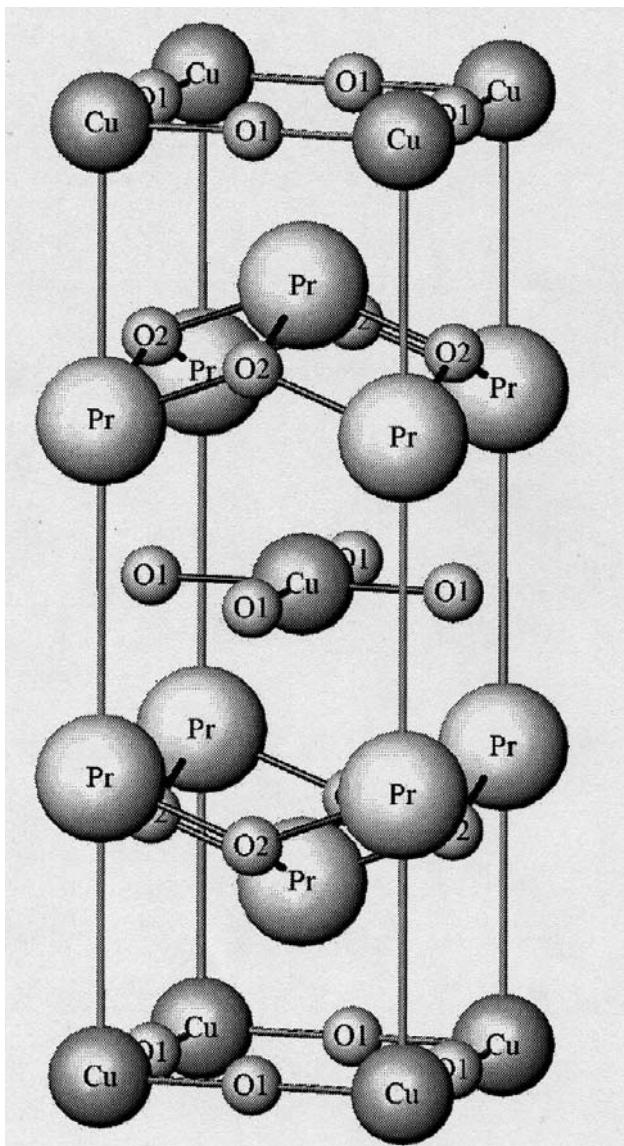
# Computational methods and destruction of the Fermi liquid in systems of correlated lattice electrons

- I. Introduction
  - Fermi liquid
- II. Experimental results from cuprates and model
- III. Strong and weak coupling pseudogap (CPT)
- IV. Weak coupling pseudogap (QMC,TPSC)
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## II-Experimental results from cuprates



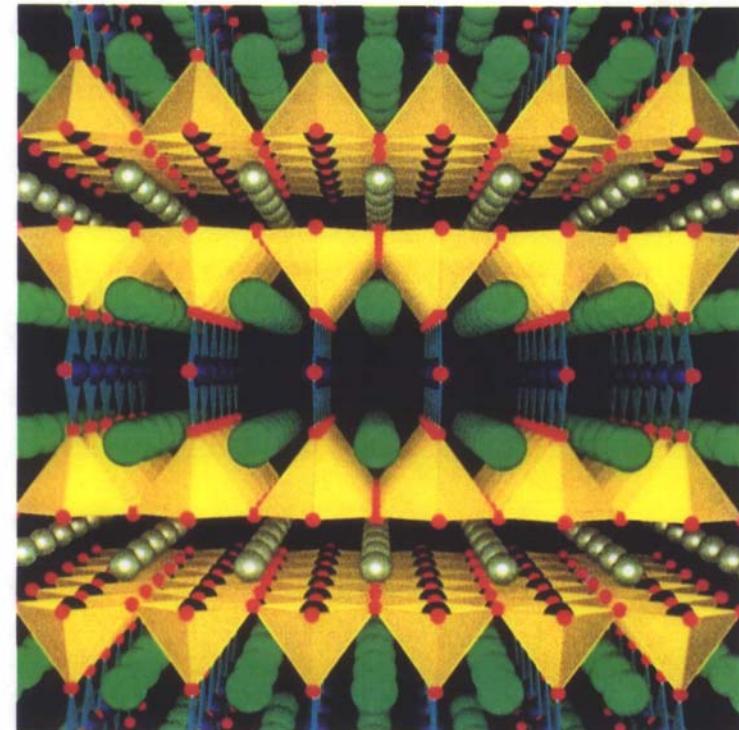
**SCIENTIFIC  
AMERICAN**

*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



$YBa_2Cu_3O_{7-\delta}$

# Phase diagram

Electron doping       $\longleftrightarrow$       Hole doping

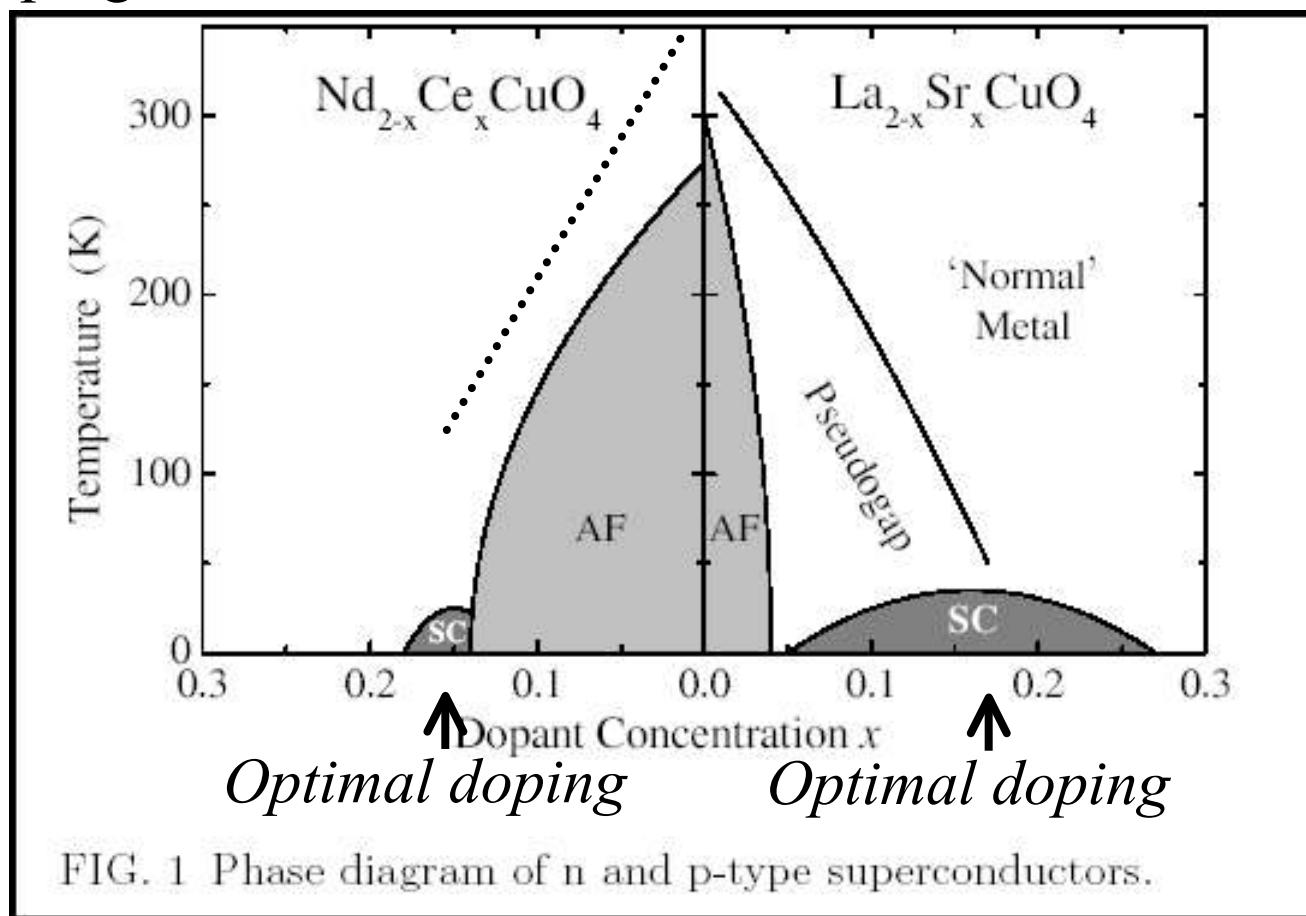


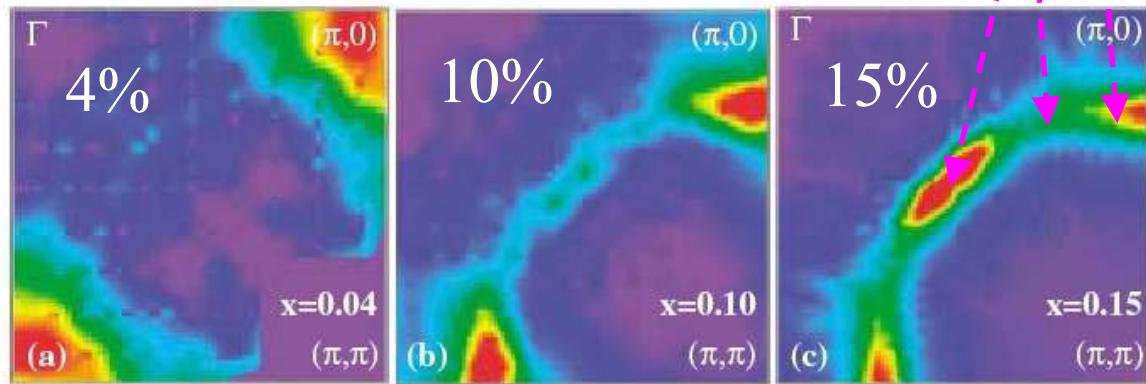
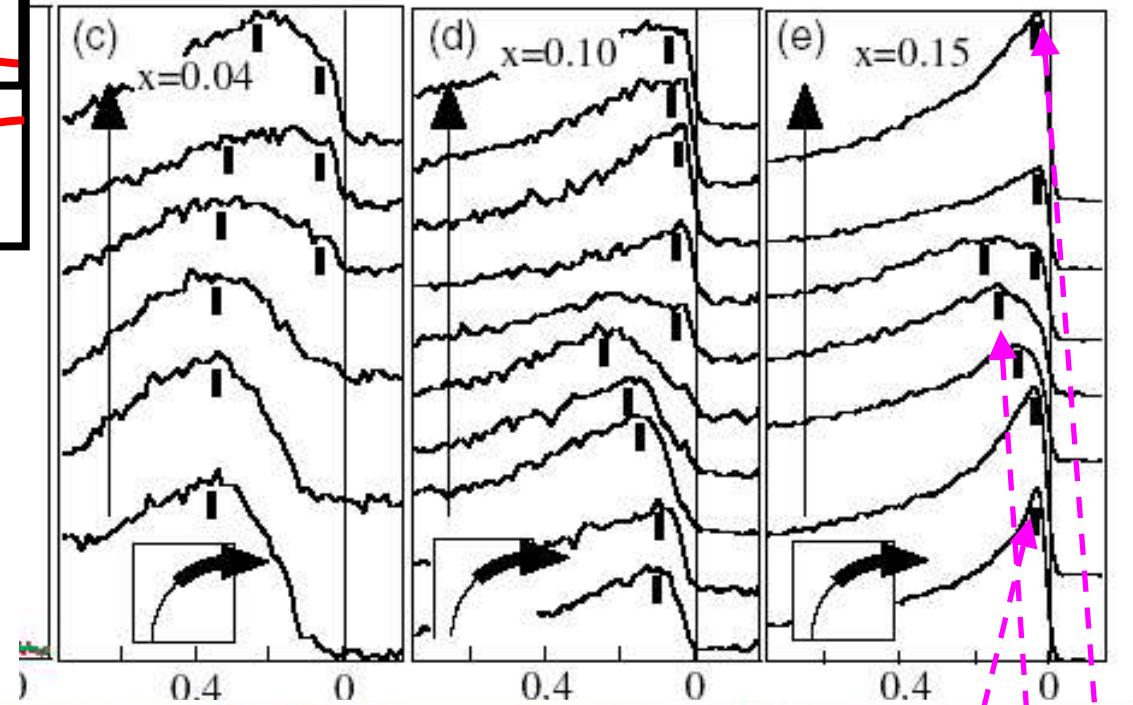
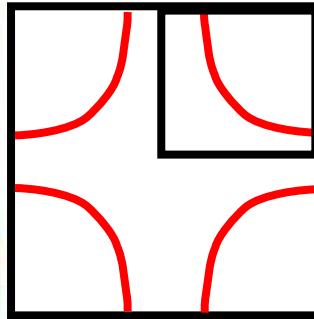
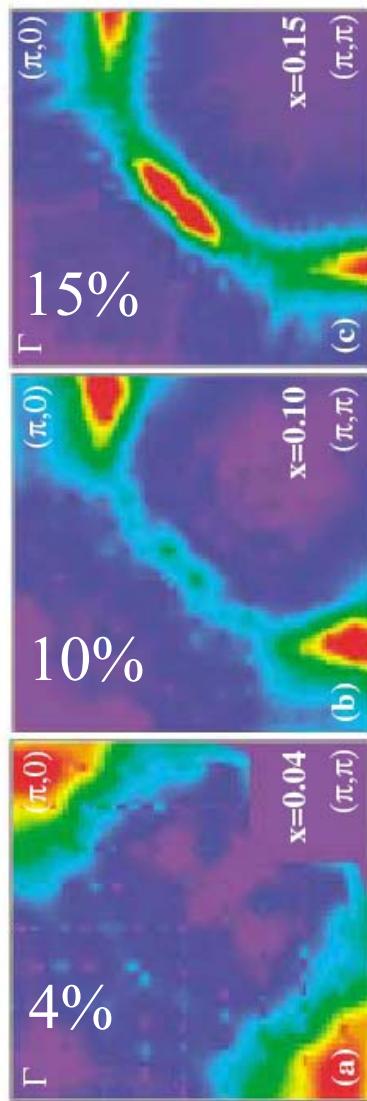
FIG. 1 Phase diagram of n and p-type superconductors.

$n$ , electron density

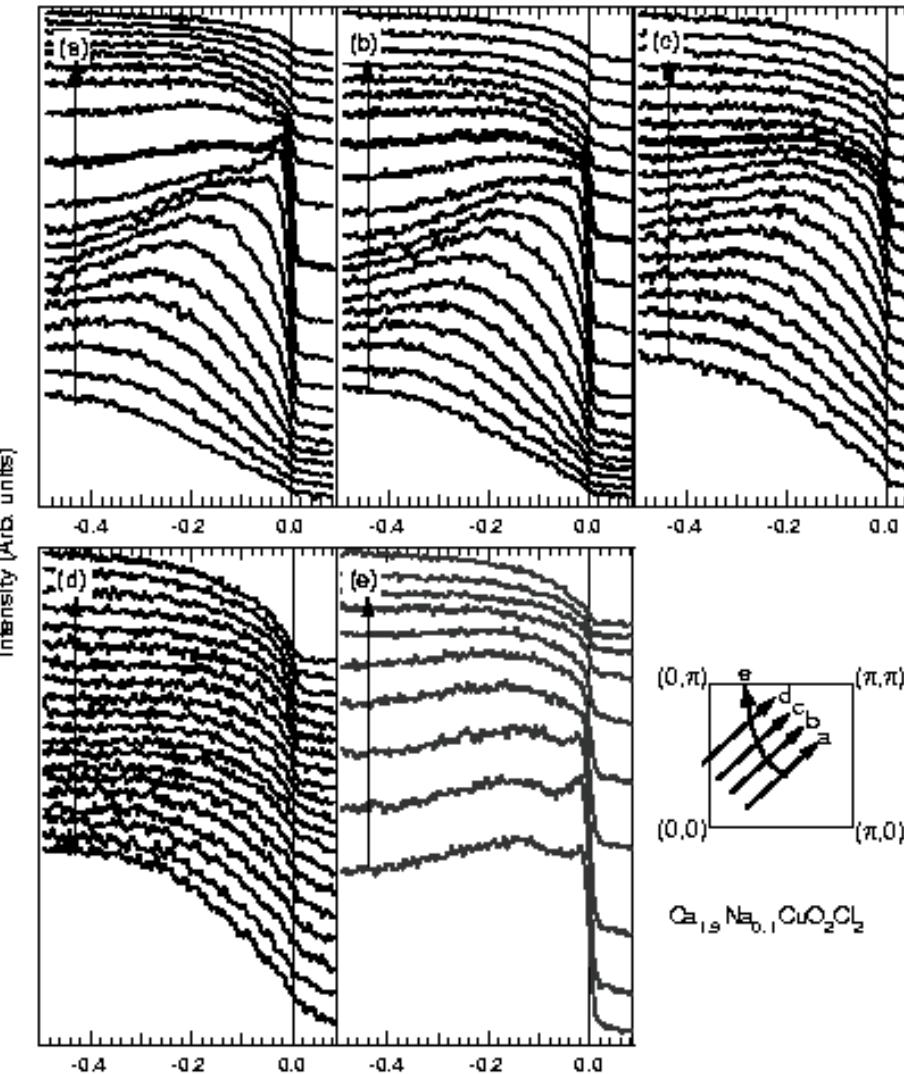
Damascelli, Shen, Hussain, 2002.

# Fermi surface, electron-doped case

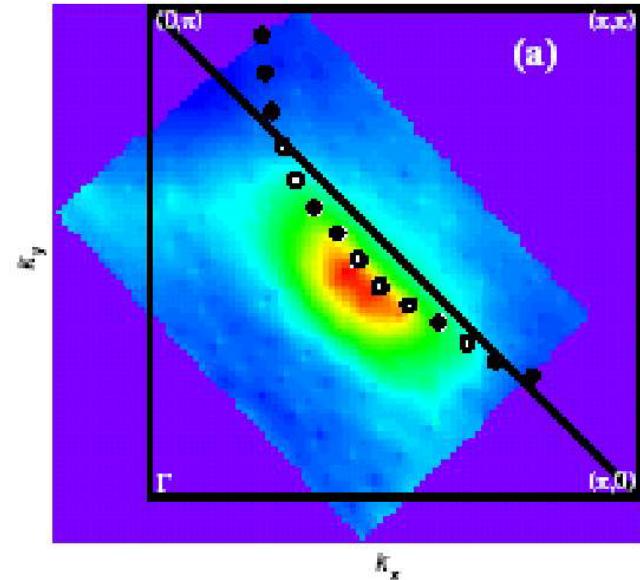
Armitage *et al.* PRL 2002.



# 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 »

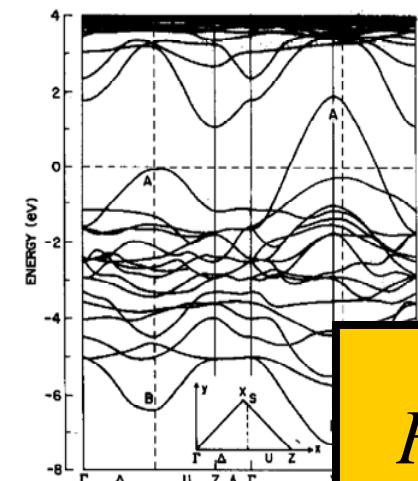
**SCIENTIFIC  
AMERICAN**

JUNE 1988  
\$3.50

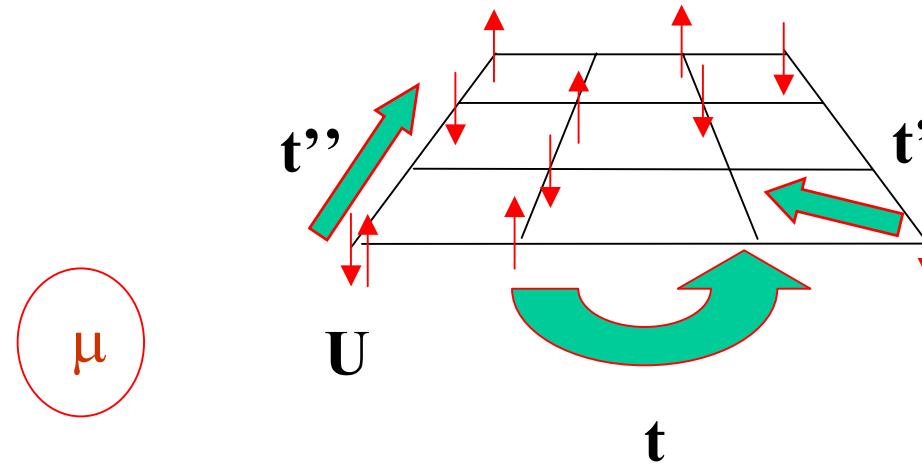
How nonsense is deleted from genetic messages.  
R for economic growth: aggressive use of new technology.  
Can particle physics test cosmology?



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



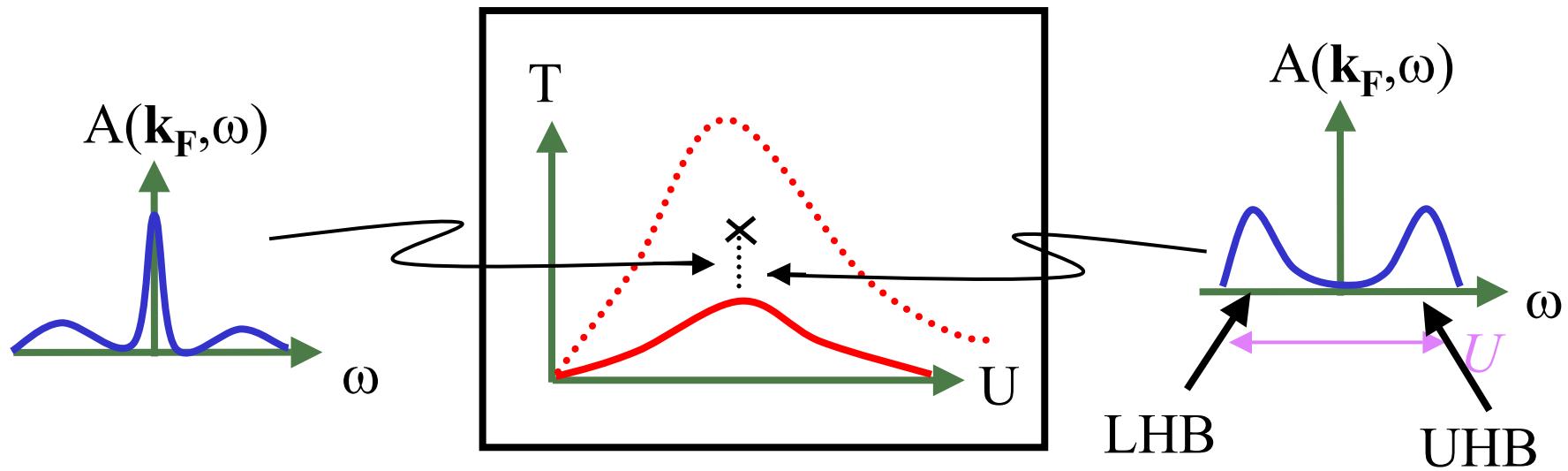
Simplest microscopic model for  $Cu$   $O$  planes.



- 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

# Questions: not only quantitative

- What destabilizes the Fermi liquid in a paramagnetic phase?
- How do we go from a Mott insulator to a conductor as a function of doping?
  - Hot spots and pseudogaps in the Hubbard model?

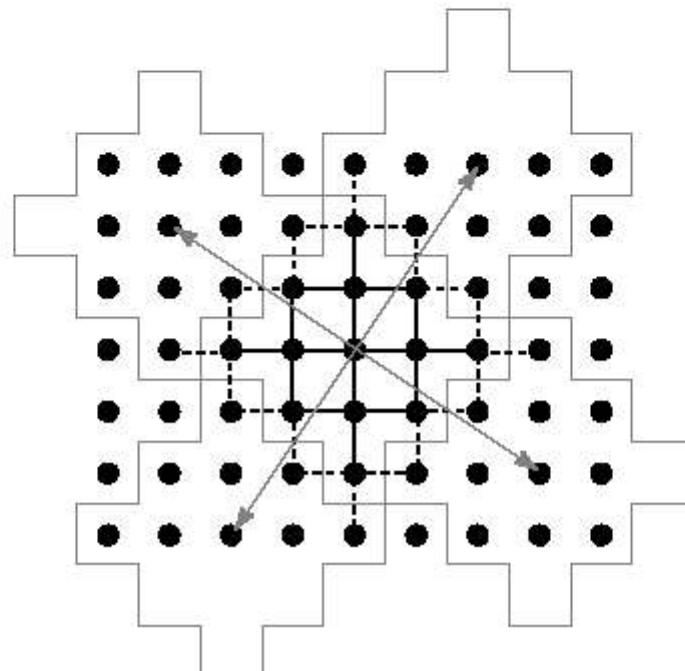
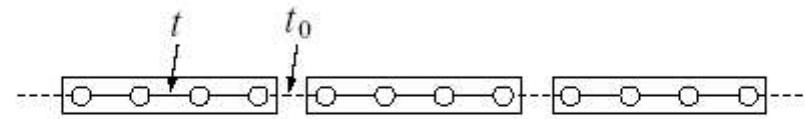
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# Cluster perturbation theory (CPT)

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

Vary  
cluster  
shape and  
size



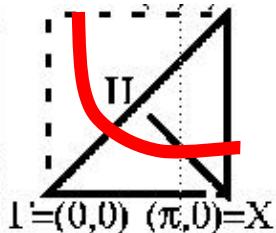
Sénéchal *et al.*  
PRL 2000,  
PRB 2002

# CPT

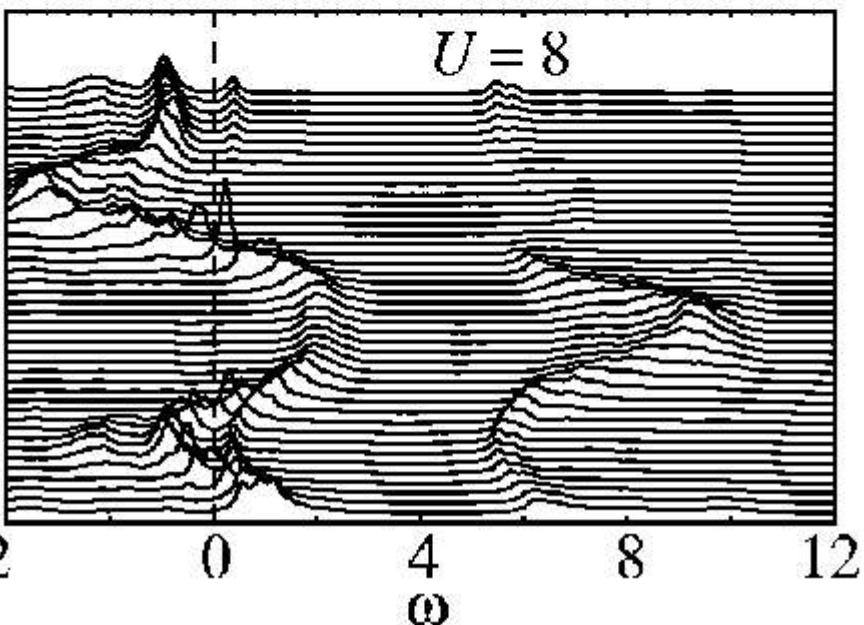
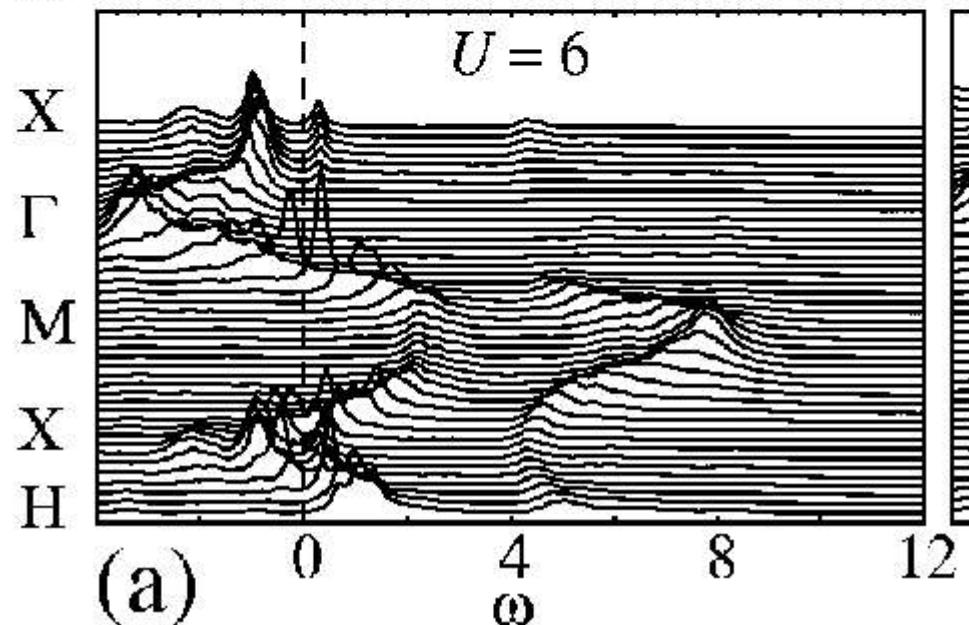
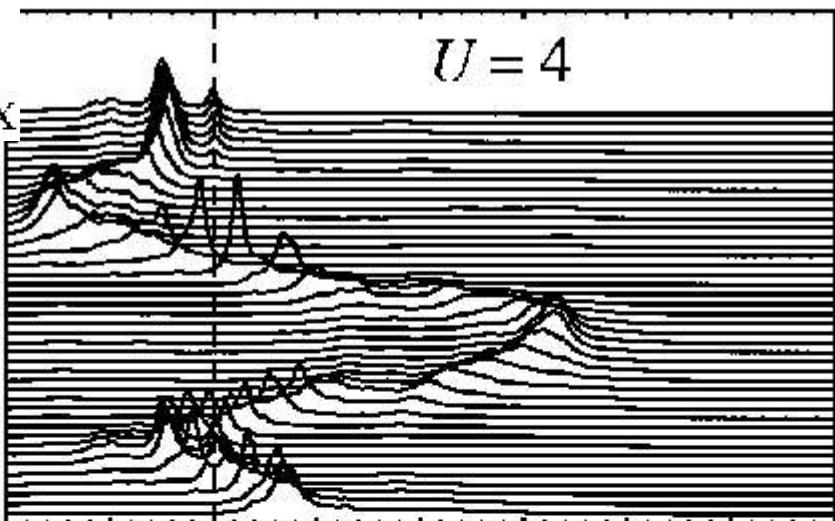
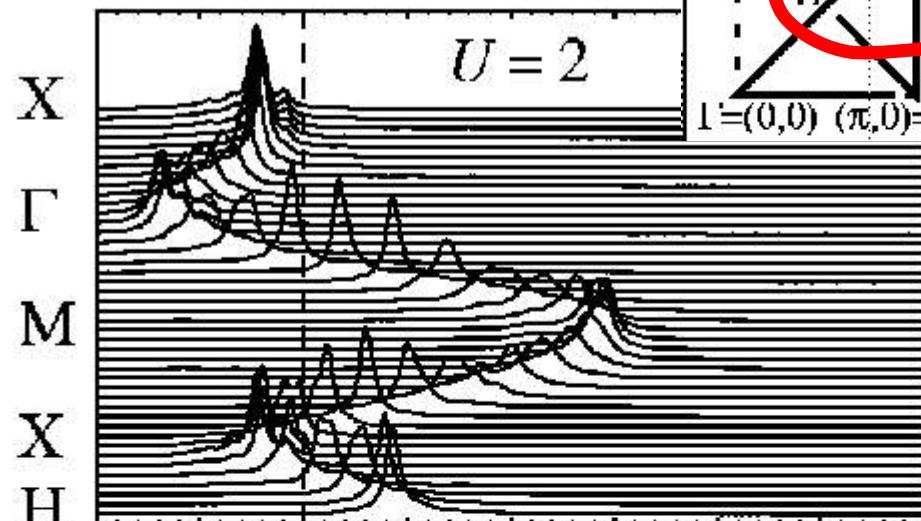
- Wave vector is continuous
  - Underlying cluster  $3 \times 4$  and  $4 \times 4$
- Exact for  $t=0$  and  $U=0$ .
- Finite energy resolution
  - Here about 40 meV (as in experiment).  
*Sénéchal et al.*  
PRL 2000,  
PRB 2002
- Tests:
  - spin-charge separation in  $d = 1$ .
  - $U=\text{infinity}$  limit.

# Hole-doped (17%)

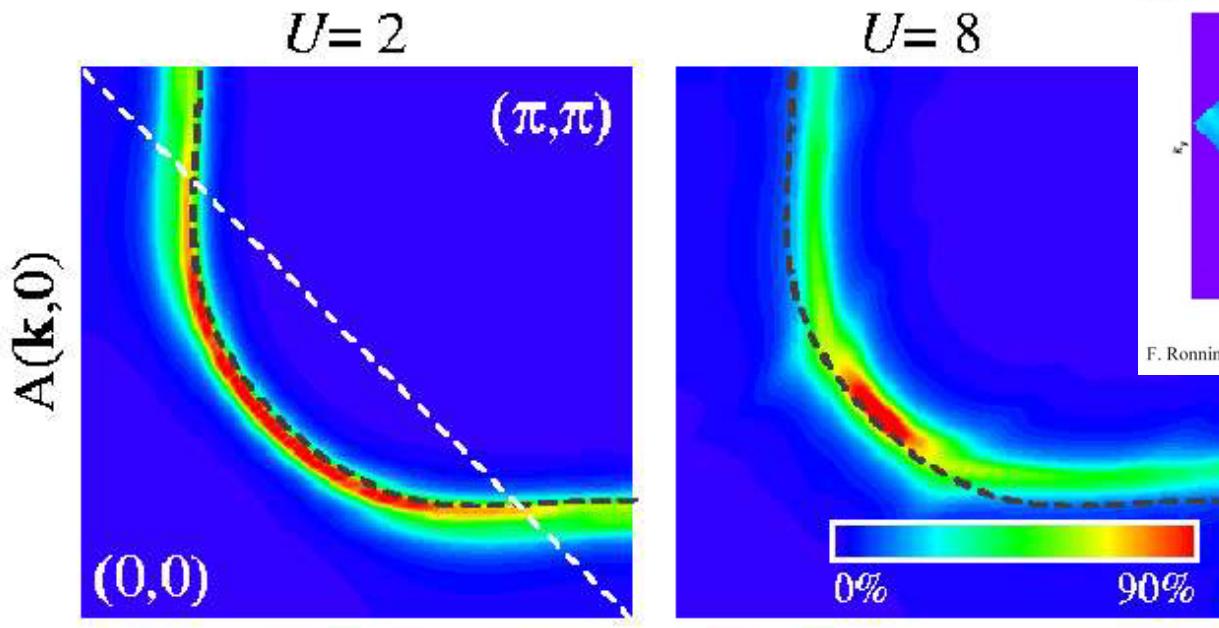
$t' = -0.3t$  ,  $t'' = 0.2t$



Sénéchal, AMT, PRL, in press



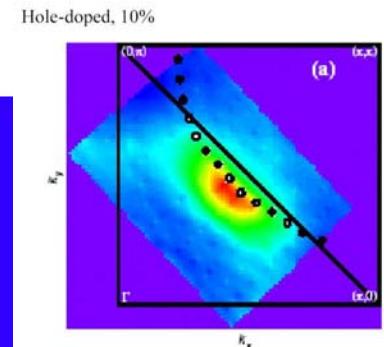
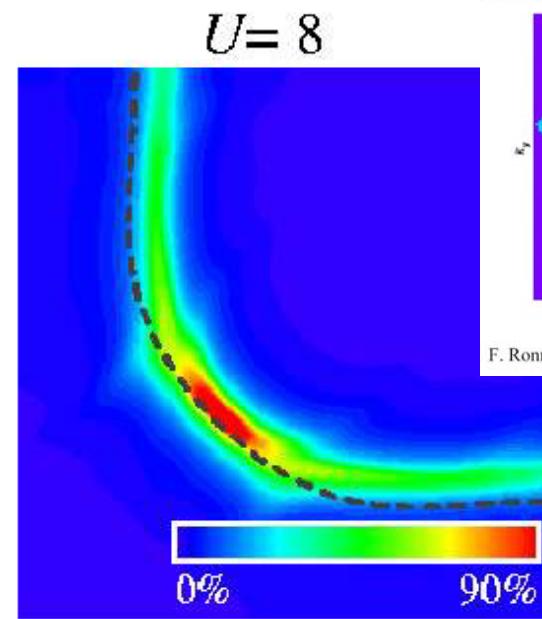
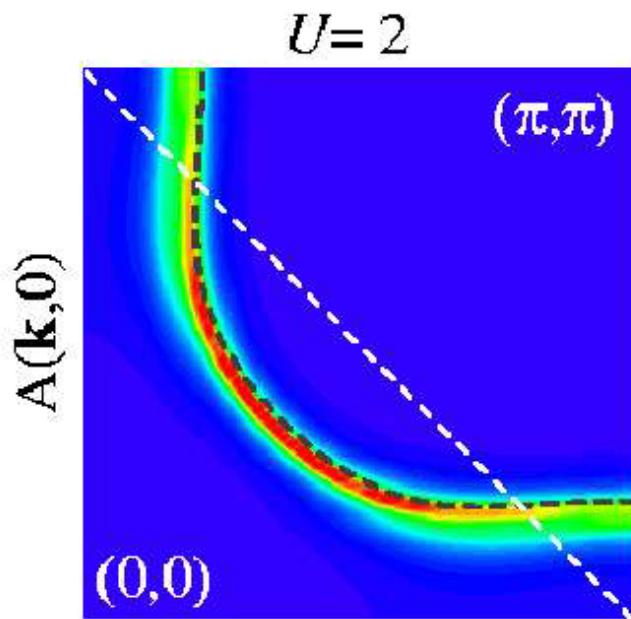
# Hole-doped (17%)



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

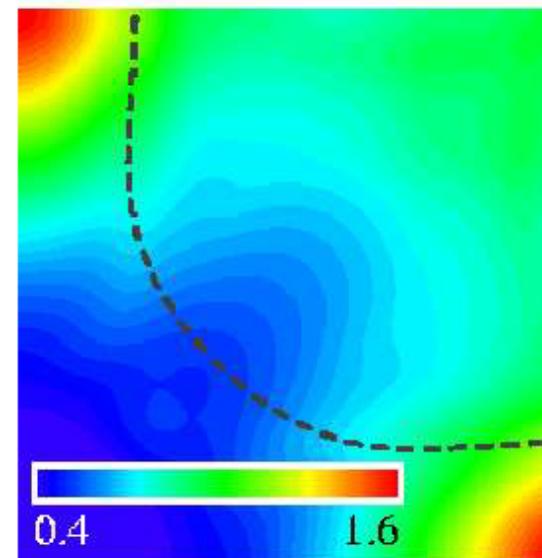
$$\eta = 0.12t$$
$$\eta = 0.4t$$

# Hole-doped (17%)



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

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



Sénéchal, AMT,  
PRL in press

# Hole-doped 17%, U=8t

$U=8$

Frequency  $\omega=-1$

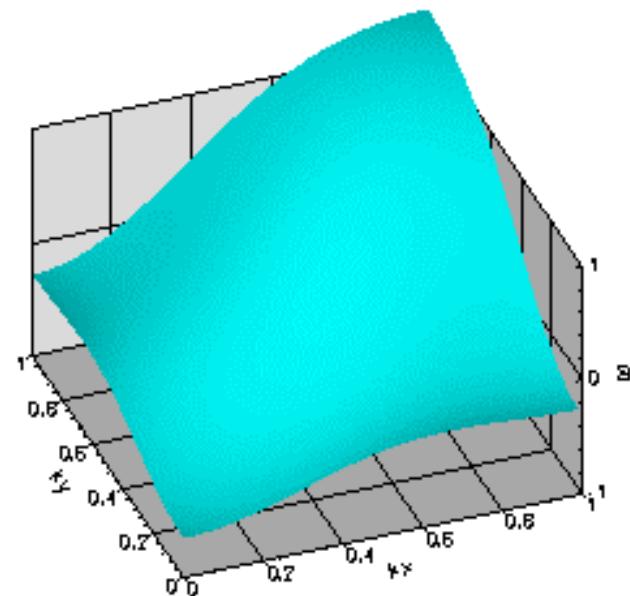
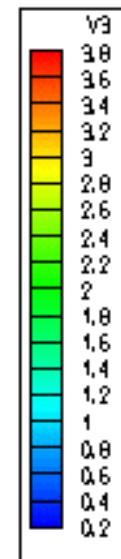
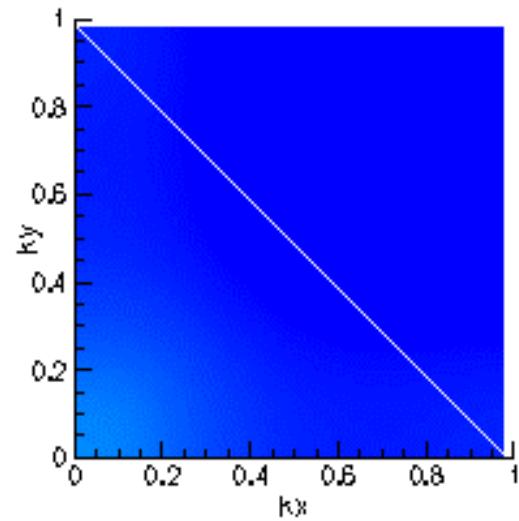
$U=2, n=10, t=0.25$   
 $t_d=-0.075, t_2=0.05$

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



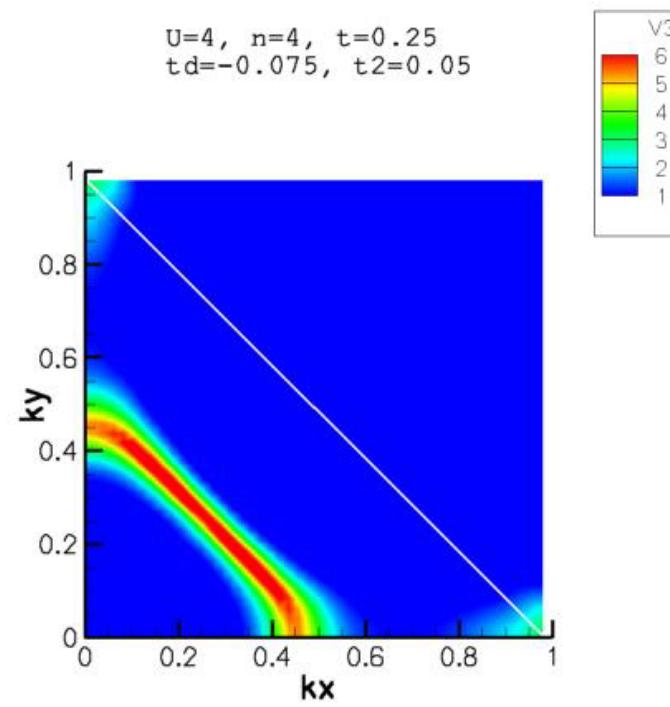
0%

90%



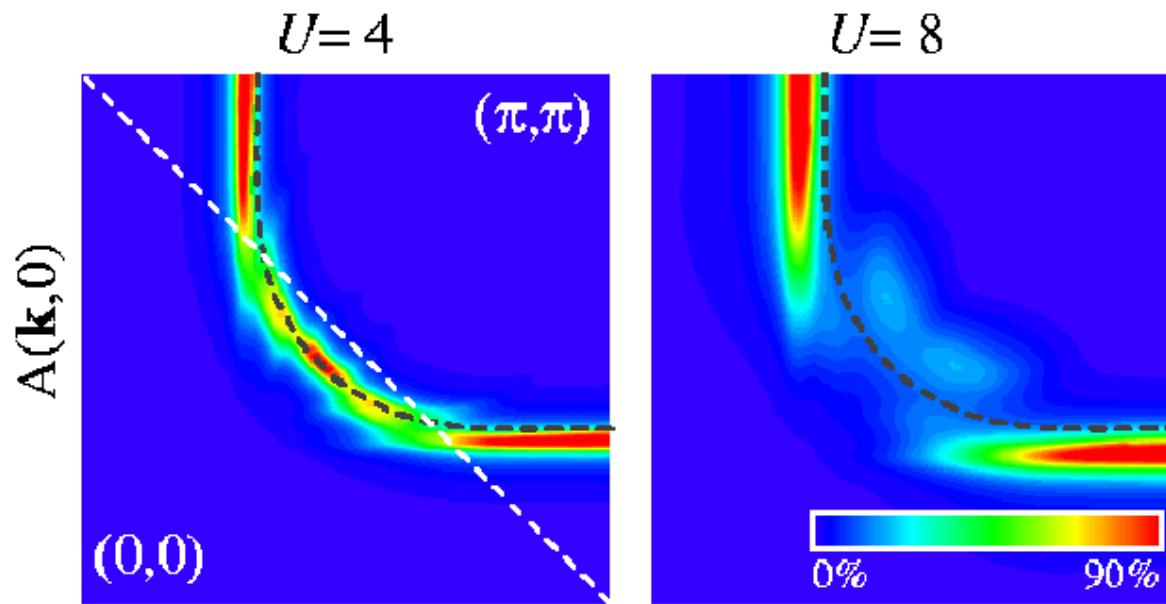
# Hole doped, 75%, $U = 16 t$

Frequency  $w=6.245e-17$



Frequenc

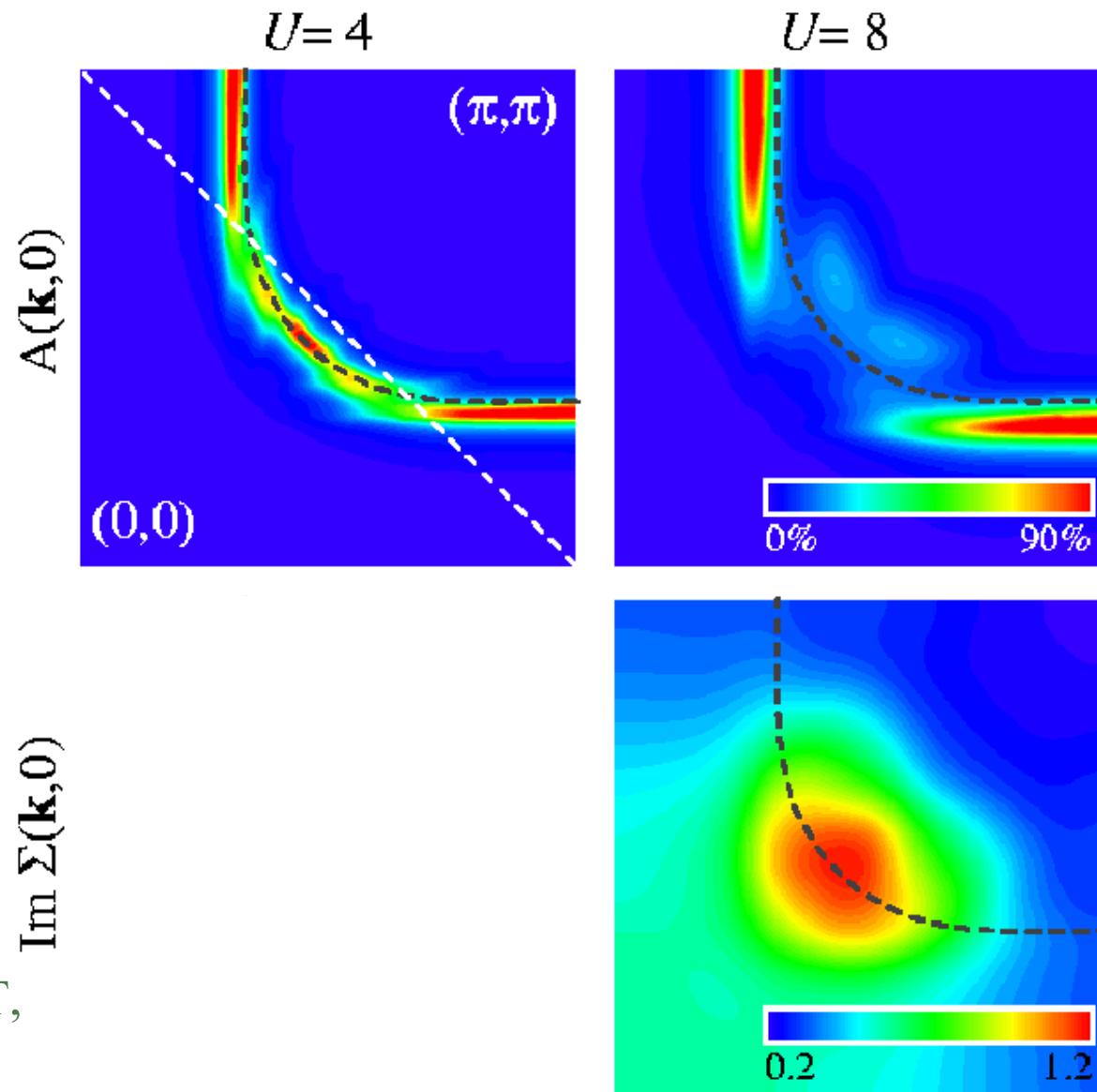
# Electron-doped (17%)



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

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

# Electron-doped (17%)

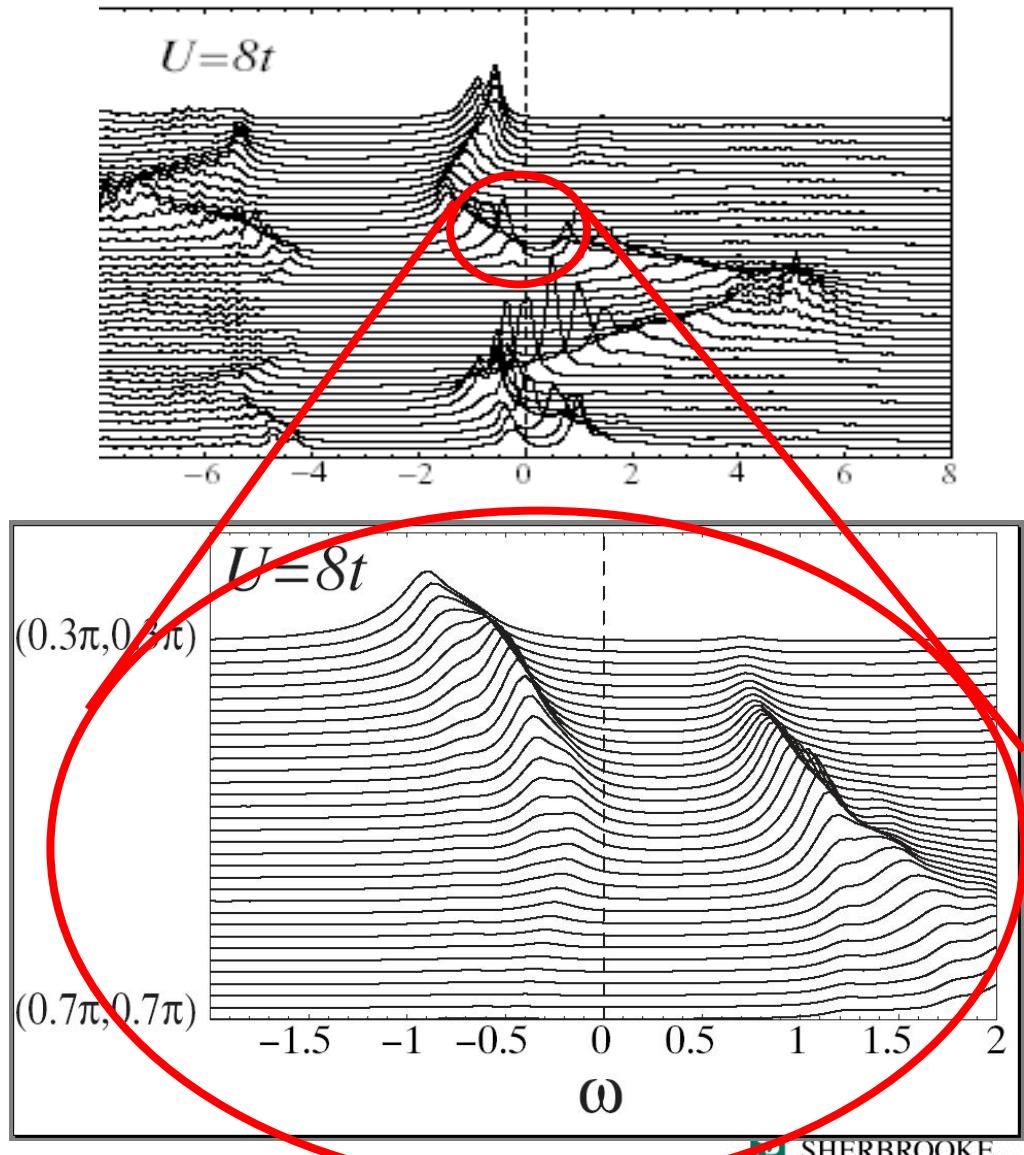
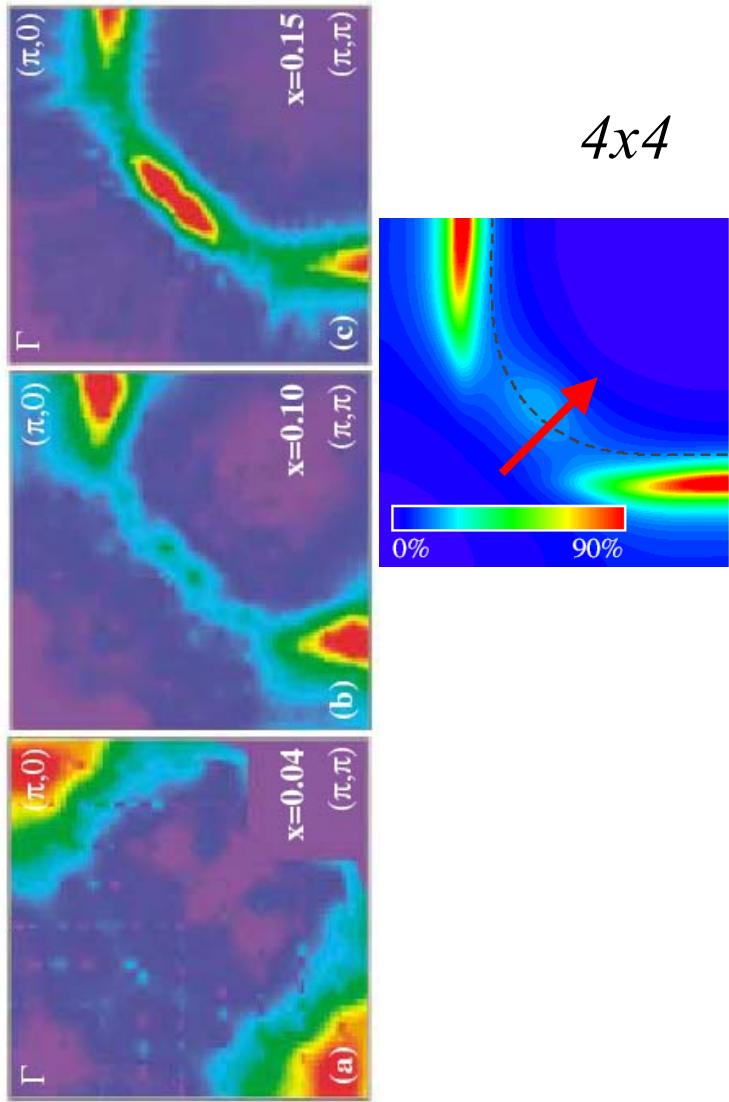


$$t' = -0.3t$$
$$t'' = 0.2t$$

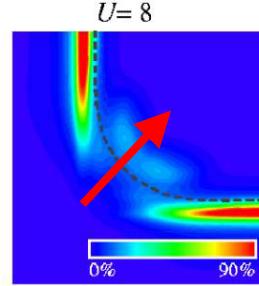
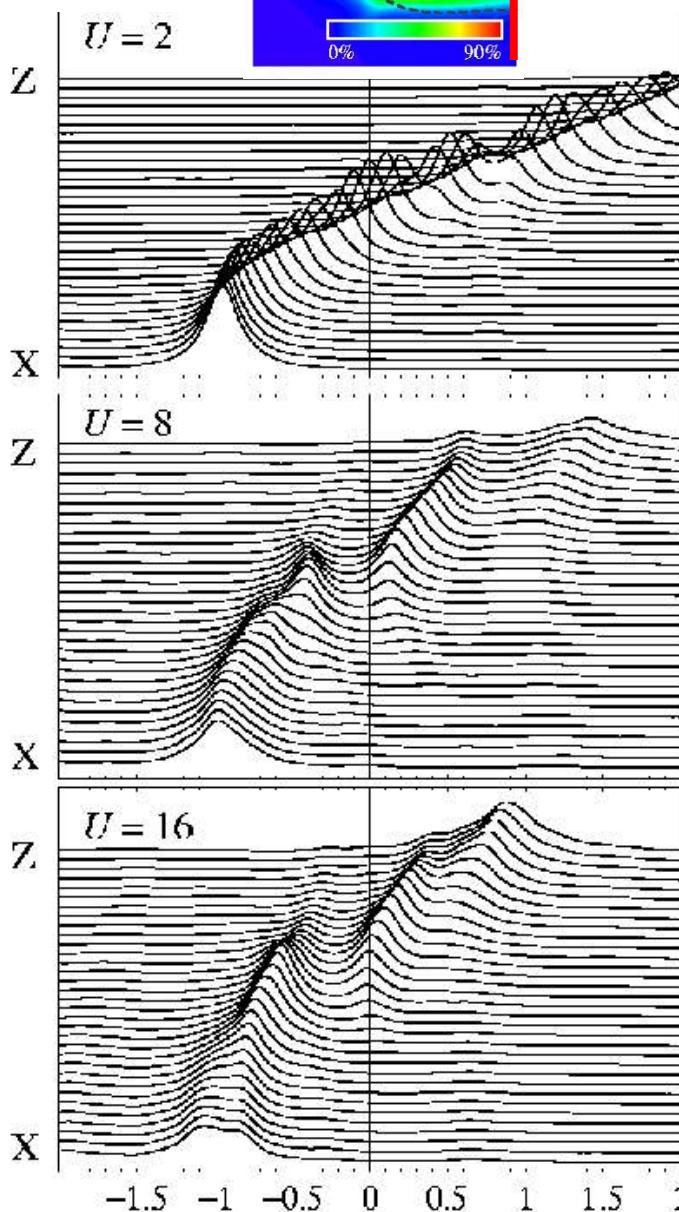
$$\eta = 0.12t$$
$$\eta = 0.4t$$

Sénéchal, AMT,  
PRL in press

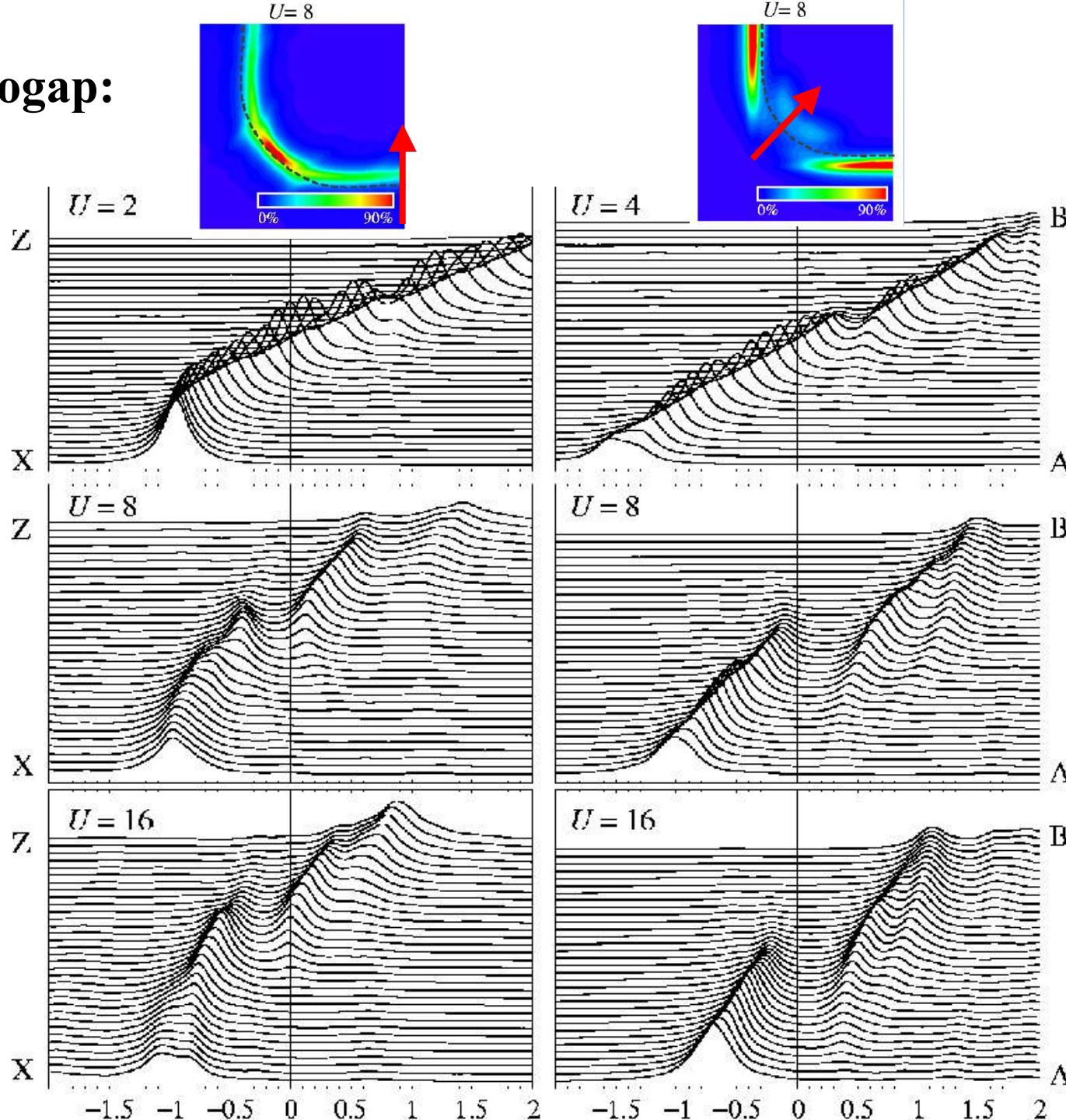
# Electron-doped 12.5%, $U=8t$



# Pseudogap:

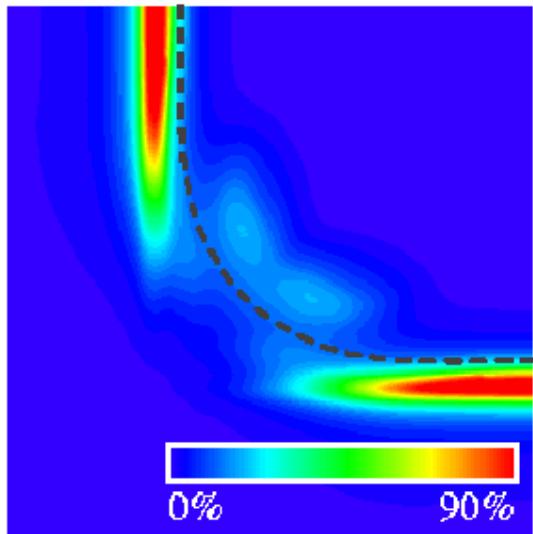


# Pseudogap:

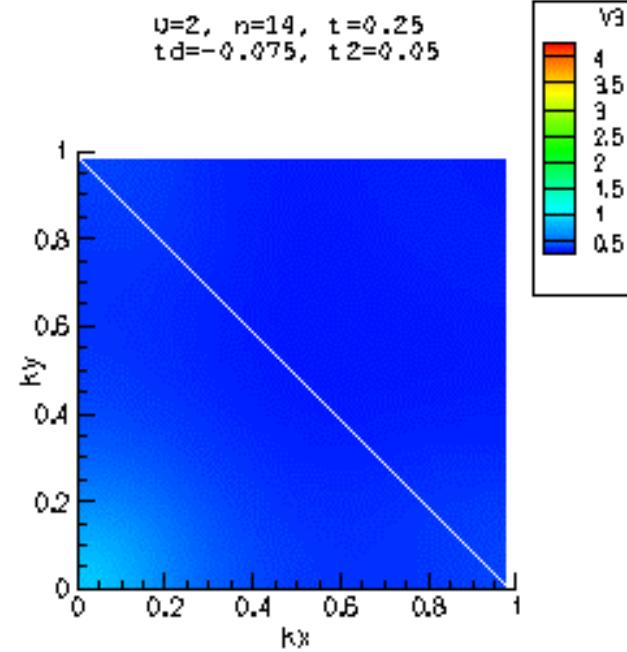


# Electron-doped, 17%, $U=8t$

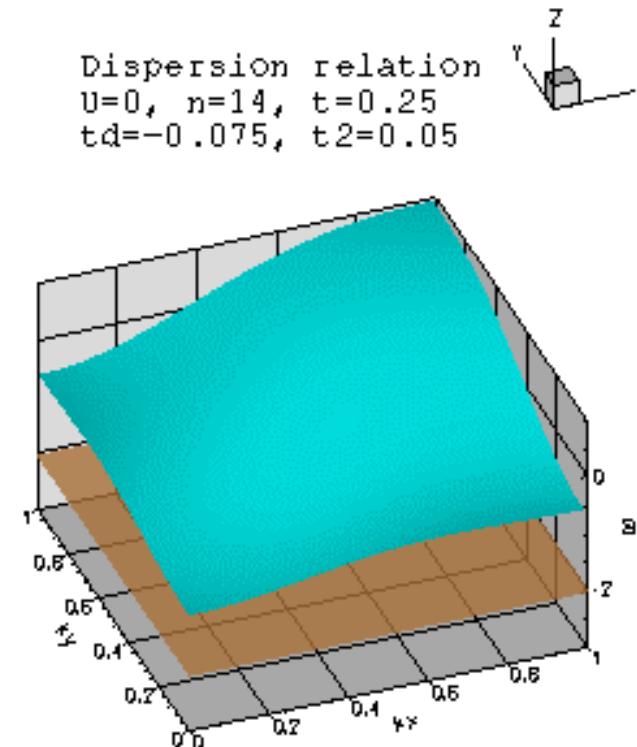
$U=8$



Frequency  $\omega=-2$

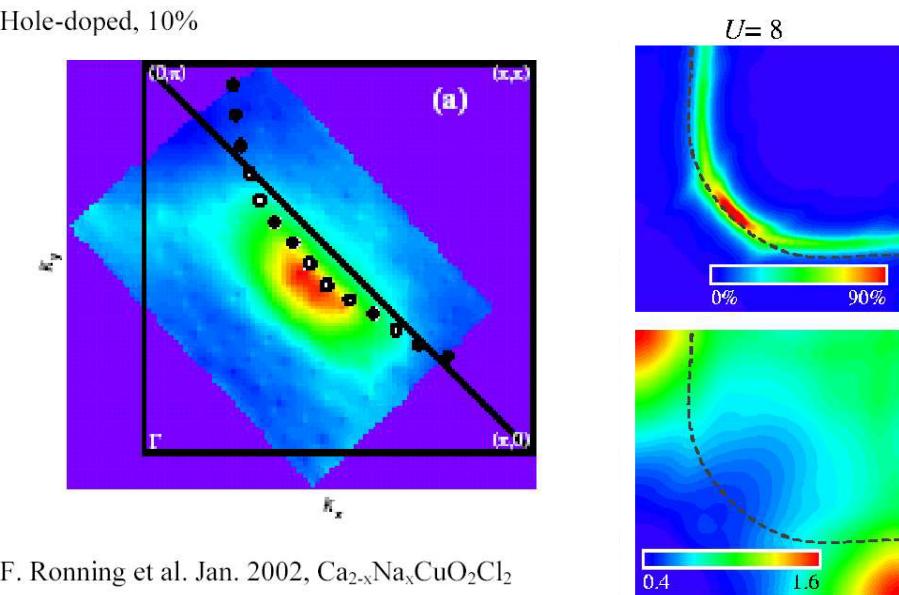


Dispersion relation  
 $U=0$ ,  $n=14$ ,  $t=0.25$   
 $t_d=-0.075$ ,  $t_2=0.05$



# Strong coupling pseudogap ( $U > 8t$ )

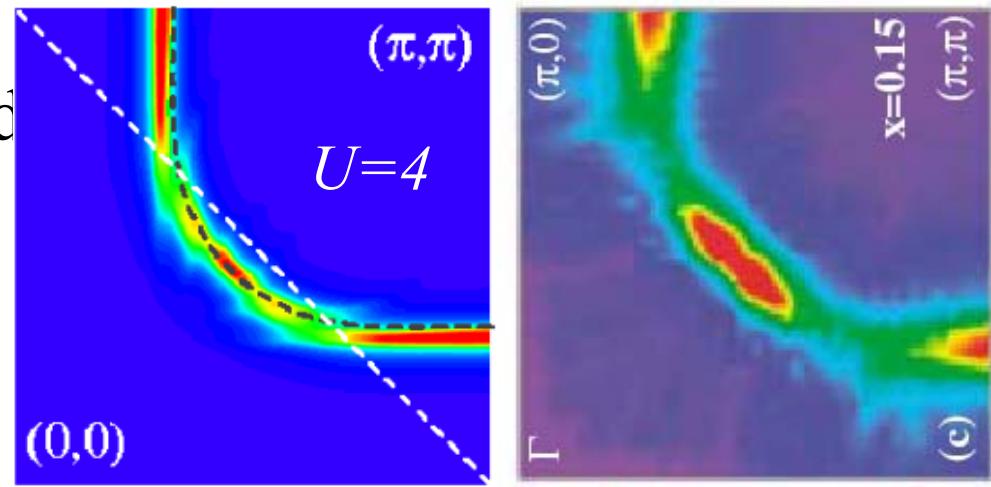
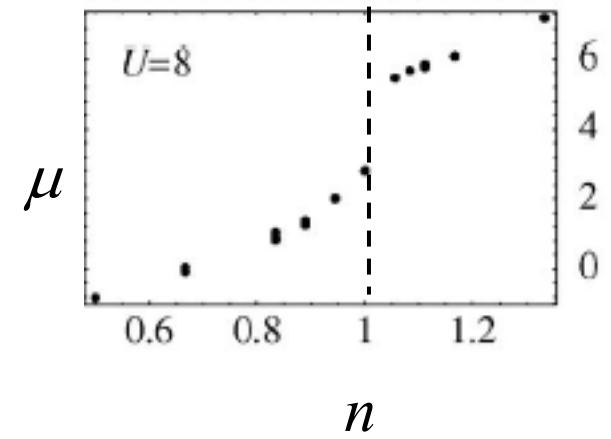
- Mott gap local (all  $k$ ) not tied to  $\omega=0$ .
- Pseudogap tied to  $\omega=0$  and only in regions nearly connected by  $(\pi,\pi)$ . (e and h),
- Pseudogap is independent of cluster shape (and size) in CPT.
- Not caused by AFM LRO
  - No LRO, few lattice spacings.
  - Not very sensitive to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



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

# Weak-coupling pseudogap

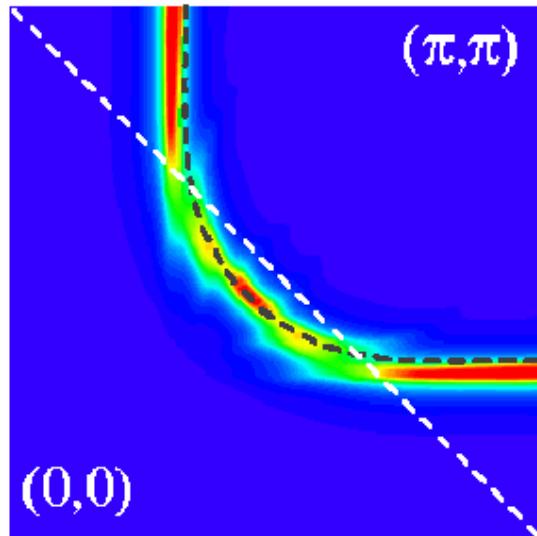
- In CPT
  - is mostly a depression in weight
  - depends on system size and shape.
  - located precisely at intersection with AFM Brillouin zone
- Coupling weaker because better screened  
 $U(n) \sim d\mu/dn$



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

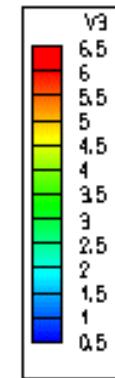
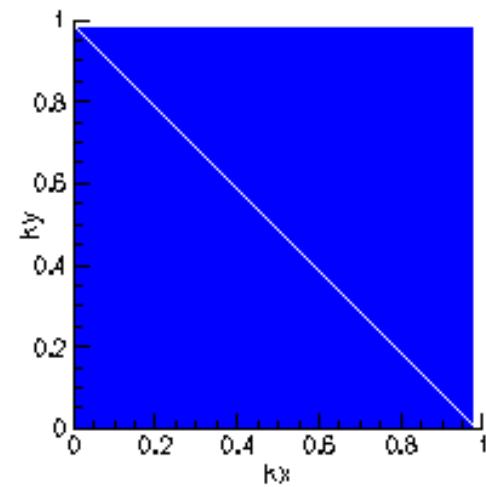
$U=4$

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

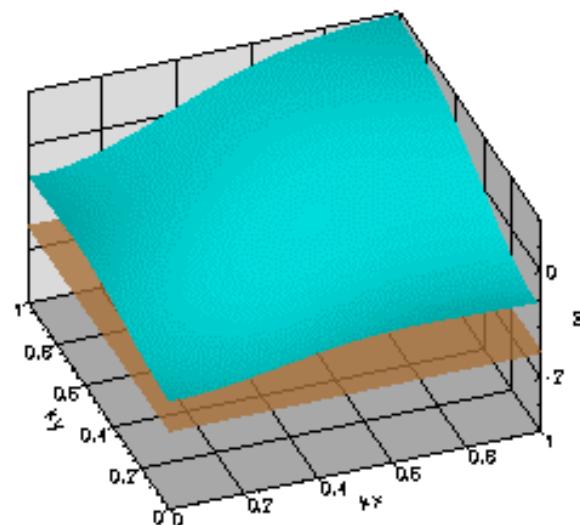
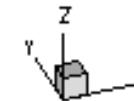


Frequency  $w=-1.5$

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



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



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# Quantum Monte Carlo, advantages and disadvantages

- Advantages
  - Sizes much larger than exact diagonalizations
  - As accurate as needed
- Disadvantages
  - Cannot go to very low temperature (except in special cases) (sign problem)
- **Use as benchmark for analytical approaches**

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

## - How it works

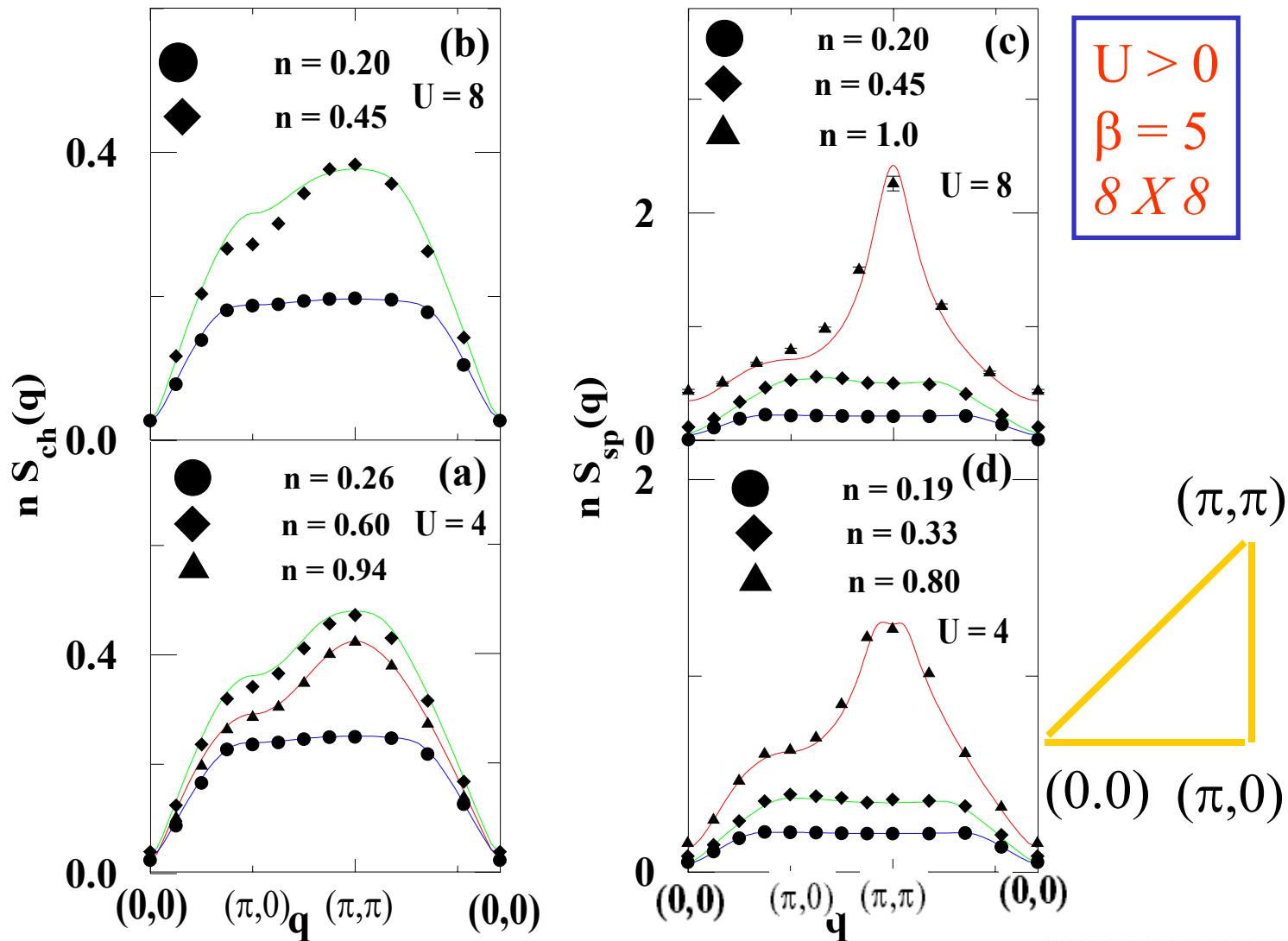
- General philosophy
  - Drop diagrams
  - Impose constraints and sum rules and try to satisfy them.
    - Pauli principle
    - Conservation laws
    - Mermin-Wagner theorem

Vilk, AMT J. Phys. I France, 7, 1309 (1997).

# Proof that TPSC is accurate. (Compare with QMC)

Notes:

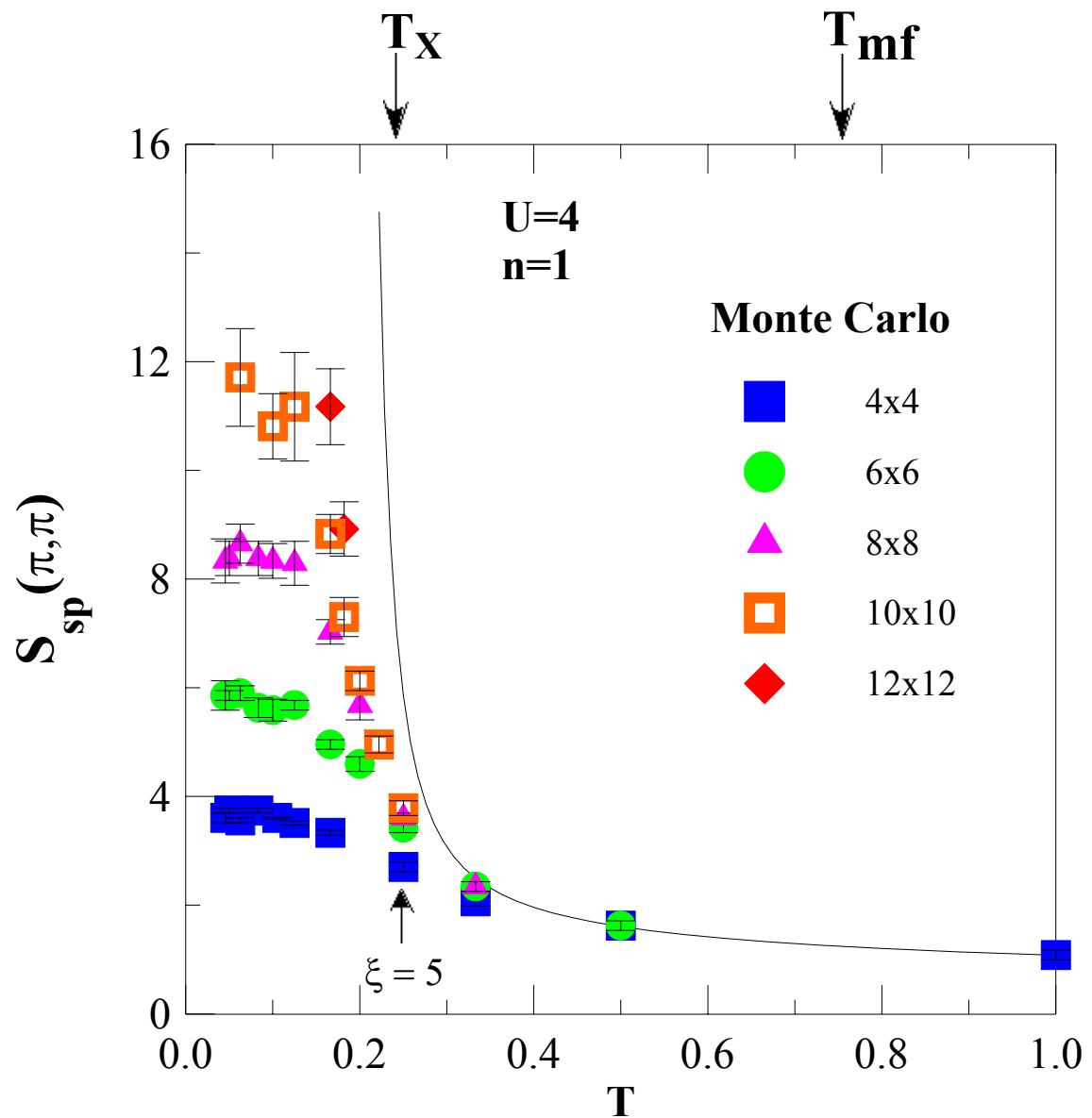
- F.L. parameters
- Self also Fermi-liquid



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

$n=1$

$$\xi \sim \exp(C(T) / T)$$

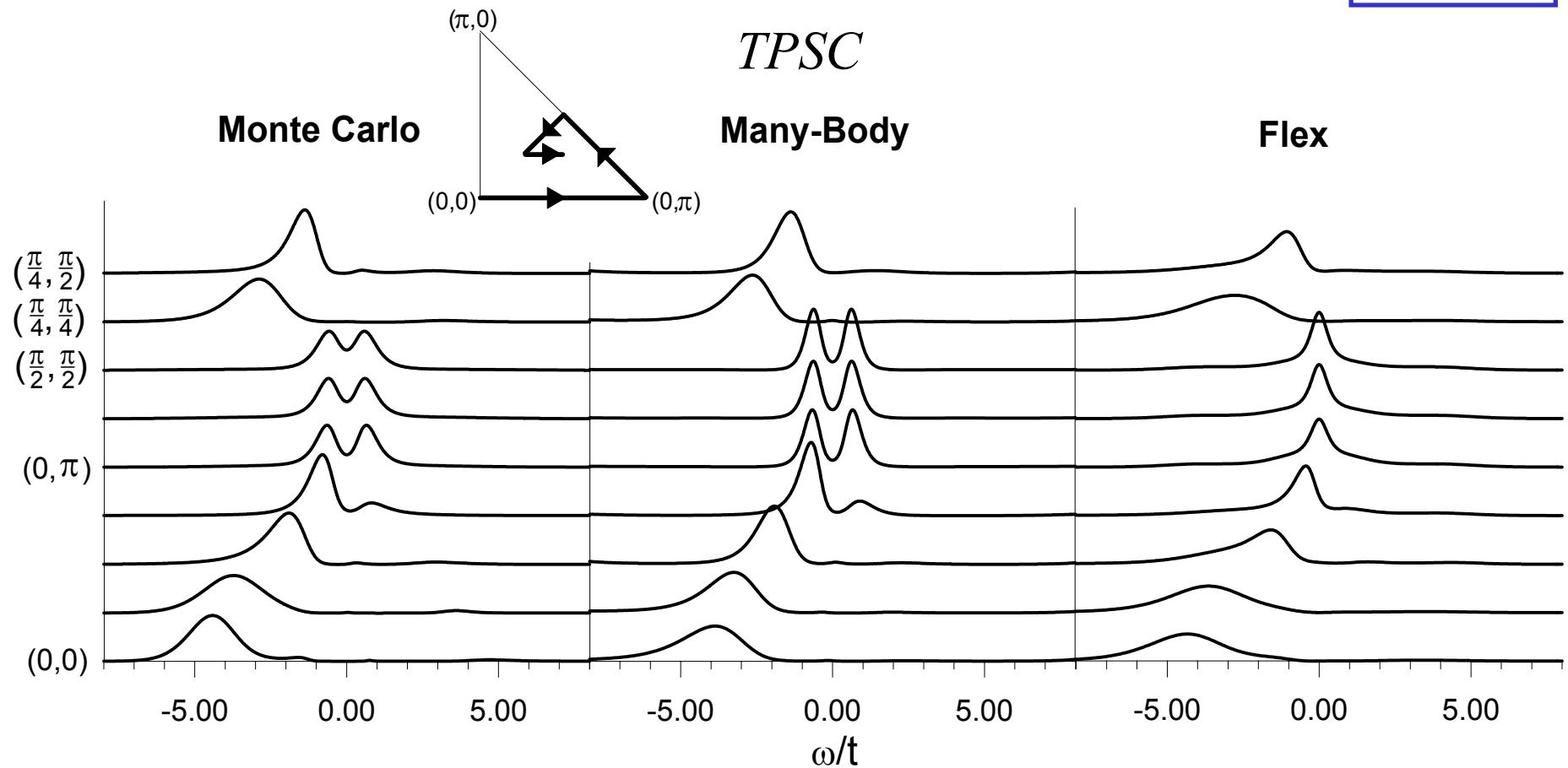


Calc.: Vilk et al. P.R. B **49**, 13267 (1994)

QMC: S. R. White, et al. Phys. Rev. **40**, 506 (1989).

Proofs...

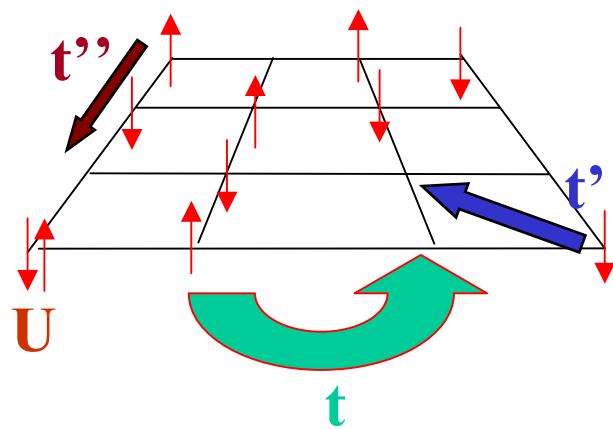
$U = +4$   
 $\beta = 5$



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

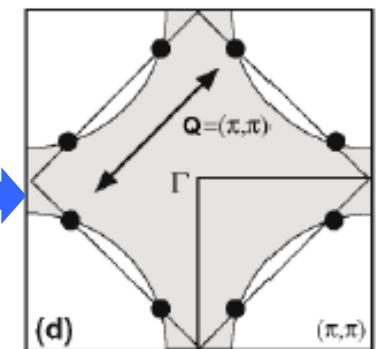
# The 2D Hubbard model

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



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

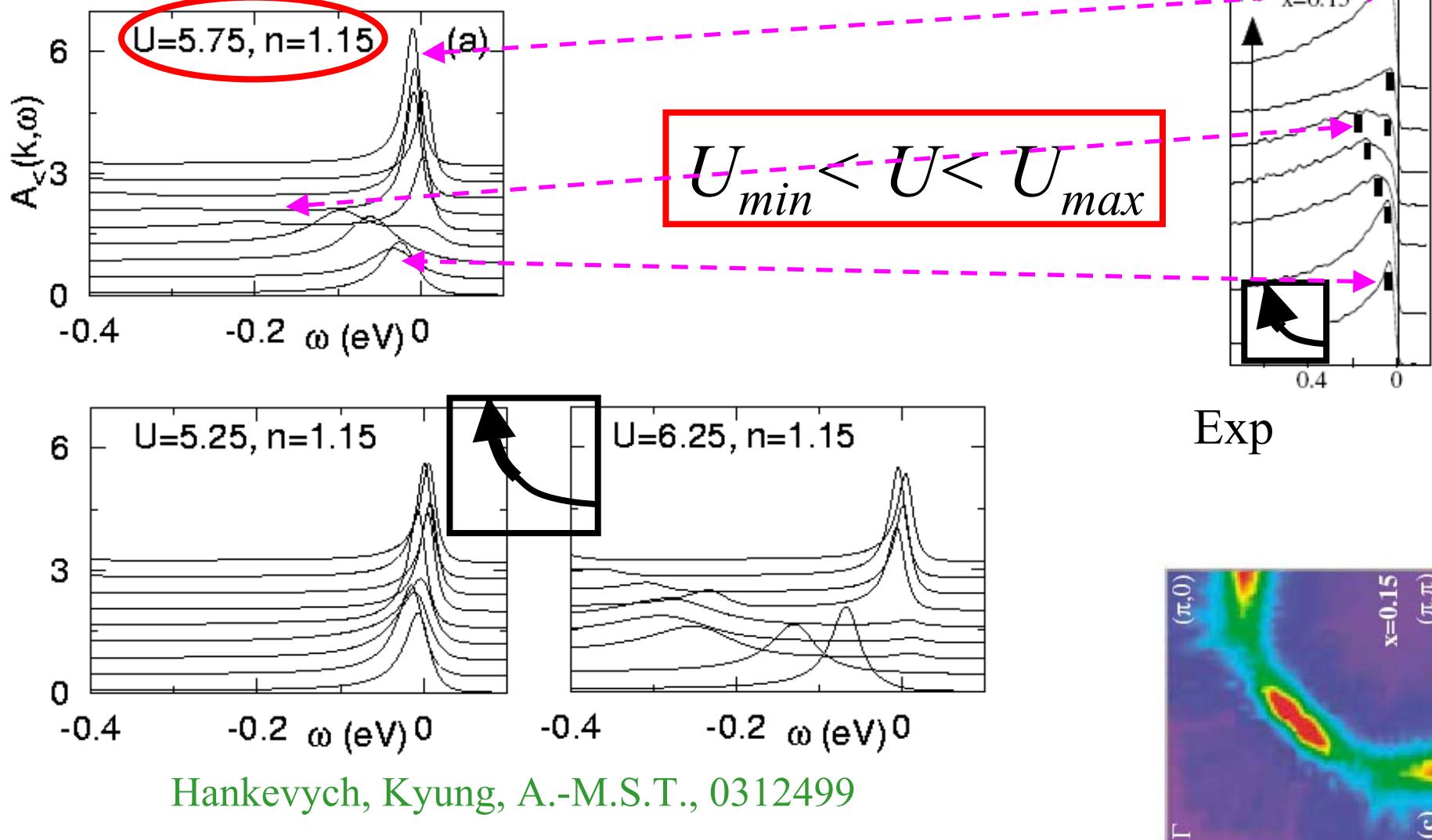
fixed



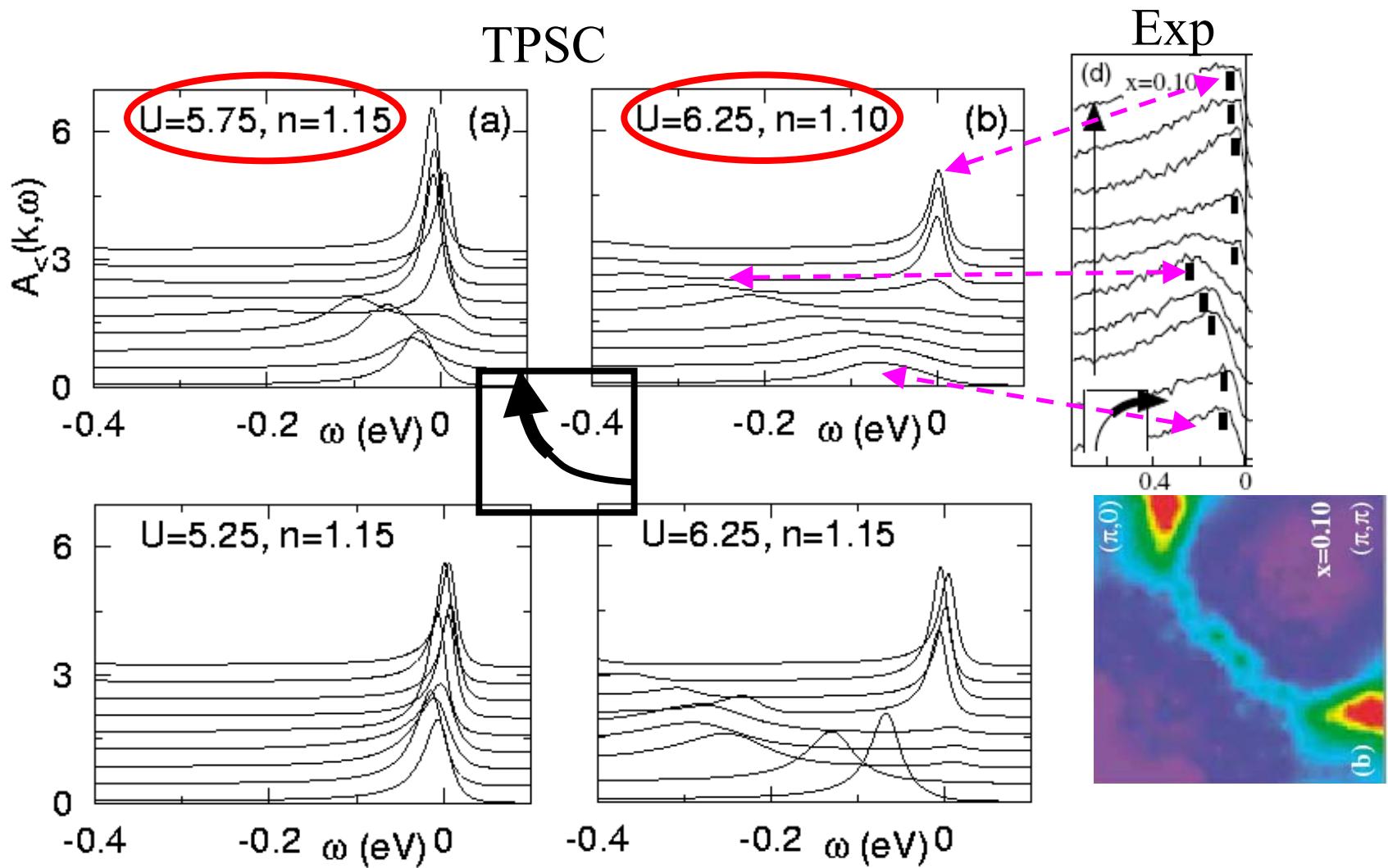
Weak coupling  $U < 8t$

$n = 1 + x$  – electron filling

# 15% doping: EDCs along the Fermi surface TPSC

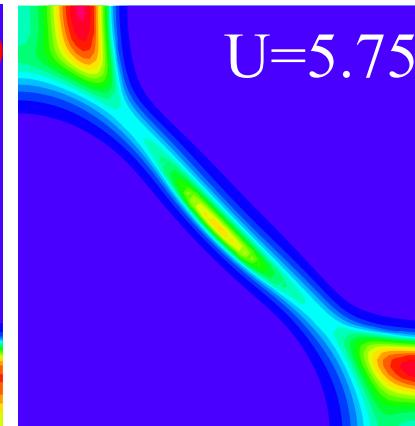
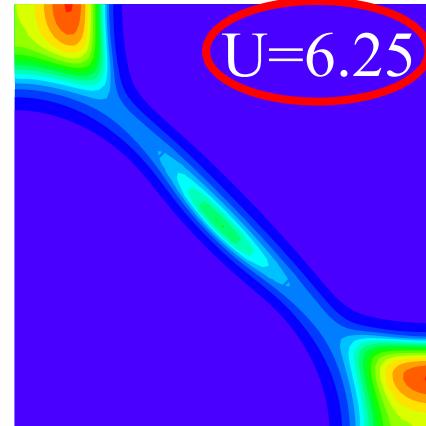
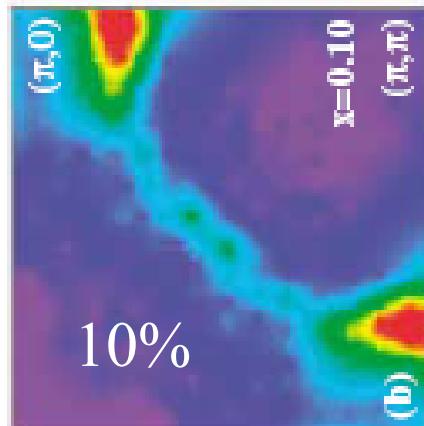
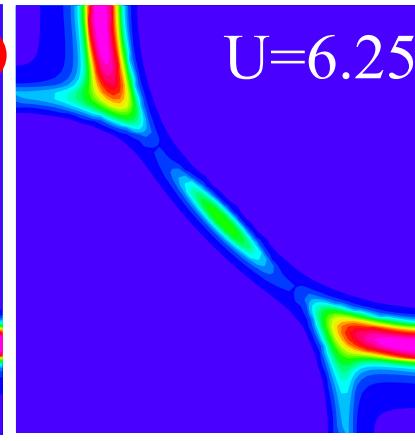
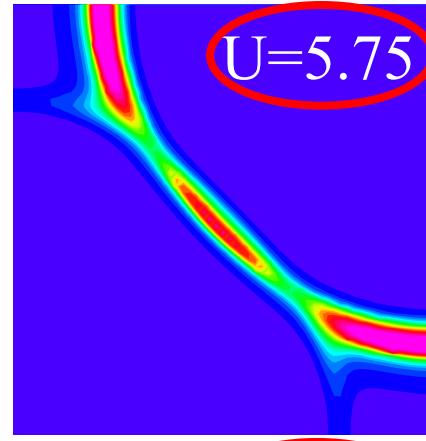
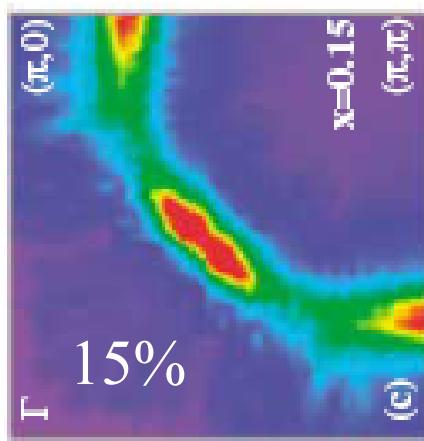


# EDCs along the Fermi surface TPSC

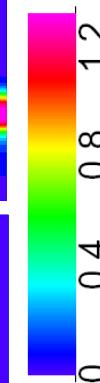


# Fermi surface plots

Hubbard repulsion  $U$  has to...

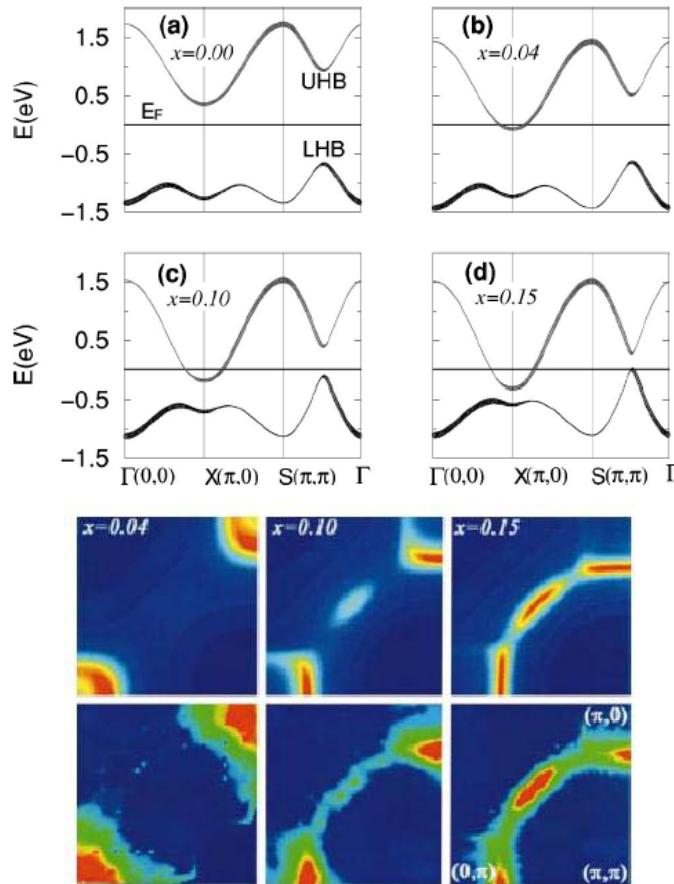


be not too large



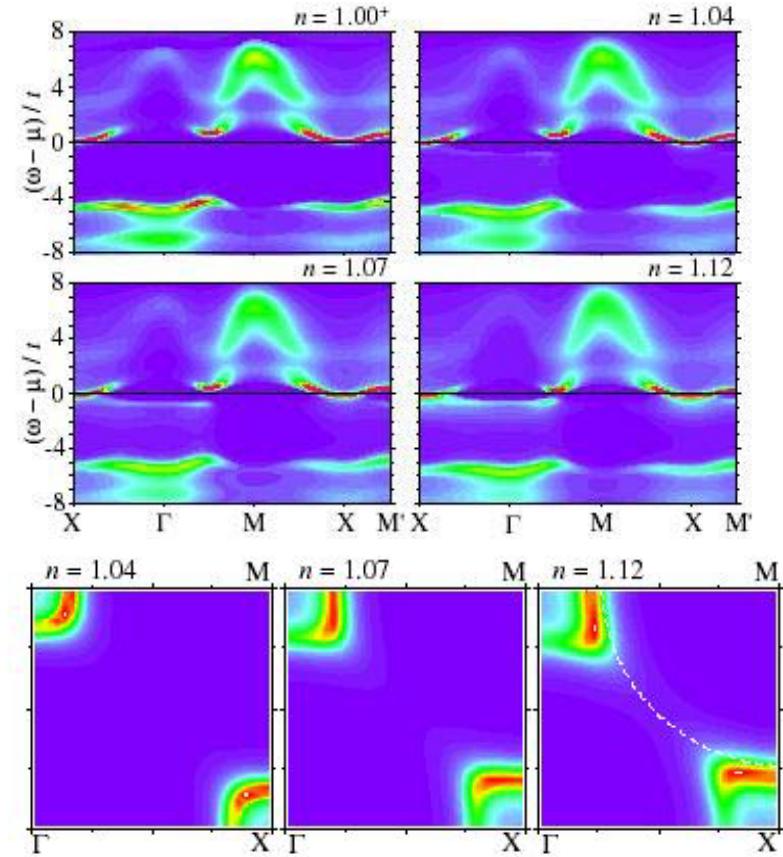
increase for  
smaller doping

# Contrast

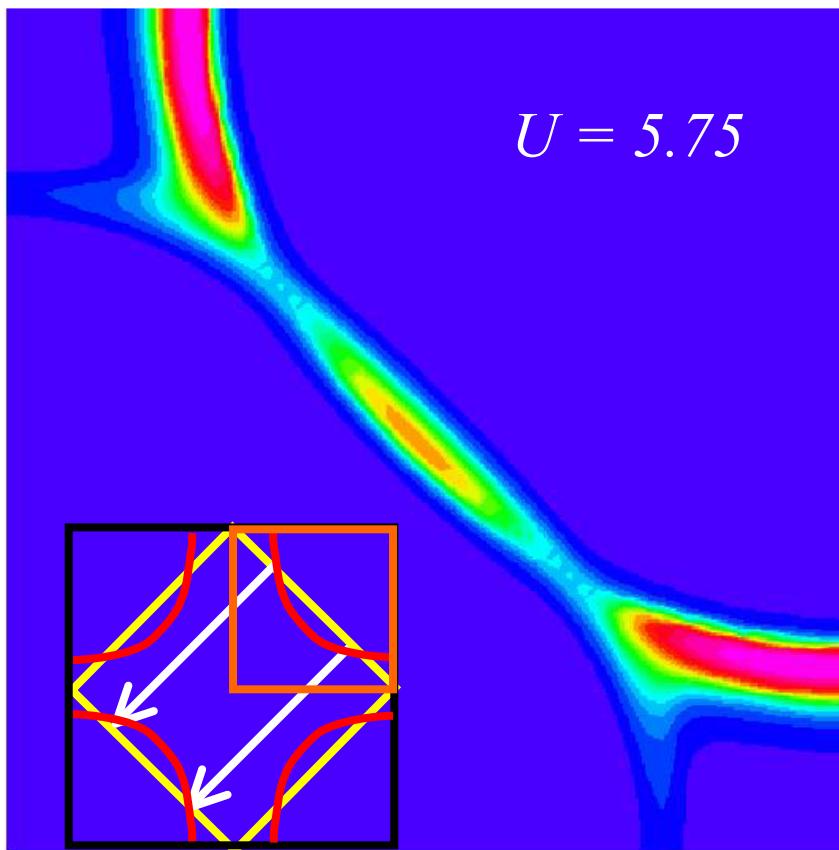


Kusko, Markiewicz, Bansil, PRB 2002,

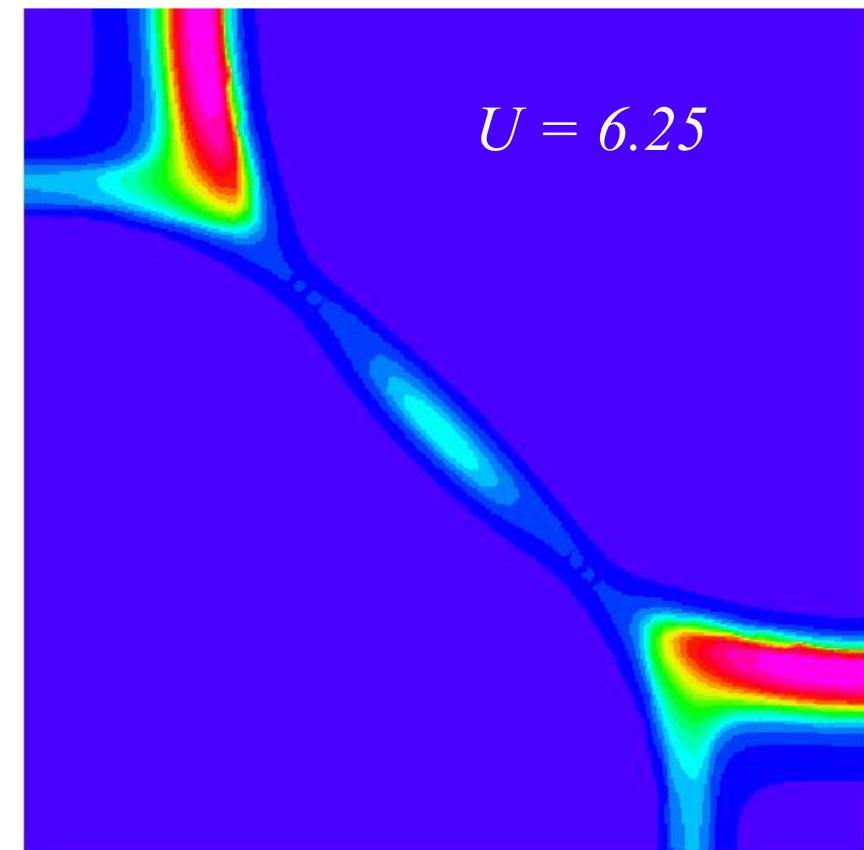
Kusunose, Rice, Phys. Rev. Lett. (2003).



# TPSC for electron-doped, 15%



$$U = 5.75$$



$$U = 6.25$$

$$t' = -0.175, t'' = 0.05$$

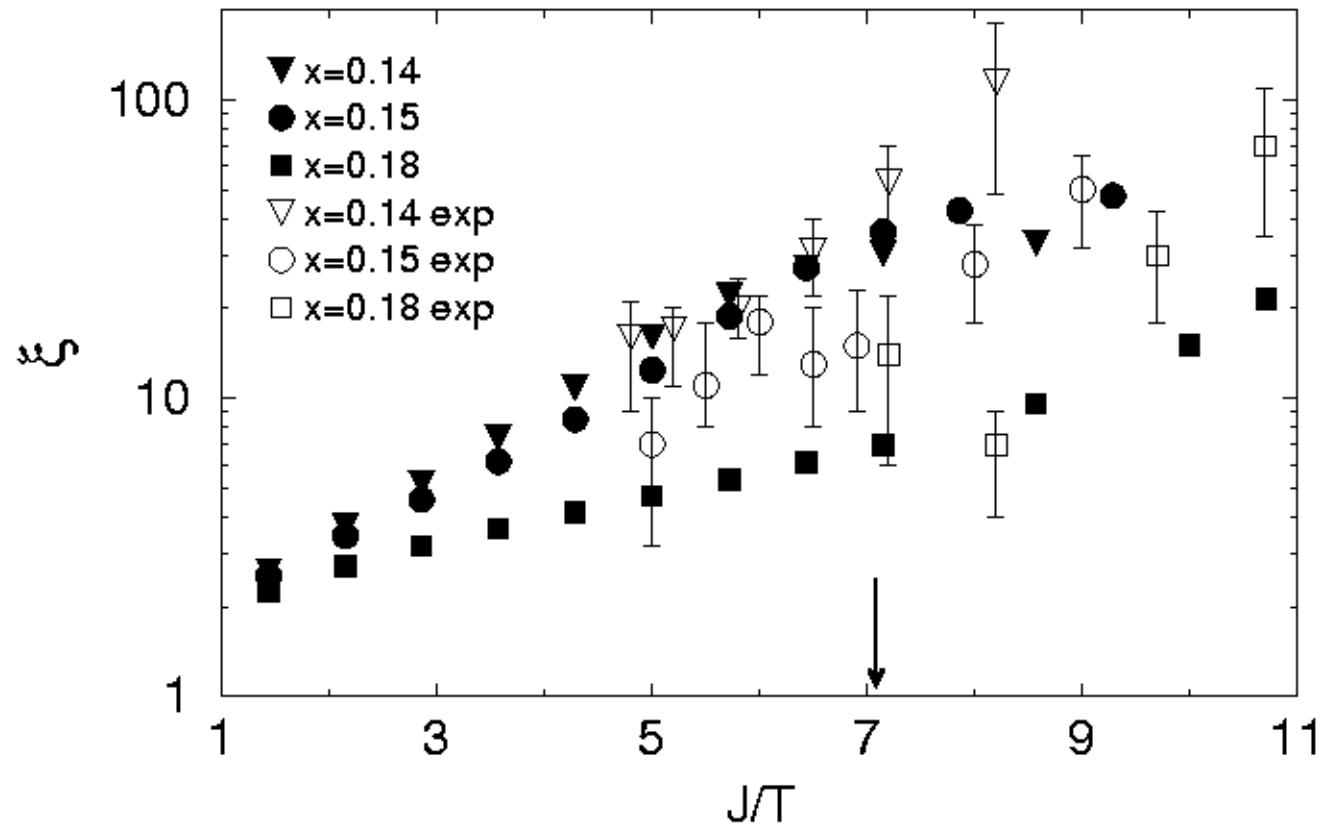
$$n = 1.15$$

$$\beta = 40$$

**$U$  cannot be too large to have three spots!**

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

# AFM correlation length (neutron)



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

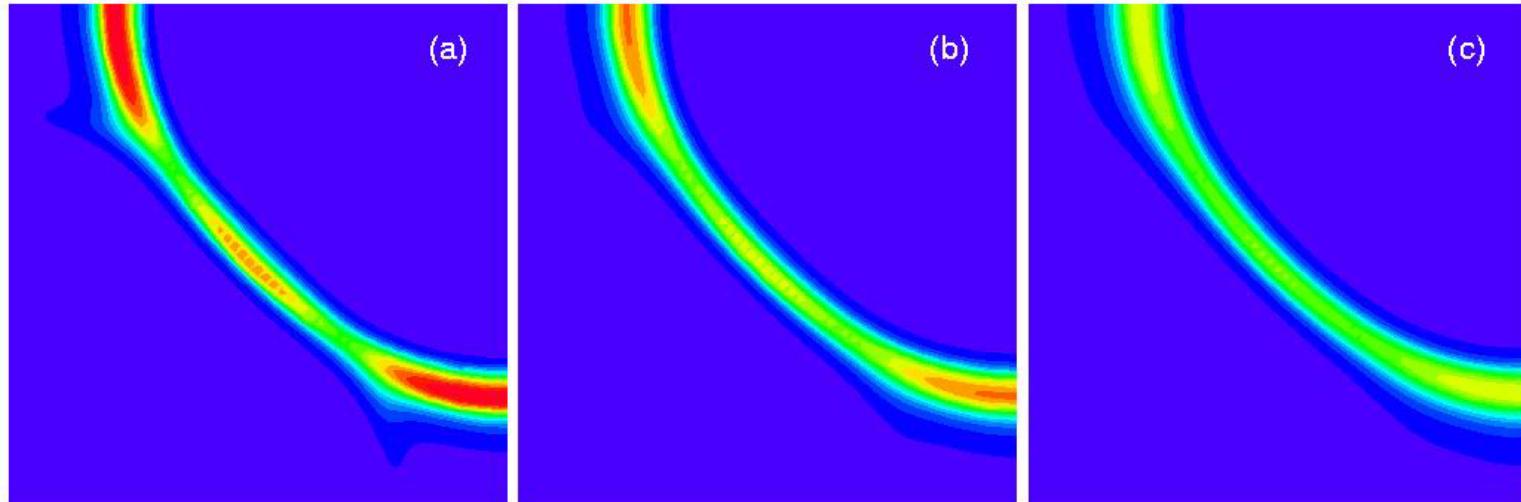
Expt: P. K. Mang et al., cond-mat/0307093, Matsuda (1992).

# Temperature dependence of ARPES

$\beta = 15$

$\beta = 10$

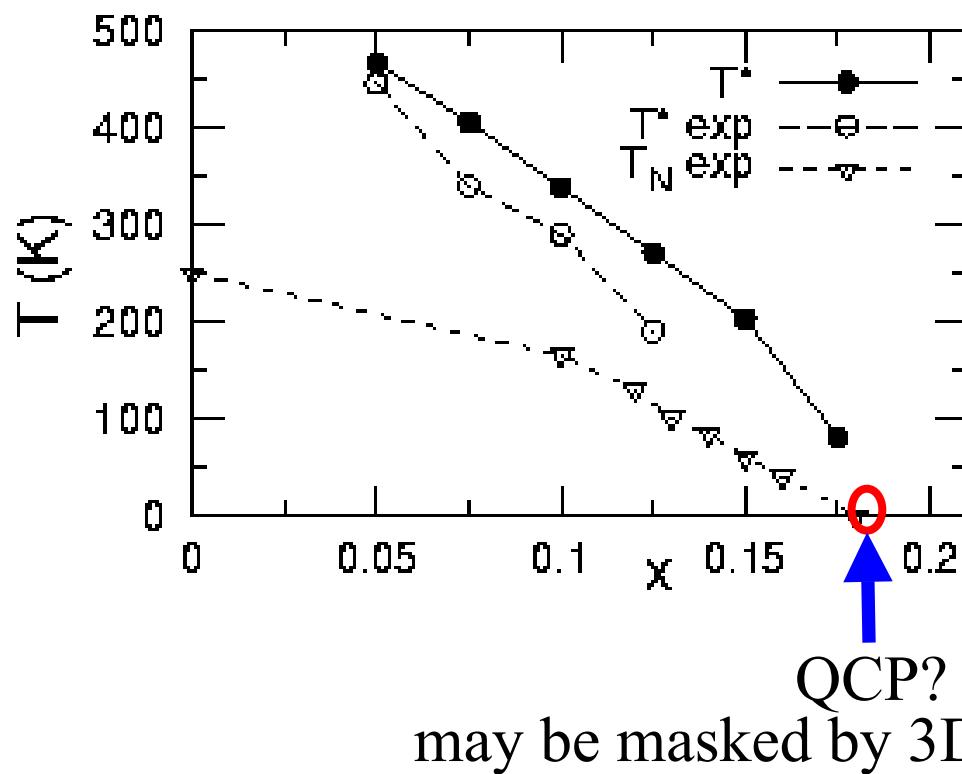
$\beta = 7.5$



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

Kyung, Hankevych, AMT, cond-mat/0312499

# Pseudogap temperature and QCP



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



supports further AFM  
fluctuations origin of PG

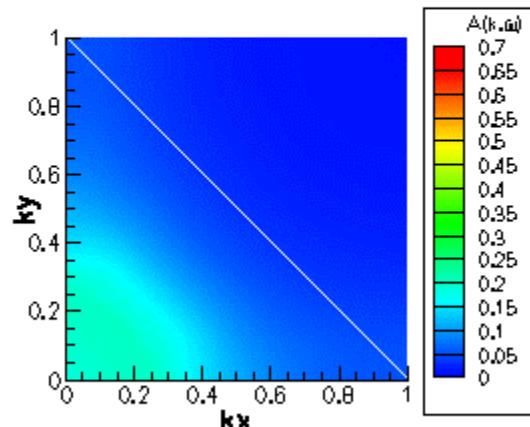
➤ ARPES to do:  
when does PG disappear  
with increasing  $T$

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

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

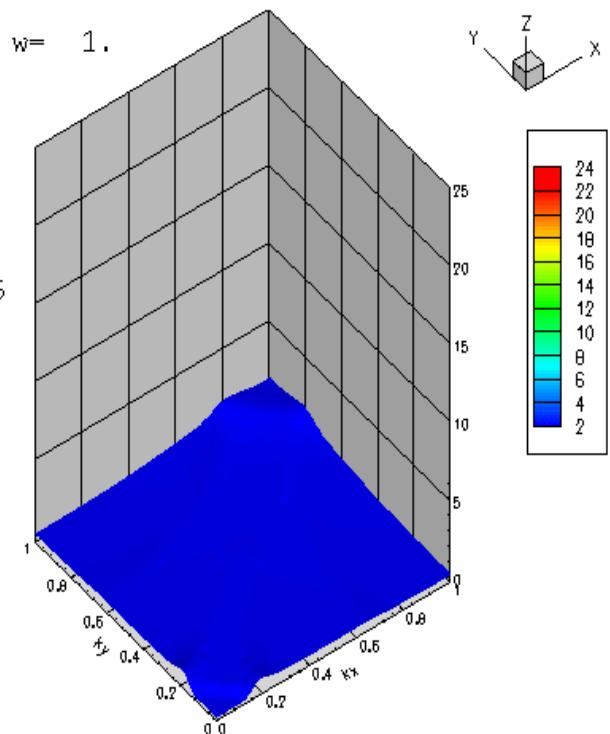
Frequency  $w = -4$ .

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



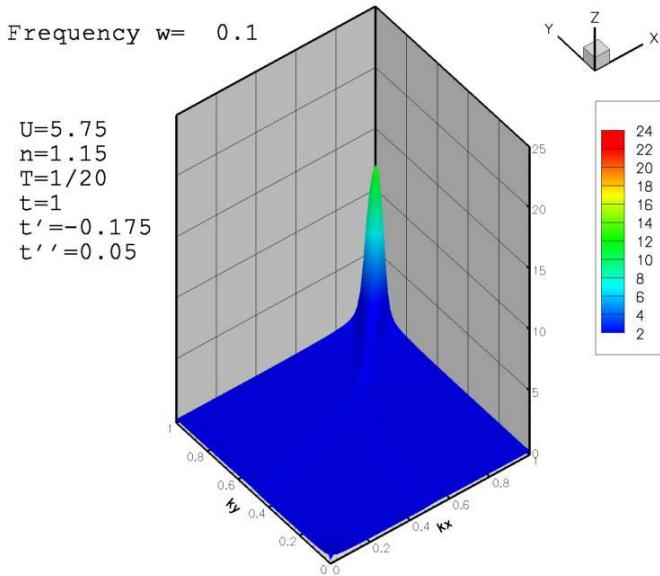
Frequency  $w = 1$ .

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

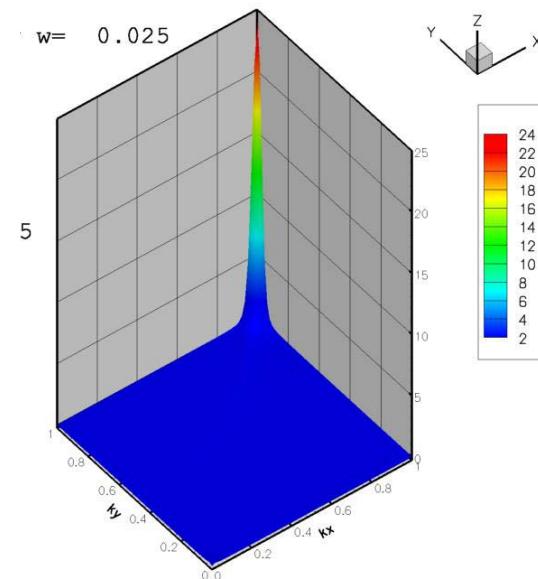


# Electron doped 15% low $T=0.05t$

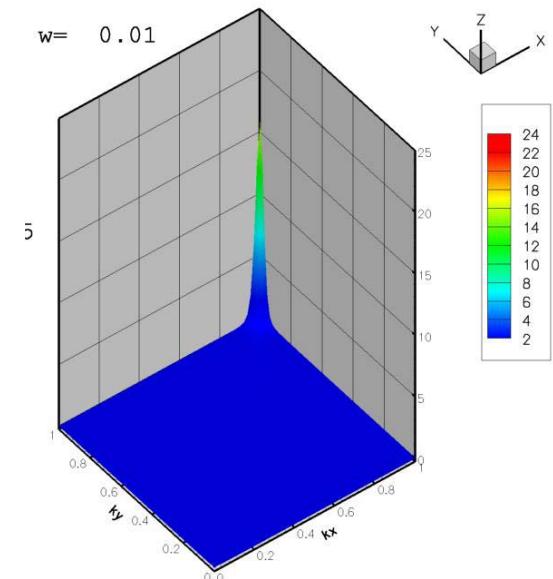
$\omega = 0.1t$



$\omega = 0.02t$



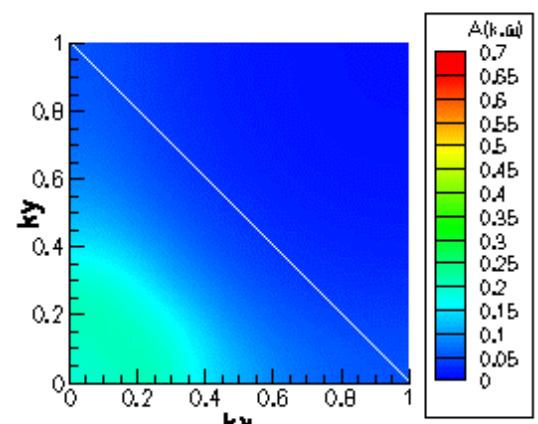
$\omega = 0.01t$



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

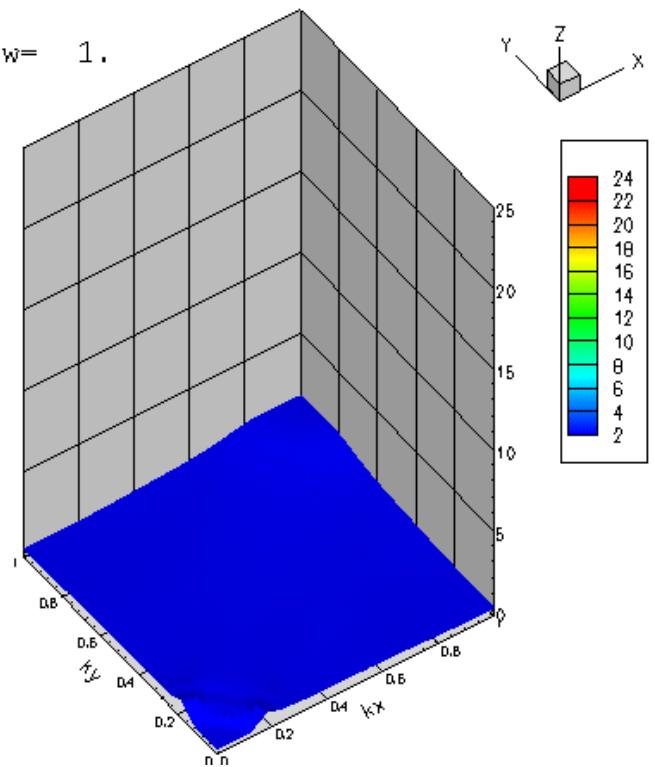
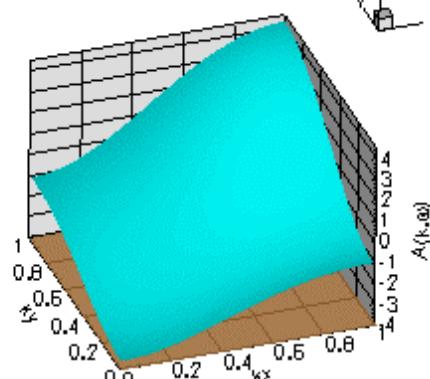
Frequency  $\omega = -4$ .

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



Frequency  $\omega = 1$ .

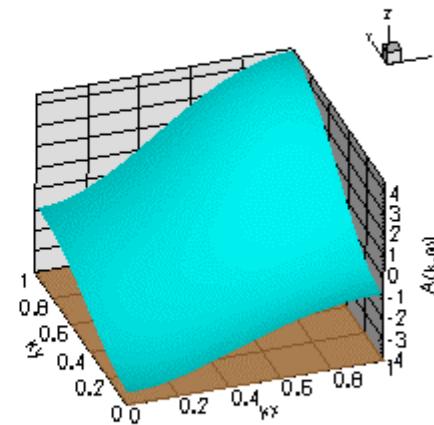
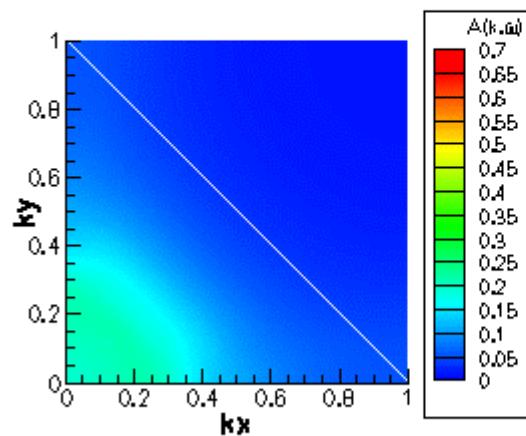
$U=5.75$   
 $n=1.15$   
 $T=1/5$   
 $t=1$   
 $t'=-0.175$   
 $t''=0.05$



# Electron-doped 10%

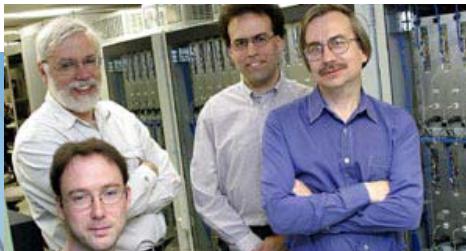
Frequency  $\omega = -4$ .

$\Omega=6.25$ ,  $n=1.10$ ,  $T=1/20$   
 $t=1$ ,  $t'=-0.175$ ,  $t''=0.05$



# Computational methods and destruction of the Fermi liquid in systems of correlated lattice electrons

- 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. Computational resources**
- VI. Conclusion



Un noeud d'Elix2

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



Elix2 vu de profil

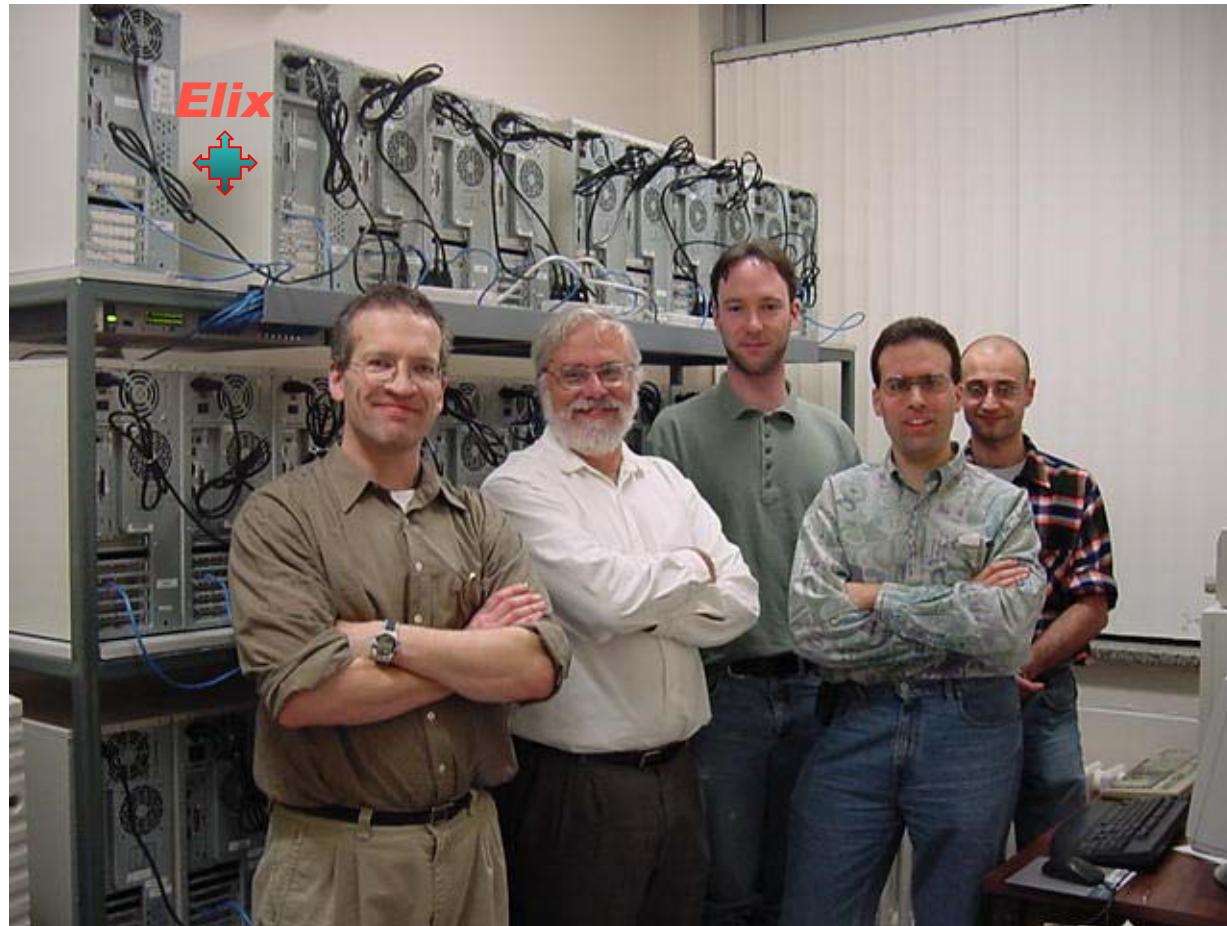
Equipe du CCS devant Elix2. Al'arrière: Patrick Vachon, Minh-Nghia Nguyen, David Lauzon, Michel Barrette, Mehdi Bozzo-Rey, Simon Lessard, Alain Veilleux. A l'avant: Patrice Albaret, Karl Gaven-Venet, Benoît des Ligneris, Francis Giraldeau. Etait absent de la photo: Jean-Philippe Turcotte, Carol Gauthier,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

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



Michel Barrette

Mehdi Bozzo-Rey



David Sénéchal

A.-M.T.

Alain Veilleux

# Elix 2 (CCS Sherbrooke)

<http://www.ccs.usherbrooke.ca/>

- Elix : 1998- 2000:
  - One of the first diskless cluster
- Elix 2 (2003), diskless. Software:
  - Cluster management system: OSCAR 2.3.1
  - Queuing system: OpenPBS 2.3.16, Torque 1.0.1
  - MPI communication library: MPICH 1.2.5.2

# bqtools (CCS Sherbrooke)

<http://www.ccs.usherbrooke.ca/>

- BQTools:
  - Multiple instances of the same code
  - Without major modification
    - generate the needed inputs files
    - transfer file to the cluster
    - submit them with the appropriate queueing system syntax.
  - Can be used for both serial and parallel (MPI) jobs
  - Same user interface, can be used with different queueing systems
  - Automatic file transfert and remote use of any number of clusters on the user side

# bqtools (CCS Sherbrooke)

- Management of data generated by the cluster.
  - BQTools can use a database to automatically store the results, the parameters used and information like the code version, computer architecture, user who run it, etc.
- The ultimate goal: only one interface to
  - get results from this database or
  - launch a new simulation on a remote cluster if the asked parameter have not been calculated yet.

<http://www.ccs.usherbrooke.ca/>

# Questions: not only quantitative

- What destabilizes the Fermi liquid in a paramagnetic phase?
- How do we go from a Mott insulator to a conductor as a function of doping?
  - Hot spots and pseudogaps in the Hubbard model?

# VI- Conclusion

- Strong-coupling pseudogap
  - h- or e- underdoped
  - CPT (+ DCA + Phillips + ...) Mott gap sufficient but not necessary. Like Mott, short-range effect (but not zero range). Scales like  $t$ .
- Weak-coupling pseudogap
  - Electron-doped high Tc in this regime near optimal  $n$ .
  - Well explained by TPSC (QMC) (Others need LRO)
  - Ratio  $\xi/\xi_{\text{th}}$  is important (precursor effect).

Liang Chen Yury Vilk



Steve Allen

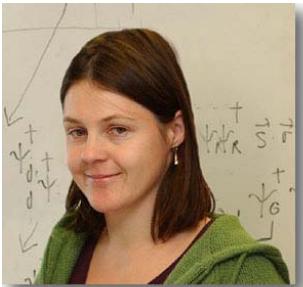


François Lemay

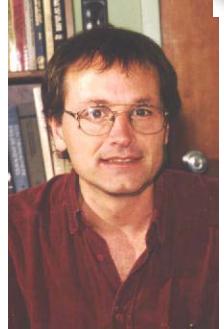


David Poulin Hugo Touchette J.-S. Landry M. Boissonnault





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*