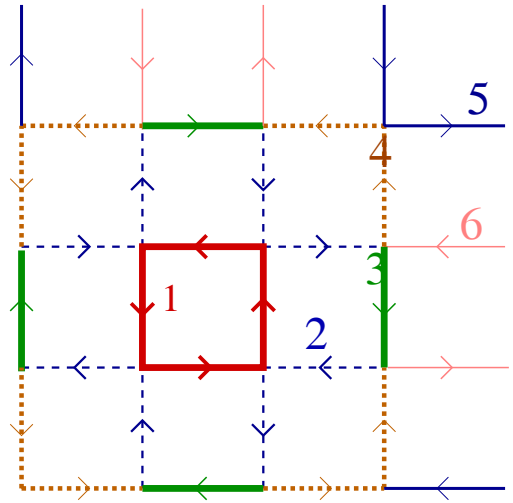
Checkerboard order in cuprate superconductors

Didier Poilblanc

Laboratoire de Physique Théorique

CNRS & Université de Toulouse

IRSAMC



Collaborators

- Cedric Weber (Lausanne)
- Sylvain Capponi (Toulouse)
- Frédéric Mila (Lausanne)
- Cyril Jaudet (Toulouse)
- Manfred Sigrist (Zürich)

References: D.P., Phys. Rev. B 72, 060508(R) (2005)

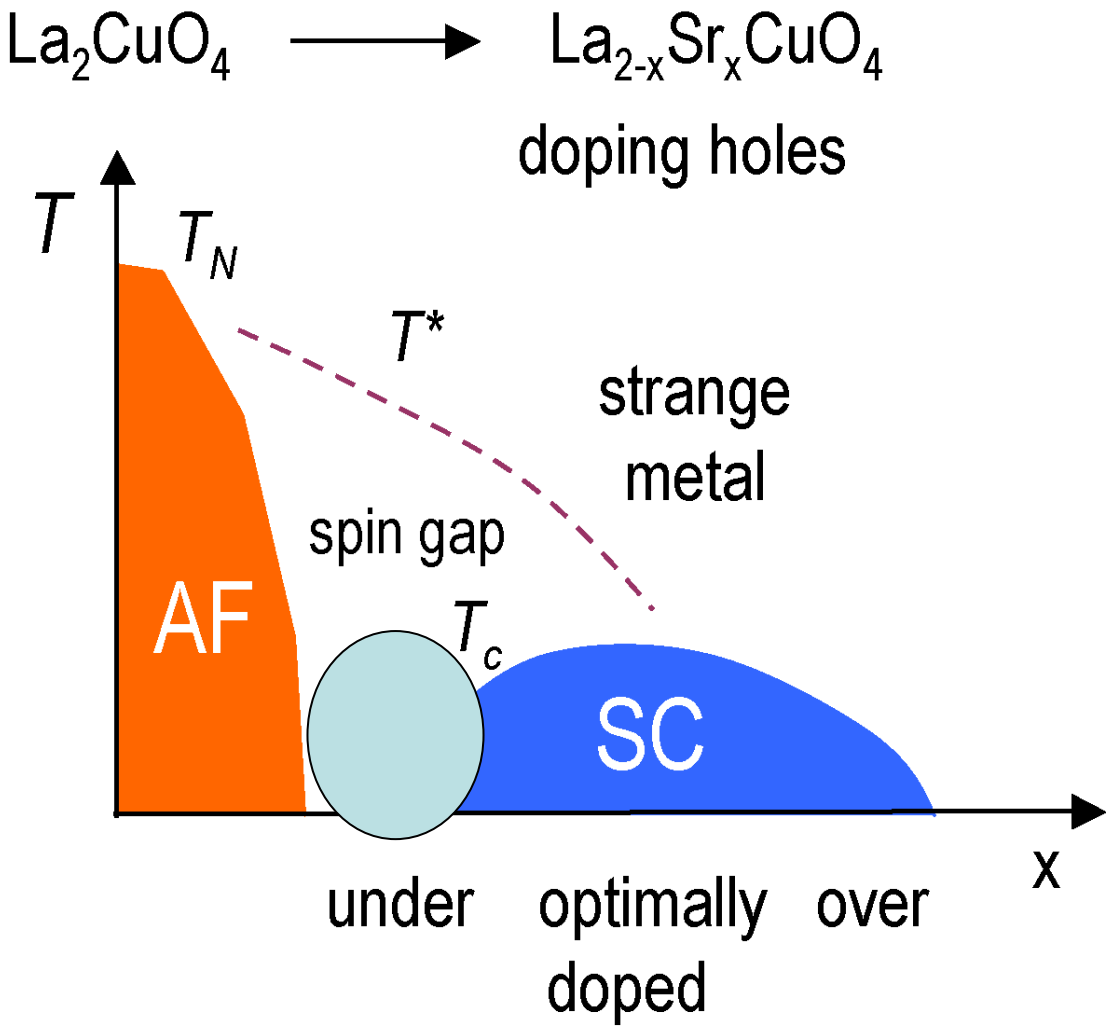
C. Weber et al., Phys. Rev. B, in press

D.P. et al., ICM proceedings

OUTLINE

- Cuprate physics and inhomogeneous states
  - STM/STS in pseudogap phase
- Renormalized mean-field theory
  - Framework similar to RVB theory
  - Results
- Variational Monte Carlo of 4x4 checkerboard
  -- Qualitative agreement with MF
- Conclusions

Generic phase diagram of the high-Tc cuprates



Doping the AF:

Basic model for lightly doped system:

t-J Hamiltonian

$$H = -t \sum_{\langle i,j\rangle,s} \left\{ c_{is}^{+} \left(1 - n_{i,-s}\right)\left(1 - n_{j,-s}\right) c_{js} + hc. \right\} + J \sum_{\langle i,j\rangle} \vec{S}_i \cdot \vec{S}_j$$

Gutzwiller approximation:
Probabilistic approximation

$$\langle c_{i\sigma}^{+} c_{j\sigma} \rangle = g_t \langle c_{i\sigma}^{+} c_{j\sigma} \rangle_0$$
$$\langle S_i \cdot S_j \rangle = g_S \langle S_i \cdot S_j \rangle_0$$

$$H_{eff} = g_t T + g_S J \sum \mathbf{S}_i \cdot \mathbf{S}_j$$

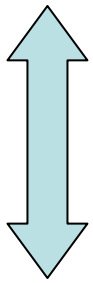
Mean field theory

F.-C. Zhang et al., Supercond. Sci. Technol. **1**, 36 (1988)

Competing phases

d-wave RVB superconductor
Anderson 87

At half-filling:
SU(2) symmetry
Kotliar 89



staggered flux phase
Affleck-Marston 88

Features of SFP detected in numerics:

- Staggered spin chirality
DP, Dagotto & Riera, PRB 91

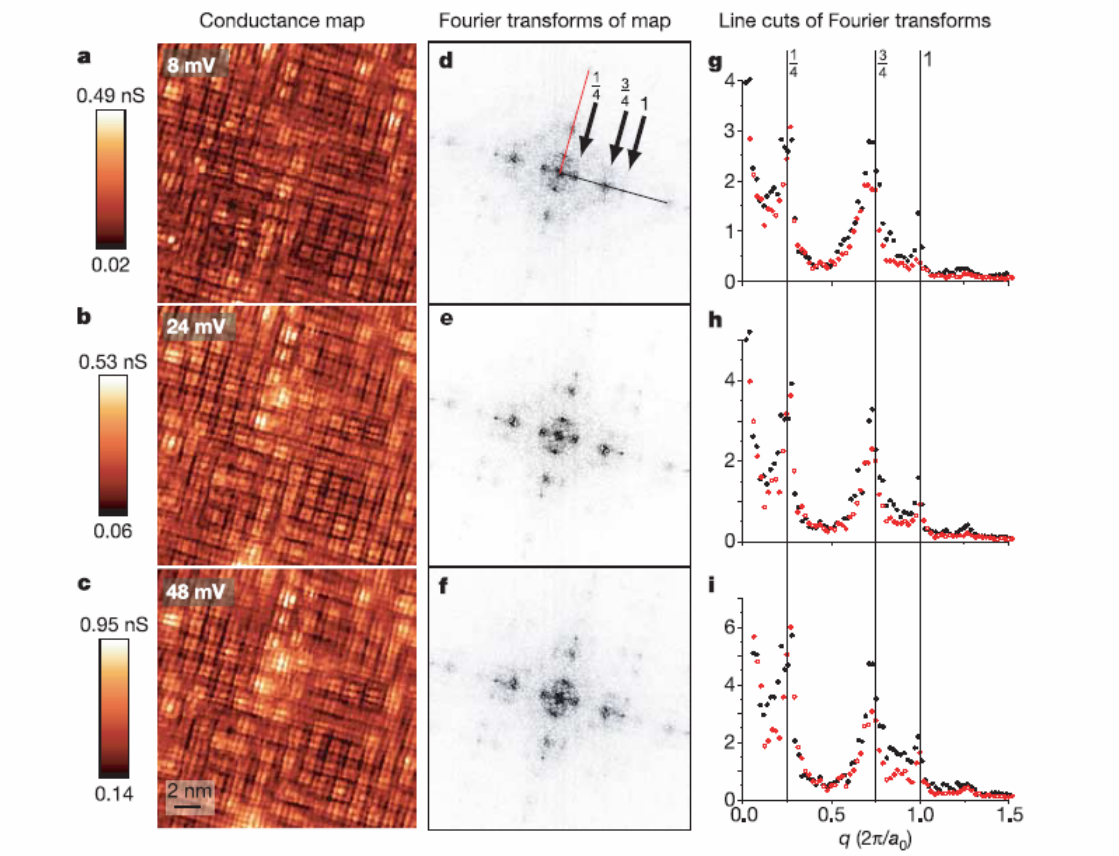
- Staggered (charge) currents
Leung, PRB 96

-Variational “flux phases” have low energy
Anderson, Hristopoulos, 89
DP, Lederer, Rice, Hasegawa, PRL 90

Charge modulation in underdoped samples

- $Ca_{2-x}Na_xCuO_2Cl_2$ (weak disorder !)
- $4a$ x $4a$ periodicity along CuO axis
- Rotation symmetry

- Non-dispersive peaks
- Weakly sensitive to doping



T. Hanaguri et al, Nature **403**, 1001 (2004).

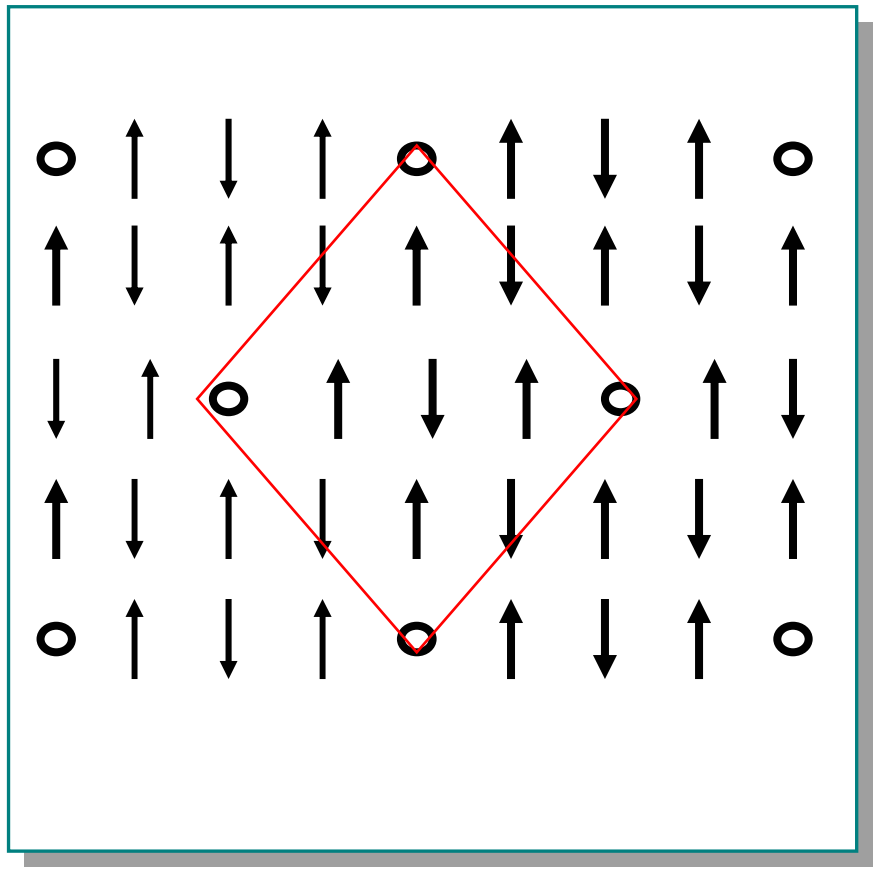
Wigner crystal of holes ?

For x=1/8:

$$\sqrt{8}a \times \sqrt{8}a$$

modulation

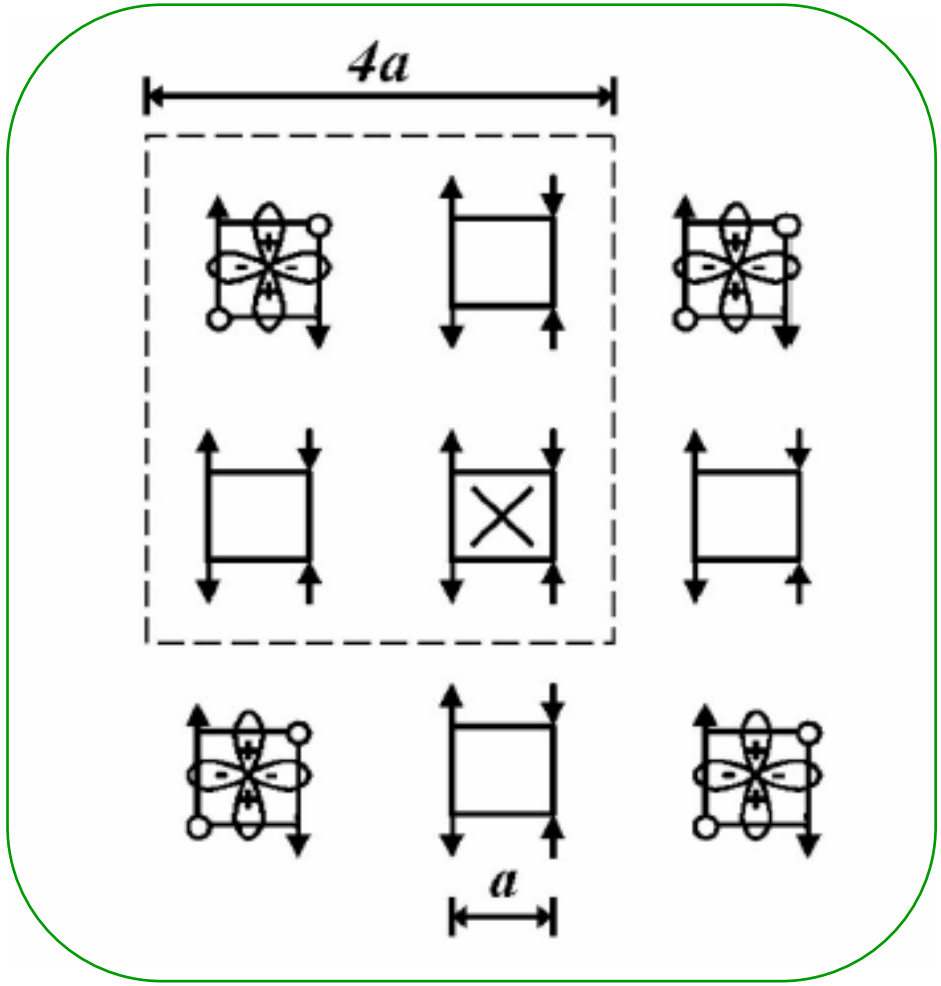
-> incompatible with experiments !



=> Pair density wave (PDW) ?

Wigner crystal of hole pairs ?

- 1 pair of holes (2 holes) per cell
- $4a$X$4a$ periodicity for hole doping of 1/8



H.-D. Chen, J.P. Hu, S. Capponi, E. Arrigoni and S.-C. Zhang, PRL 89, 137004 (2002).
H.-D. Chen, S. Capponi, F. Alet, and S.-C. Zhang, PRB 70, 024516 (2004).

Other alternative: Bond Order Wave ?

Extend renormalized MF formalism to inhomogeneous case

$$H_{\mathrm{MF}} = -t \sum_{\langle ij \rangle \sigma} g_{ij}^{t} (c_{i,\sigma}^{\dagger} c_{j,\sigma} + h.c.) - \mu \sum_{i\sigma} n_{i,\sigma}$$

$$-\frac{3}{4} J \sum_{\langle ij \rangle \sigma} g_{i,j}^{J} (\chi_{ji} c_{i,\sigma}^{\dagger} c_{j,\sigma} + h.c. - |\chi_{ij}|^2)$$

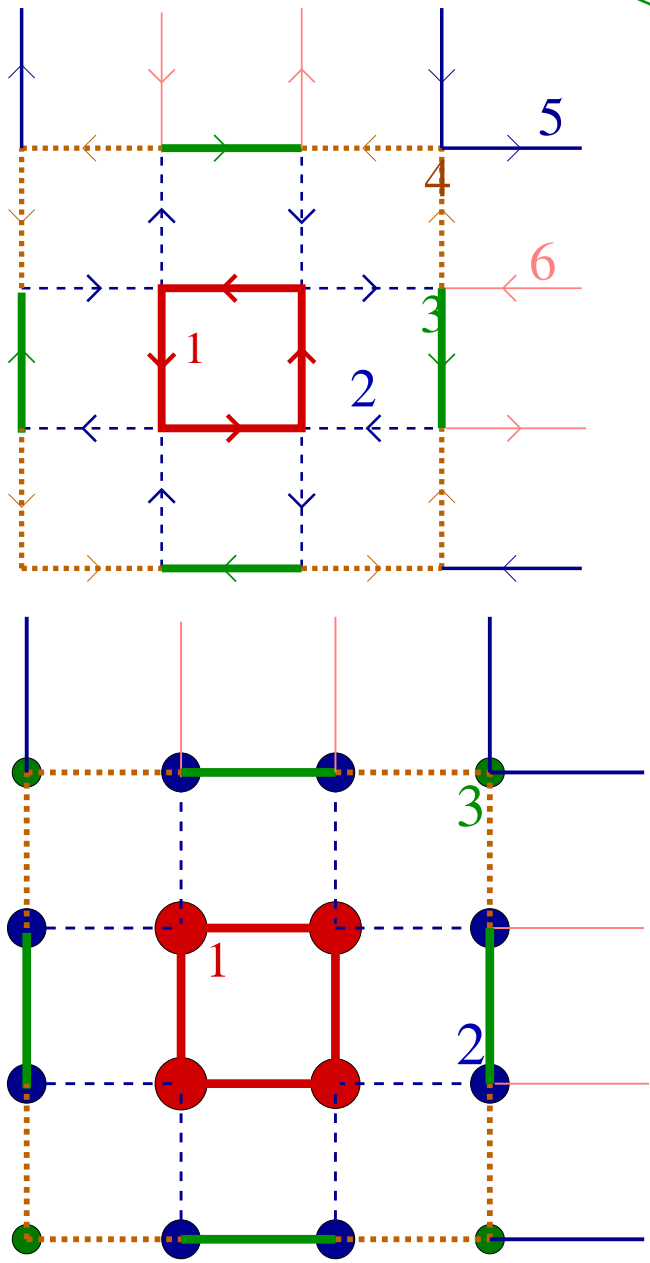
$$-\frac{3}{4} J \sum_{\langle ij \rangle \sigma} g_{i,j}^{J} (\Delta_{ji} c_{i,\sigma}^{\dagger} c_{j,-\sigma}^{\dagger} + h.c. - |\Delta_{ij}|^2),$$

→ + usual MF self-consistent equations

→ Site dependent g's, bond amplitudes and site densities

4a X 4a superstructure

- Unrestricted MF equations solved on 48 x 48 cluster
- 4x4 pattern emerges at x=1/8
- modulations of bond hopping & exchange : dominant BOW
- small CDW component: CDW ≈ BOW / 10 !
- almost-staggered charge currents: but inhomogeneous and very small amplitudes



Variational Monte Carlo: competition with Staggered flux state & RVB superconductor

- Competing phases close in energy: MF not enough! ⟹ **accurate VMC computations**

- **Order parameters** reduced compared to MF:
  - Bond Order : 10 % ⟹ strongest !
  - CDW order : 1.3 %

- **Energetics** : 4ax4a order very low energy
  - Slightly lower than SFP (a few %)
  - N.N. Coulomb repulsion stabilizes 4ax4a structure w.r.t d-wave RVB superconductor

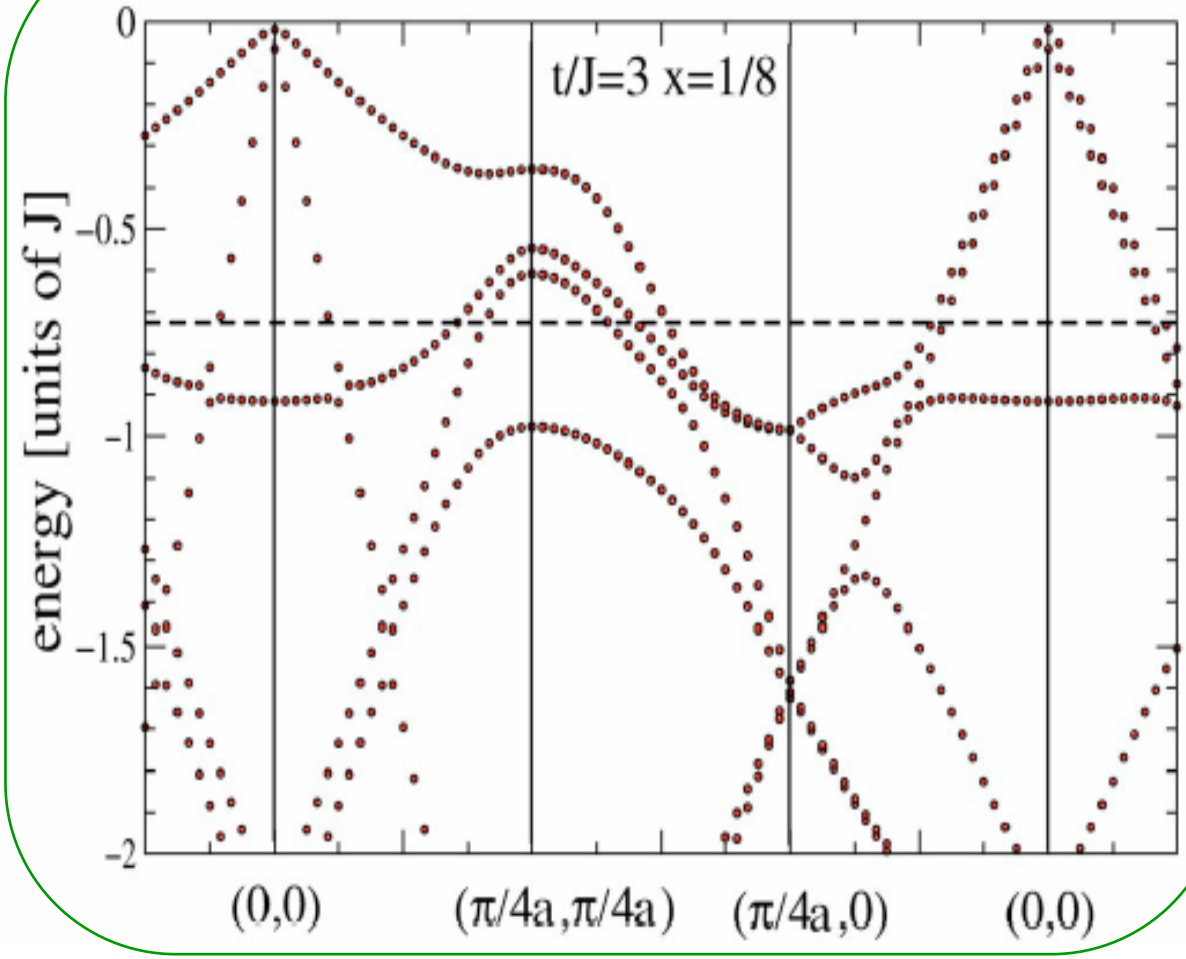
MF electronic spectrum

Some features of staggered flux state (or ddw):

Cone-like dispersion

→ Metallic character !

→ V-shape
STS spectrum



Conclusion

- 4x4 Bond Order Wave: superposition of various order parameters:
  - modulation of bond amplitudes → **Bond order wave (BOW)**
  - Very small modulation of local charge density → CDW (1/10)
  - small staggered currents → time-reversal symmetry breaking
  - **Confirmed by (exact) VMC estimates (EPFL coll.)**
- In agreement with STS/STM experiments
- 4ax4a superstructure compete with d-wave RVB SC: stabilized by Coulomb repulsion, disorder, surface, etc…
- Other possible instabilities of SFP: new domain wall ("striped") flux states (in coll. M.Raczkowski, R.Frésard & A. Oles)