Interplay between charge, pairing (and orbital current) modulations in some t-J models

CENTRE NATIONAL DE LA RECHERCHE SCIENTIFIQUE

Didier Poilblanc*

Manuela Capello, Marcin Raczkowski

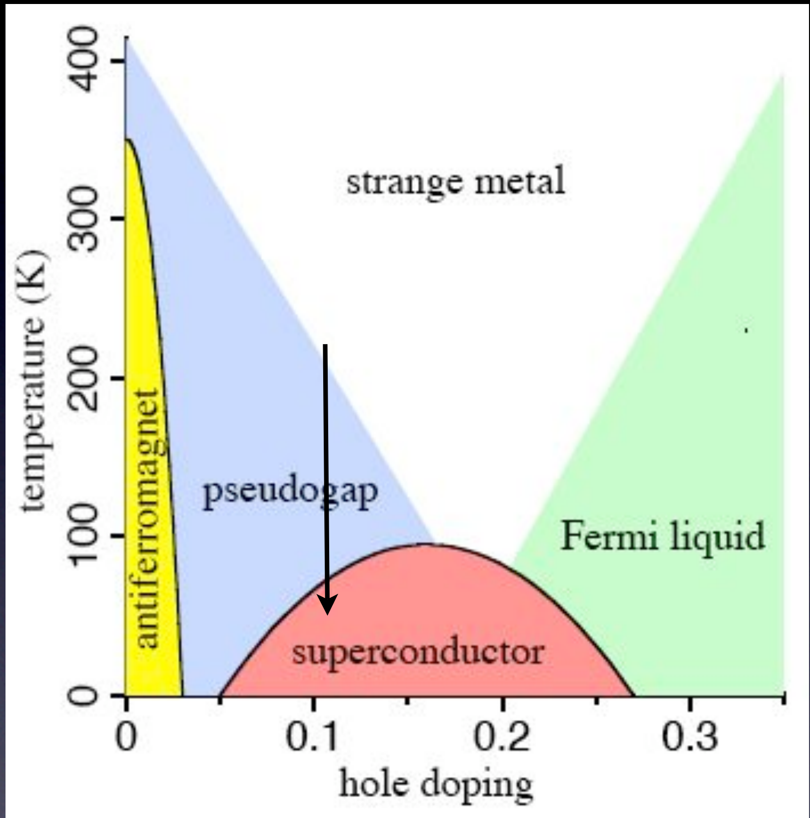
R. Frésard and A. Oleś

*CNRS and Université Paul Sabatier, Toulouse (France)

Outline

- The basics of RVB and the pseudo-gap
- Observation of charge order in High-Tc superconducting materials
- Results on superconducting RVB hole stripes
- Results for a single Zinc impurity
- Open issue: competition with orbital current states

High-Tc Phase diagram

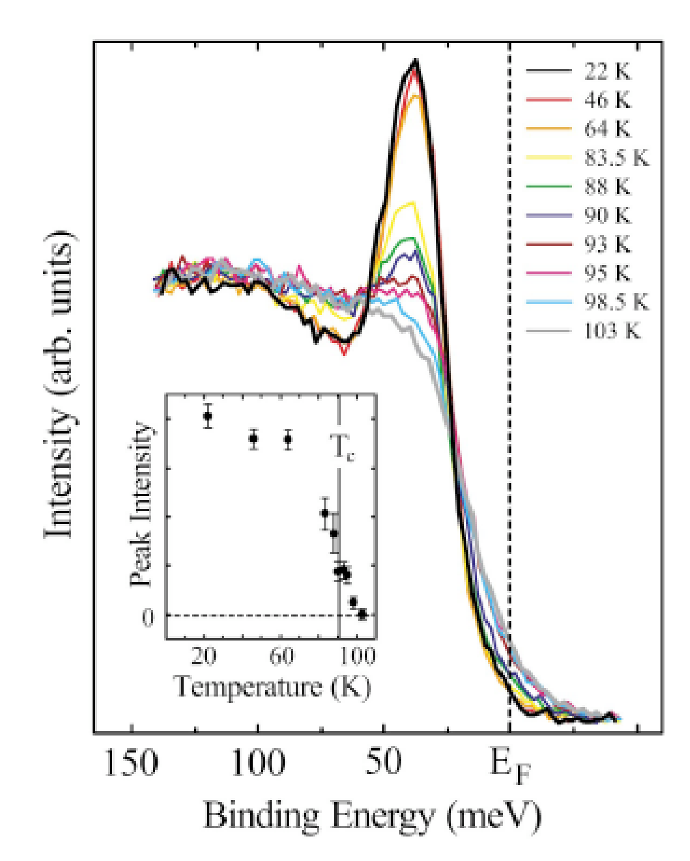


*RVB is a simple appealing theory for pseudo gap

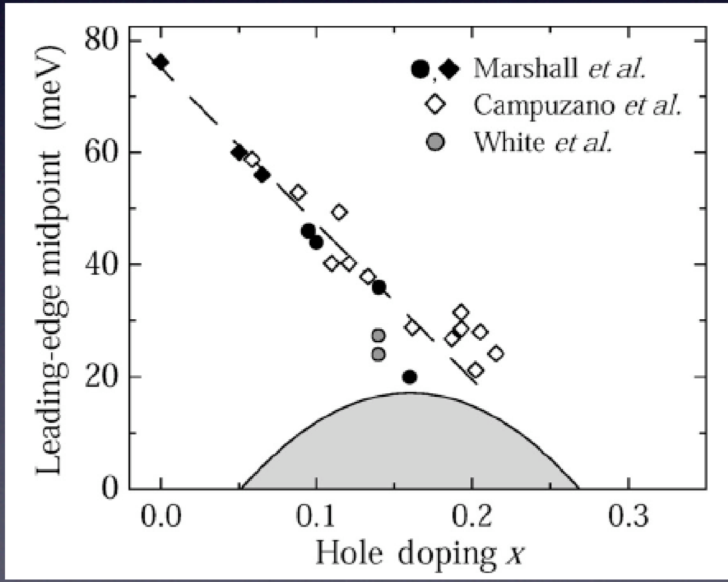
* Can we also describe inhomogeneous states with the RVB framework ?

Superconducting state emerges from doping a Mott insulator

The pseudogap phase



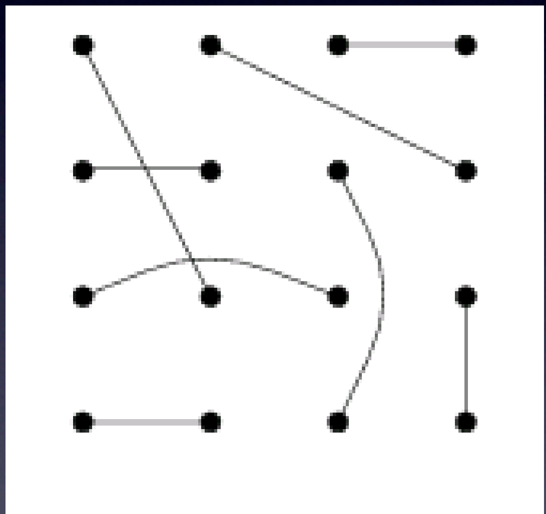
Existence of a pseudo-gap but
no superconductivity
and no quasiparticles



(pi,0) vs. T
Fedorov 1999
Bi2212
Tc=91K

Resonating Valence Bond state

* Mott physics: no double occupancies
* Antiferromagnetic term important



Non-magnetic ground state:
good for low spin,
low dimensionality

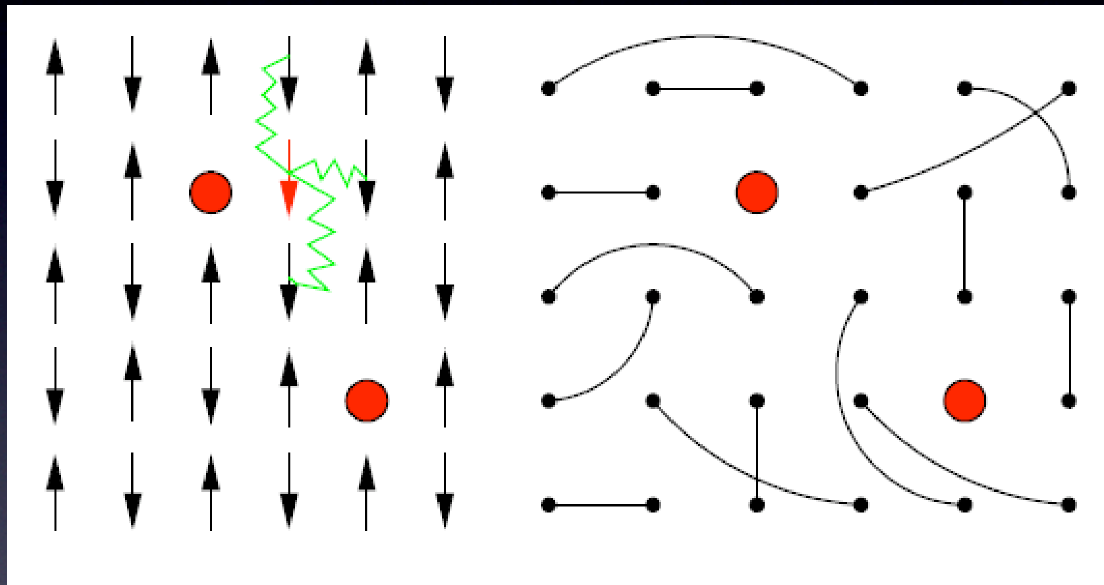
$$\bullet\!\!-\!\!\bullet = \frac{1}{\sqrt{2}}(\uparrow_i\downarrow_j - \downarrow_i\uparrow_j)$$

[Anderson, Science 1987]

RVB: liquid of singlets of spins which resonate

(Simple minded) RVB scenario

Holes frustrate antiferromagnetism

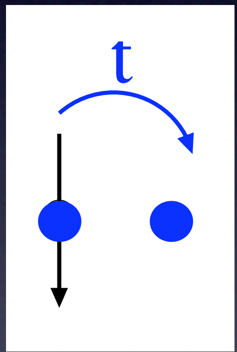


The RVB state regains the lost AF exchange
by the resonance betwen many different configurations

The RVB state naturally becomes a superconductor
since the pairing already exists

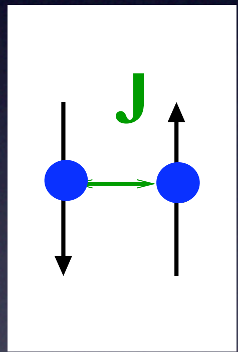
The t-J model

$$H_{tJ} = -t \sum_{\langle ij \rangle, \sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + h.c. + J \sum_{\langle ij \rangle} S_i \cdot S_j$$

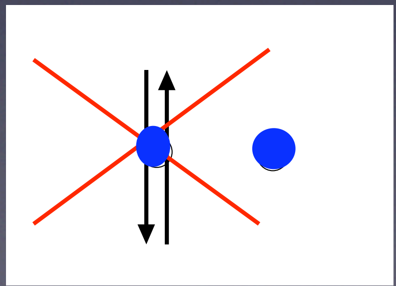


KINETIC TERM

+



AF EXCHANGE TERM



CONSTRAINT of
NO DOUBLE OCCUPANCIES

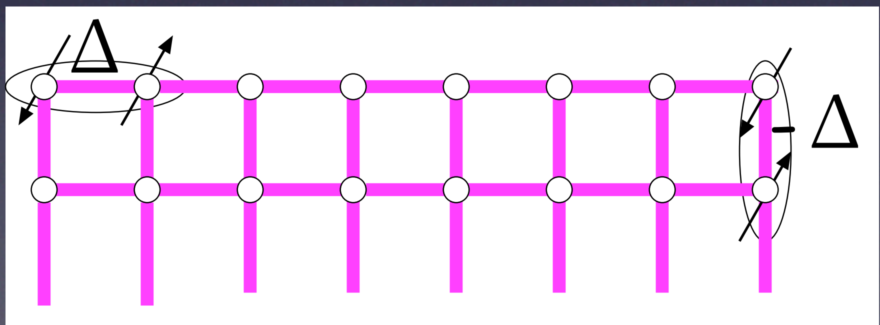
RVB variational state

$$H_{BCS} = H_{kin} + \sum_{ij} \Delta_{ij} c^\dagger_{i\uparrow} c^\dagger_{j\downarrow} + \mu \sum_i n_i + h.c.$$

Uncorrelated state | D ⟩

$$|\Psi_{RVB}\rangle = \prod_i (1 - n_{i\uparrow} n_{i\downarrow}) |D\rangle$$

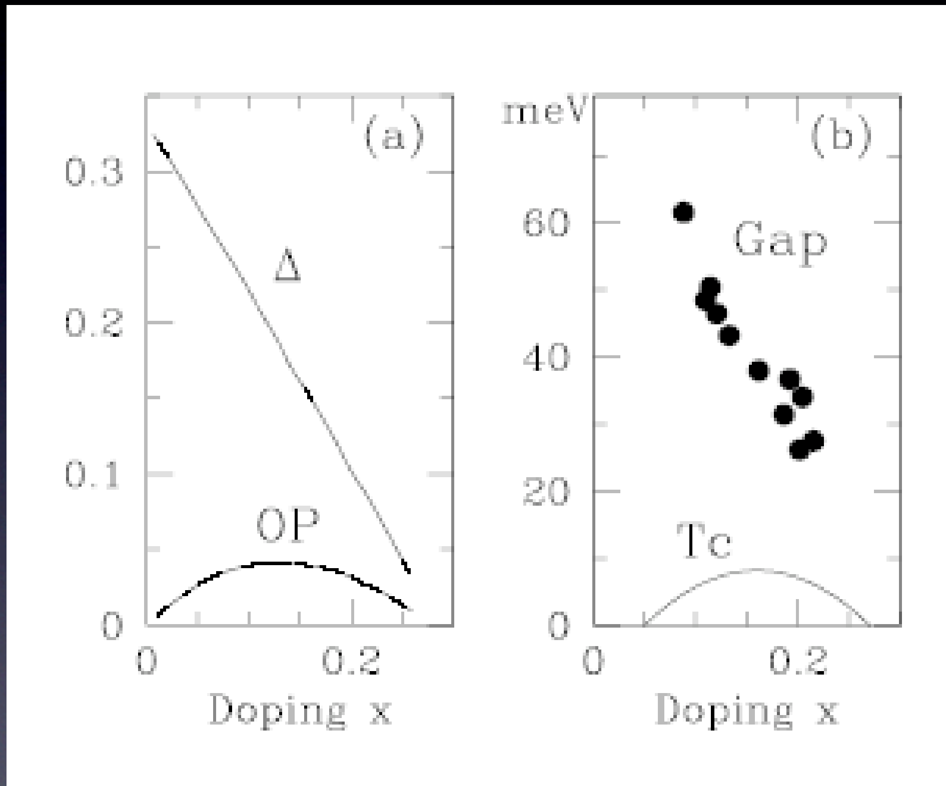
Strongly correlated wavefunction



Δ,μ are variational parameters

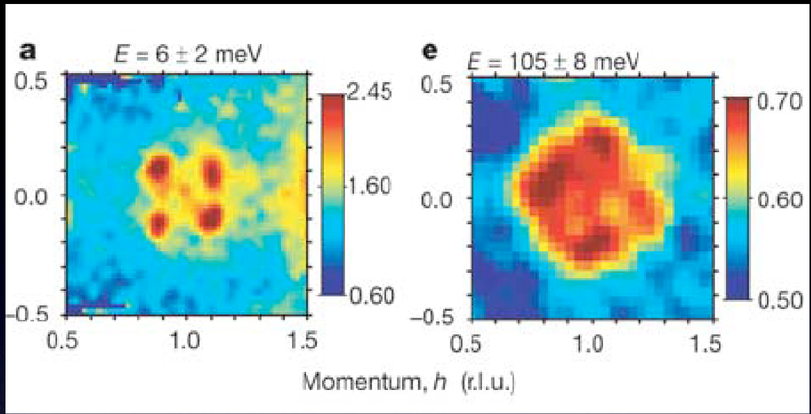
All Δ_{ij} uniform with d-wave symmetry

RVB => Correct behavior of pseudo-gap & SC order parameter



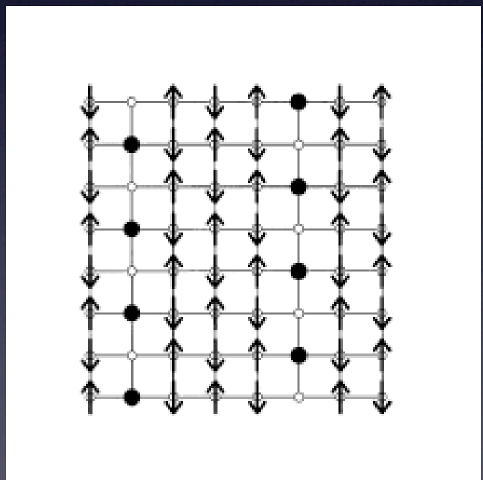
Anderson et al. J.Phys. C 2004

Neutron scattering: AF Stripes



$La_{2-x}Ba_xCuO_4$
at doping x=1/8

[Tranquada et al. Nature 1995]

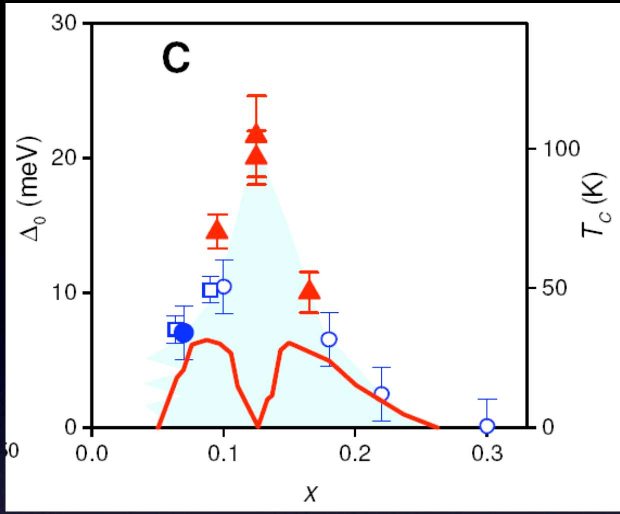


ANTIFERROMAGNETIC STRIPE SCENARIO

Spatially ordered state with holes concentrated ***unidirectionally*** between AF domains

Could the SC state become also stripy ?

Stripes are compatible with pairing !

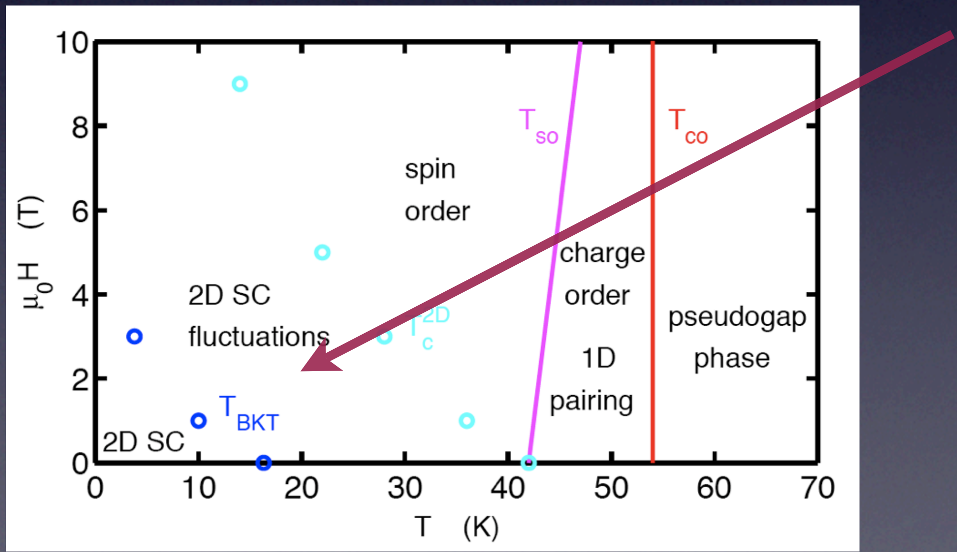


LaBaCuO: Tc~0 at doping x=1/8
but (ARPES + STM) d-wave gap
still there!

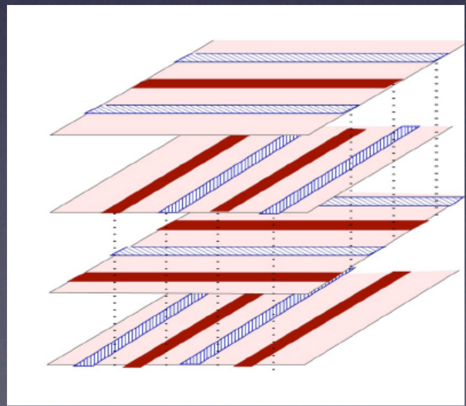
[Valla et al., Science 2006]

Planes are (Josephson) decoupled
but pairing exists!

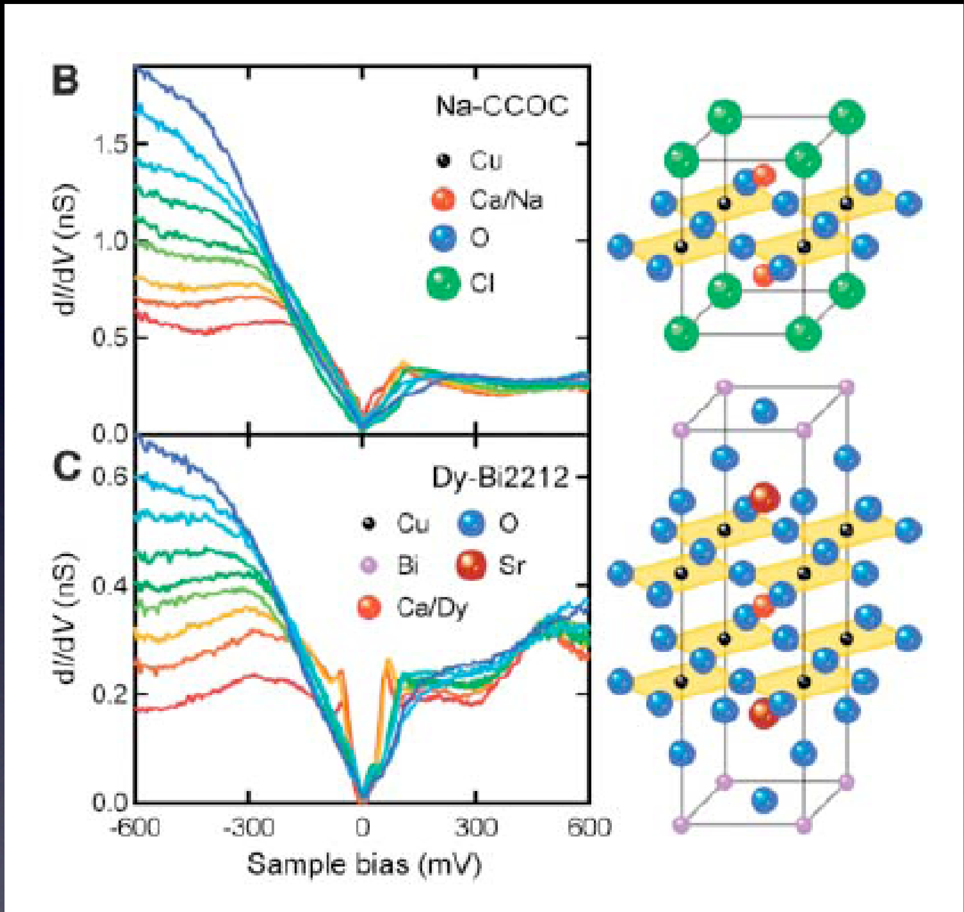
[Berg et al., PRL 2007]



[Li et al., PRL 2007]



STM Experiments:



DIFFERENTIAL CURRENT

$dI/dV(r,V) = f(r,z)\, N(r,E=eV)$

*N(r,E) LOCAL DOS

*f(r,z) tunnelling matrix element (unknown)

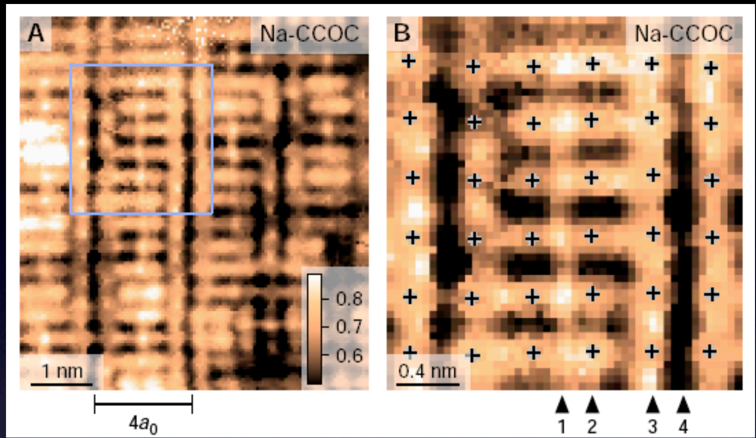
J.C. Davis' group

EXTRACT e^- INSERT e^-

Ground state properties ?

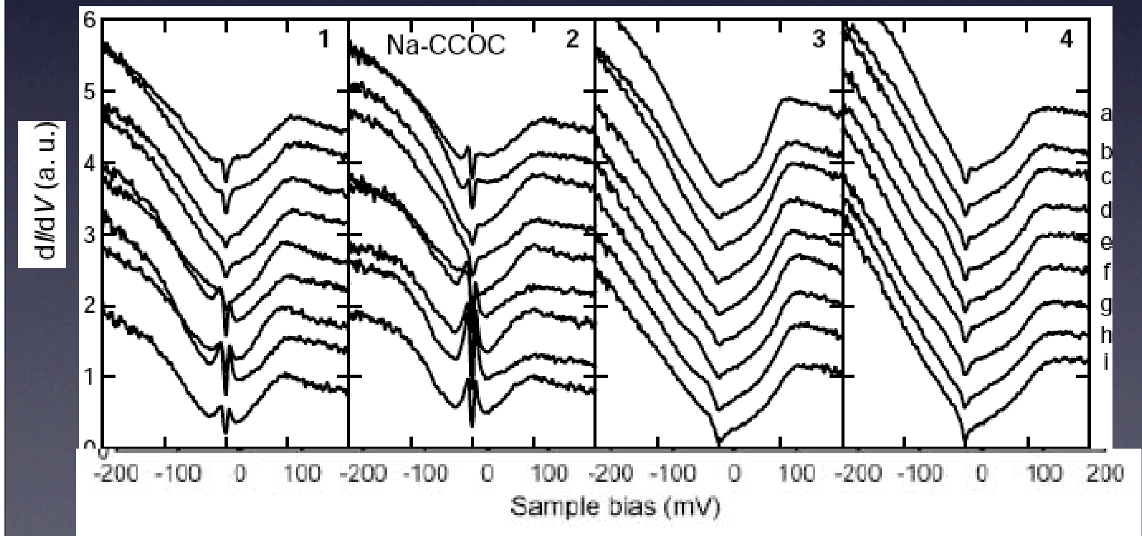
STM-experiments: R-maps

$Ca_{2-x}Na_xCuO_2Cl_2$ and Dy-Bi2212 (at T< Tc) [Kohsaka et al. Science 2007]



$$R(r,z,V) = \frac{I(r,z,+V)}{I(r,z,-V)} \sim \frac{x(r)}{1-x(r)}$$

→ Extract hole density x(r)



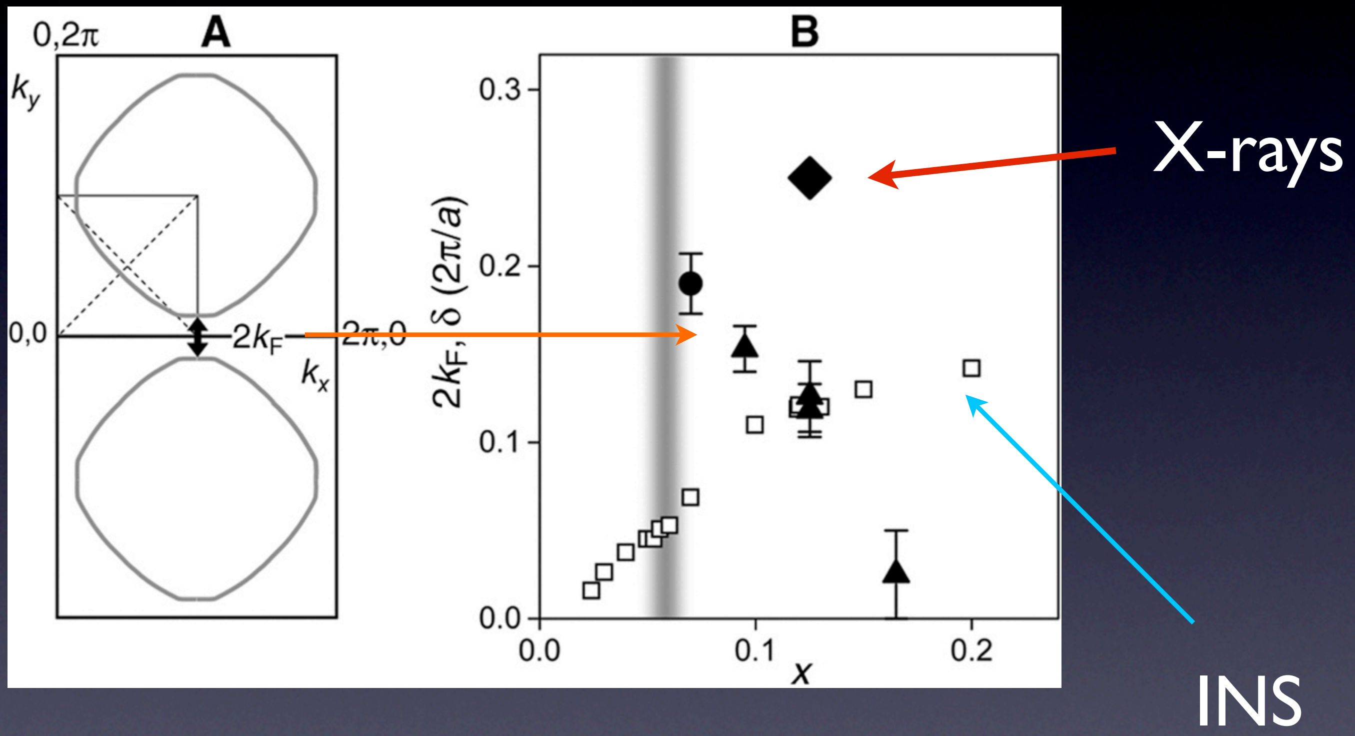
HOLE RICH

HOLE POOR

Bond-centered unidirectional patterns

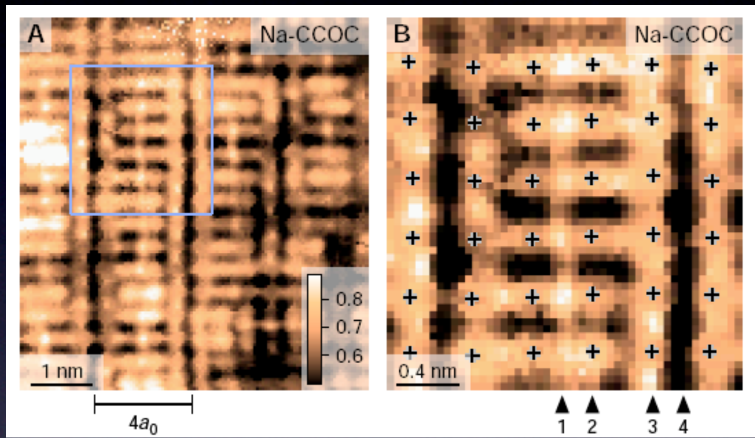
Different low-energy properties

Not a Fermi surface nesting mechanism !



[Valla et al., Science 2006]

SPATIAL ORDER + SUPERCONDUCTIVITY



GOAL: describe **superconducting hole-stripes** within RVB framework ?

RVB variational state revisited

$$H_{BCS} = H_{kin} + \sum_{ij} \Delta_{ij} c^{\dagger}_{i\uparrow} c^{\dagger}_{j\downarrow} + \mu \sum_i n_i + h.c.$$

t_{ij} and Δ_{ij} become bond dependent !!

Uncorrelated state $|D\rangle$

$$|\Psi_{RVB}\rangle = \prod_i (1 - n_{i\uparrow} n_{i\downarrow}) |D\rangle$$

Strongly correlated wavefunction

A convenient guide:
Gutzwiller approximation
+
Mean-field

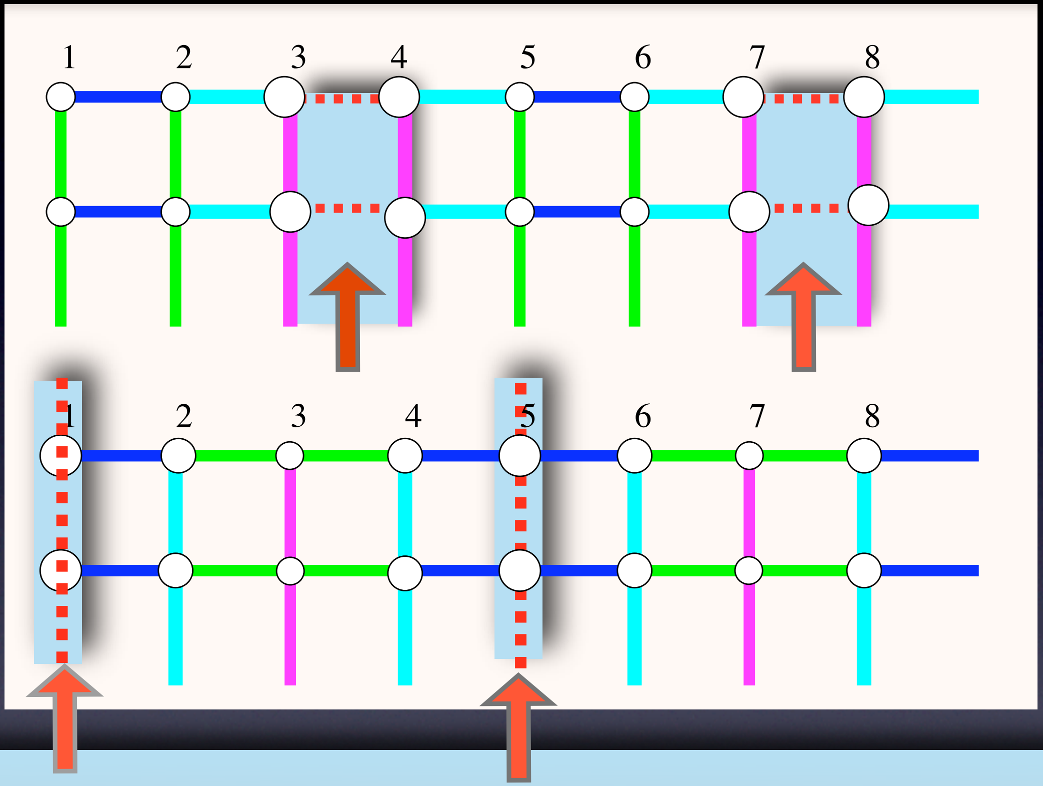
VMC : optimization scheme developped in S. Sorella's group, up to 16x16 clusters with PBC

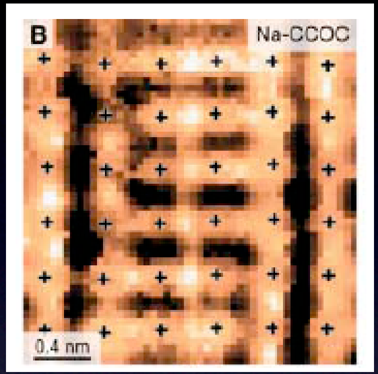
Superconducting stripes

We allow for inhomogeneous Δ_{ij}

Bond centered

Site centered





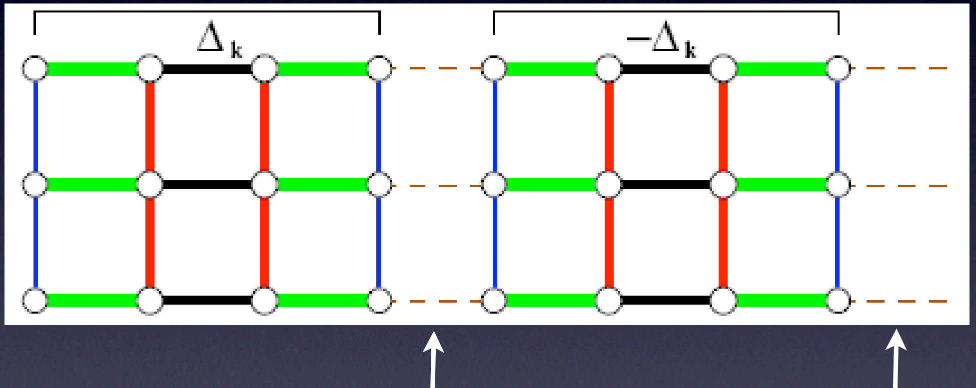
Create line-defects in the RVB state

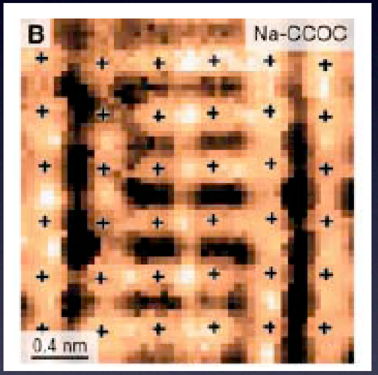
Impose $\Delta_{ij}=0$ along one direction,

with periodicity 1/2x

Superconducting stripes (II): pi-domain RVB stripes

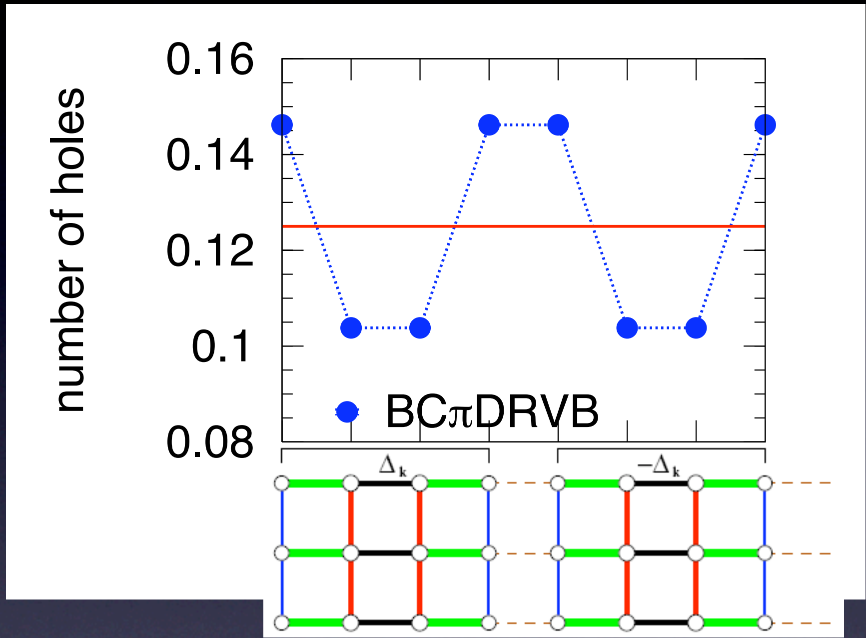
Bond-centered symmetry





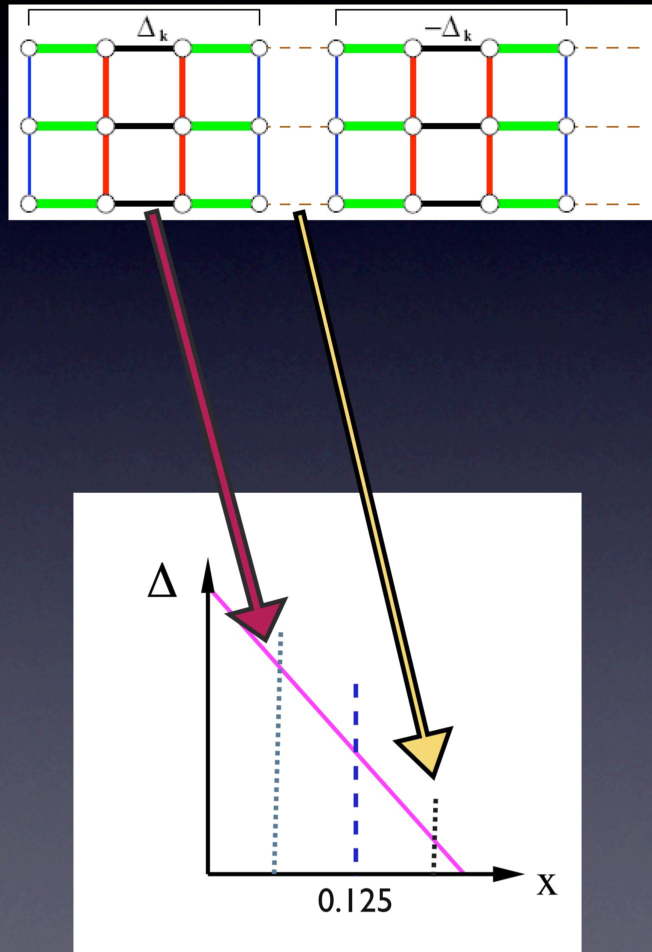
The pi-phase shift in Δ_k implies regions with domain walls in the pairing, with $\Delta_{ij}=0$

Charge modulation is there!

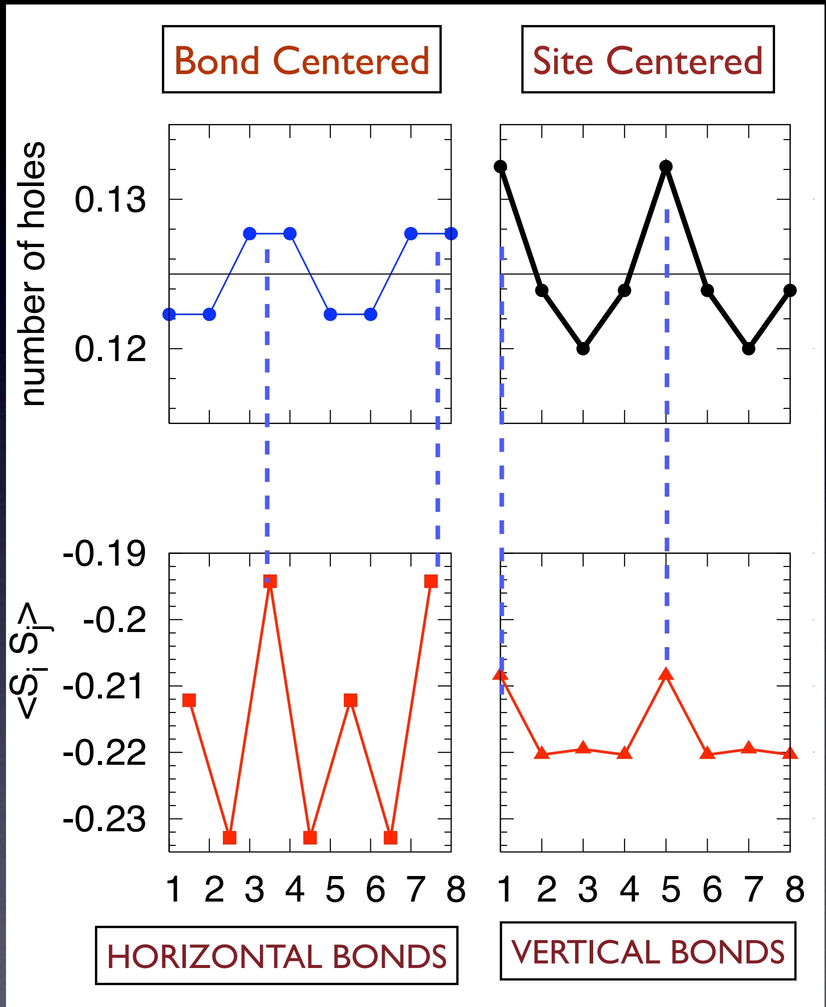


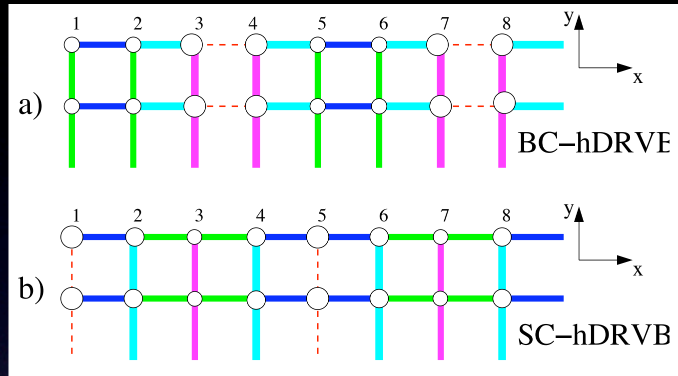
2 NON-EQUIVALENT SITES

Holes concentrate where spin-pairing is smaller (around the domain walls)

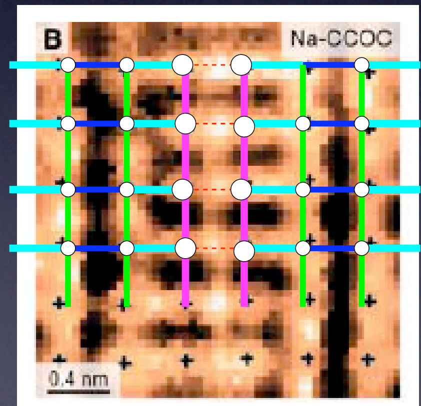


In-phase domains





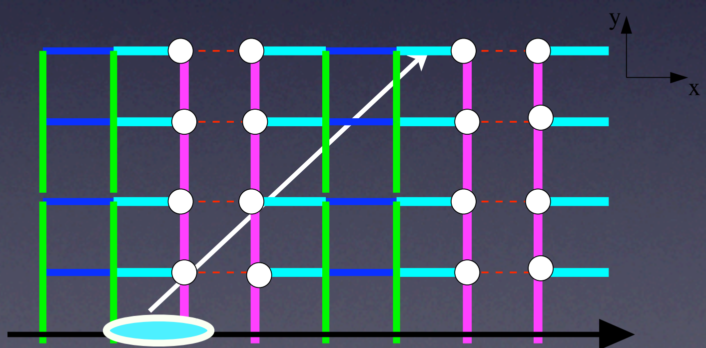
Hole stripes emerge

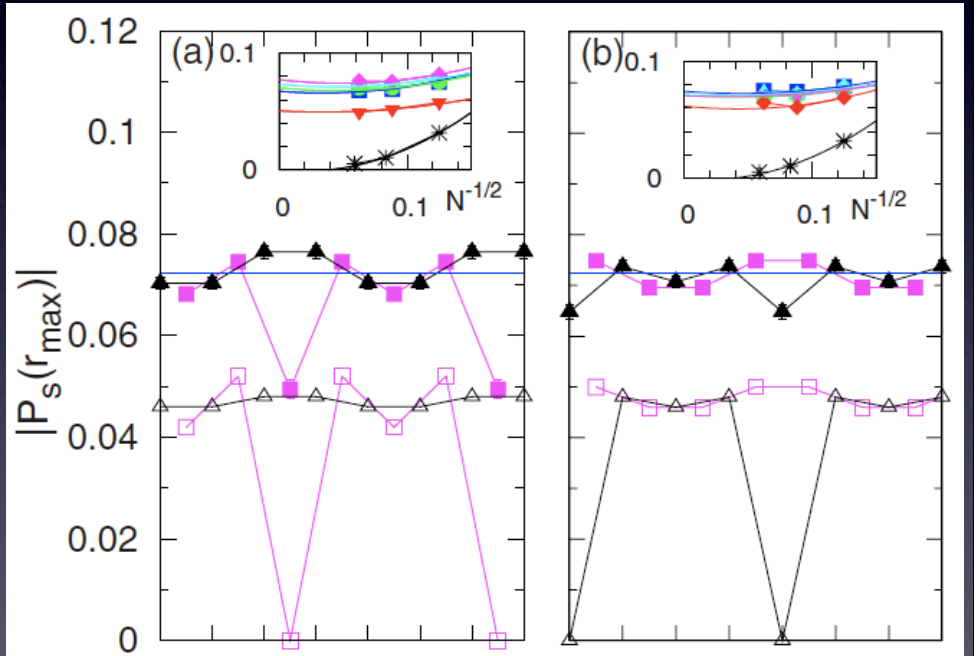


Superconductivity is modulated !

$$P_s^2(r) = \langle \tilde{\Delta}_{s+r}^\dagger \tilde{\Delta}_s \rangle$$

$$\tilde{\Delta}_s^\dagger = c_{s\uparrow}^\dagger c_{s+a\downarrow}^\dagger - c_{s\downarrow}^\dagger c_{s+a\uparrow}^\dagger$$

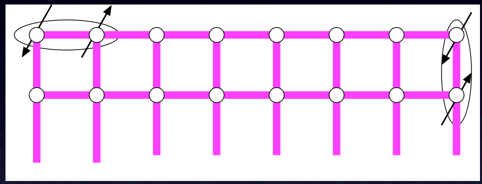




Energies are really close (~10^{-4} t)

t/J=3,
doping 1/8
up to
16x16 clusters

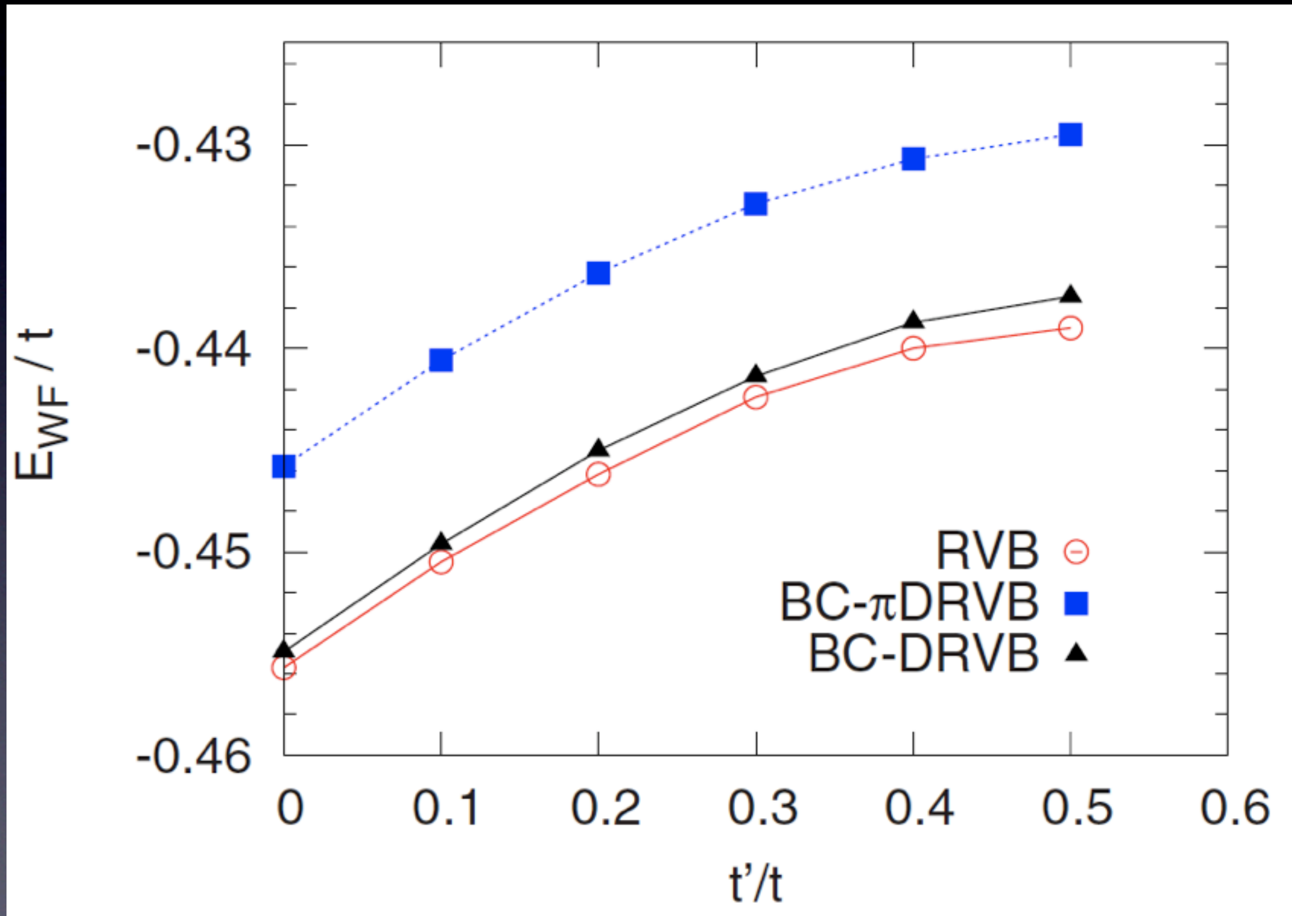
WF	E_{VMC} [t]
RVB	-0.45564(3)
SFP	-0.44630(3)
pi-DRVB	-0.44529(3)
BC-hDRVB	-0.45490(3)
SC-hDRVB	-0.45530(3)



Anti-phase

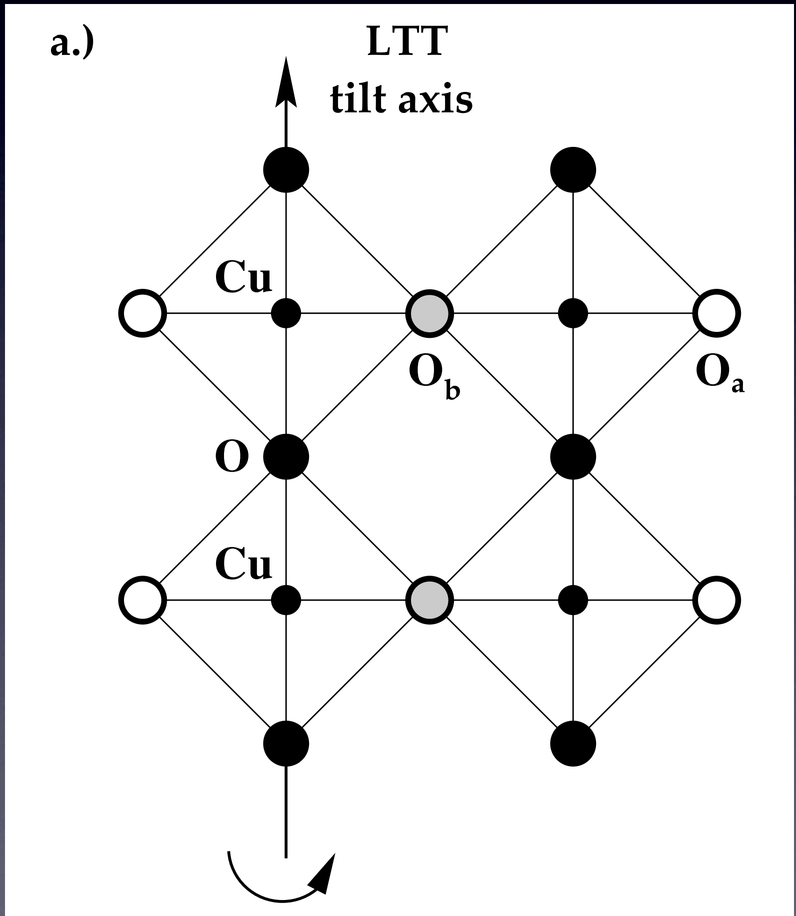
In-phase

Role of t’



Lattice distortion

$$H_{tJ}^{\alpha} = -t \sum_{<ij>,\sigma} \alpha_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + h.c. + J \sum_{<ij>} \alpha_{ij}^{2}\, S_i \cdot S_j$$

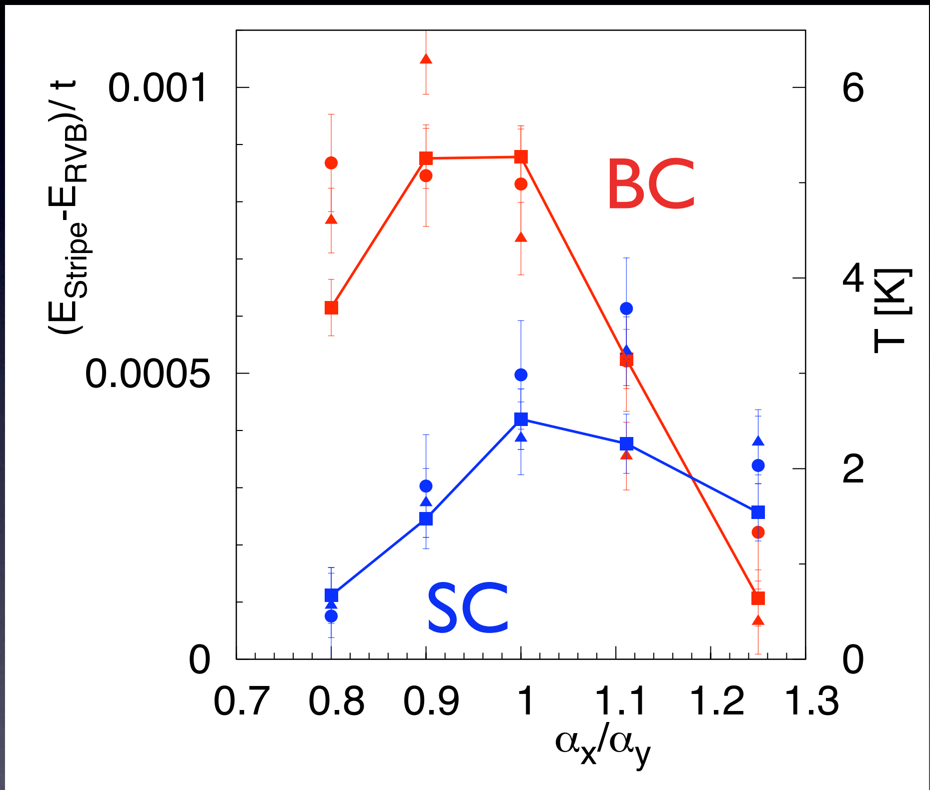


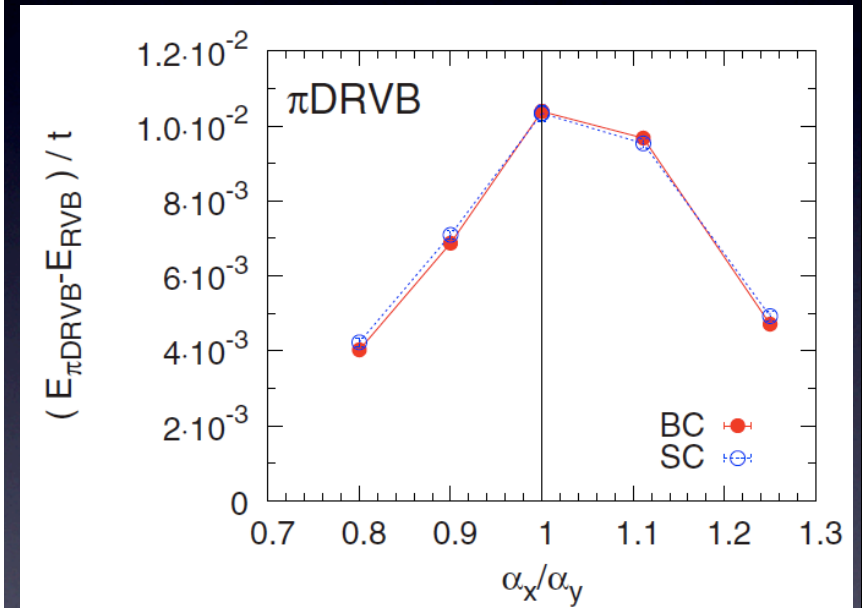
The tilt in the oxygen octahedra induces a different t and J along x and y:

tilt axis along y:
$\alpha_x < 1$ and $\alpha_y = 1$

Lattice LTT distortion further stabilizes the superconducting stripes

In-phase





Anti-phase

Tilt axis along y

Tilt axis along x

Other related work

* Himeda, Kato & Ogata, PRL 2002
  [simple cosine modulation of SC]

* Berg, Fradkin, Kim, Kivelson, Oganesyan, Tranquada & Zhang, PRL (2007)
  [Dynamical layer decoupling scheme]

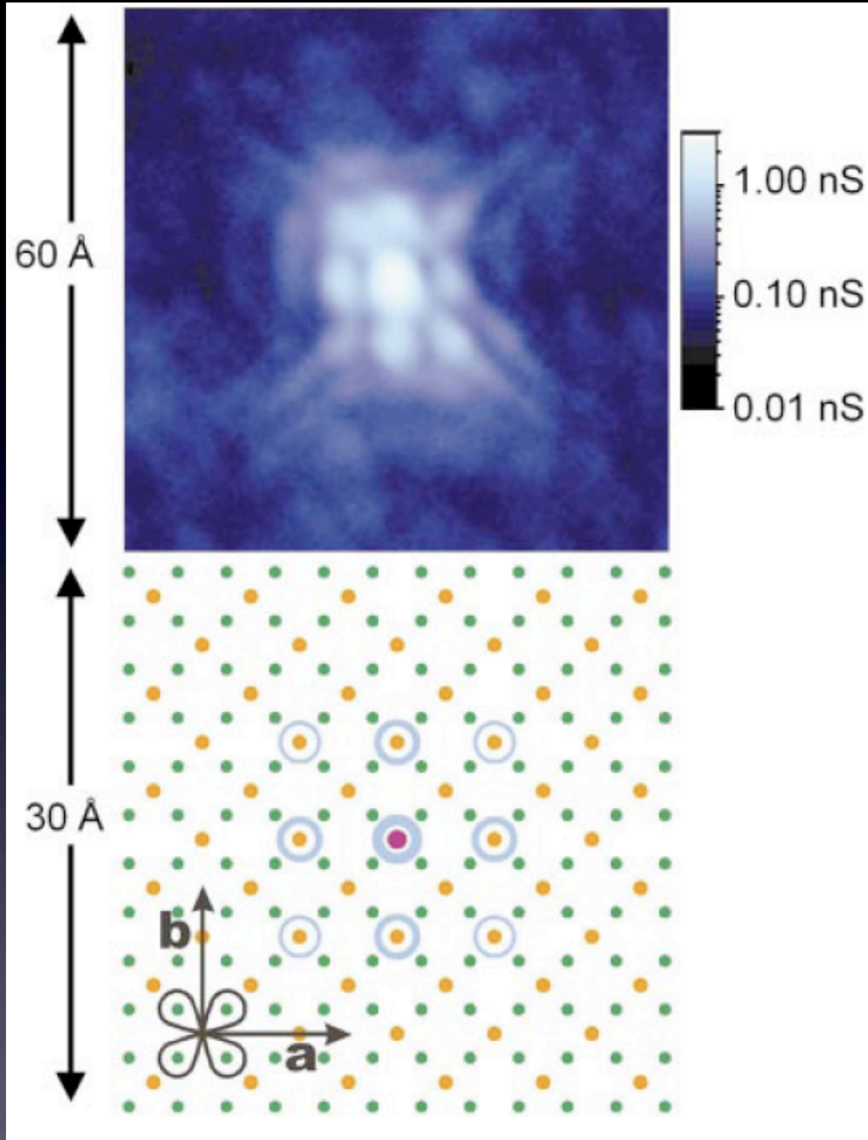
* Yang, Chen, Rice, Sigrist and Zhang, arXiv:0807.3789
  [Mean-field RVB including spin ordering]

Role of impurities ?

Low-energy DOS around Zinc impurity in SC state

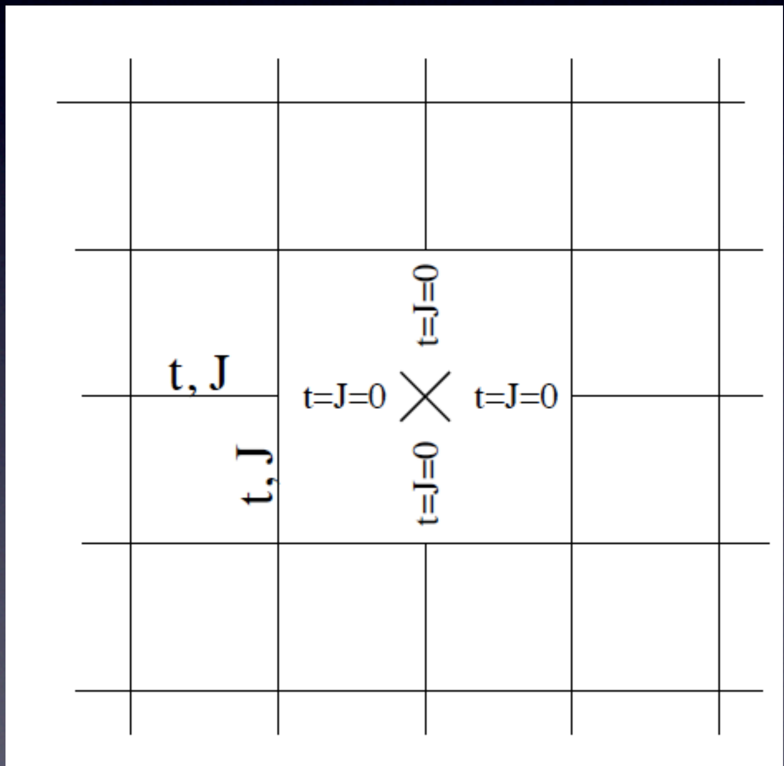
- Large DOS along nodal directions
- Suppression of SC within ~15A from Zn

Pan et al., Nature 403, 746 (2000)



$Bi_2Sr_2Ca(Cu_{1-x}Zn_x)_2O_{8+\delta}$ single crystals

Controled impurity doping offers a stringent test for correlated models and RVB wf's !



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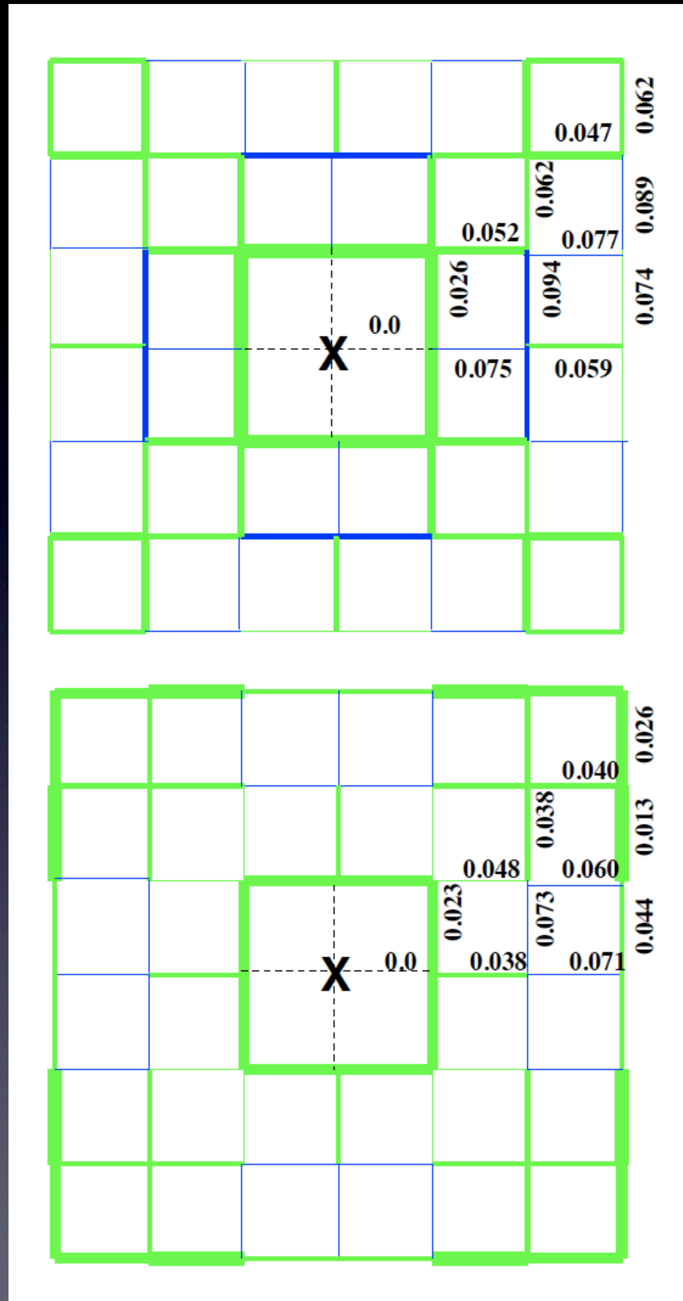
Variational Gutzwiller-projected RVB wavefunction (16x16 clusters) x=12 %

x=7 %

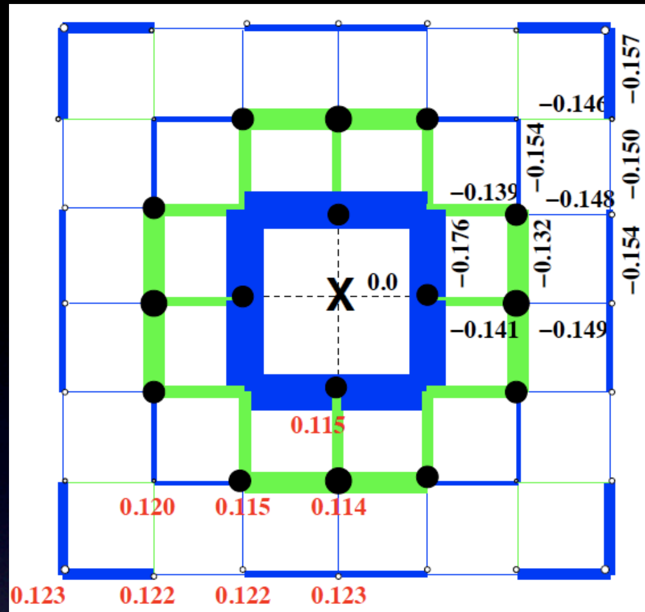


Suppression of pairing correlations over large distances

16x16 cluster
(only central region shown)

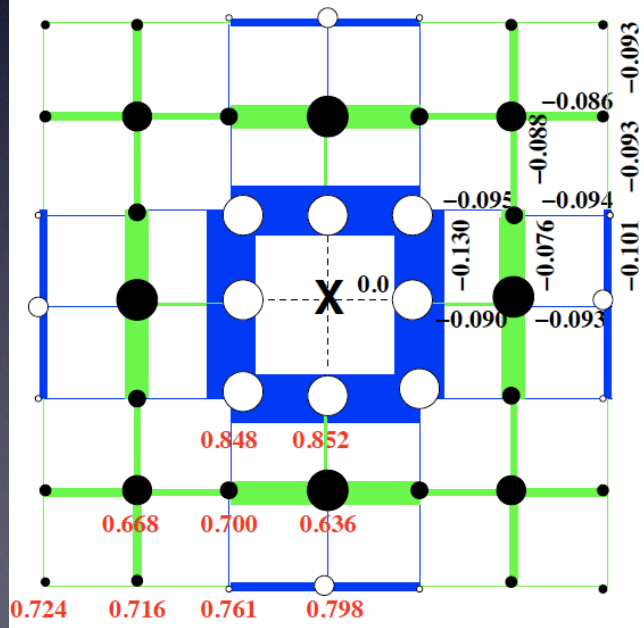
Strong modulation of local hole density

x=12 %



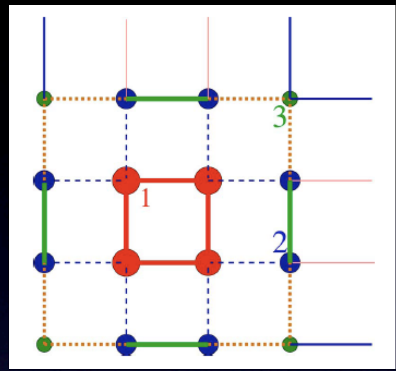
But needs STM R-maps to compare to experiments !!

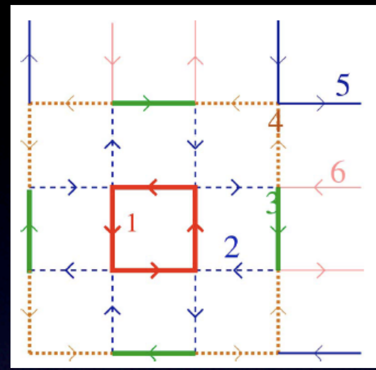
x=7 %



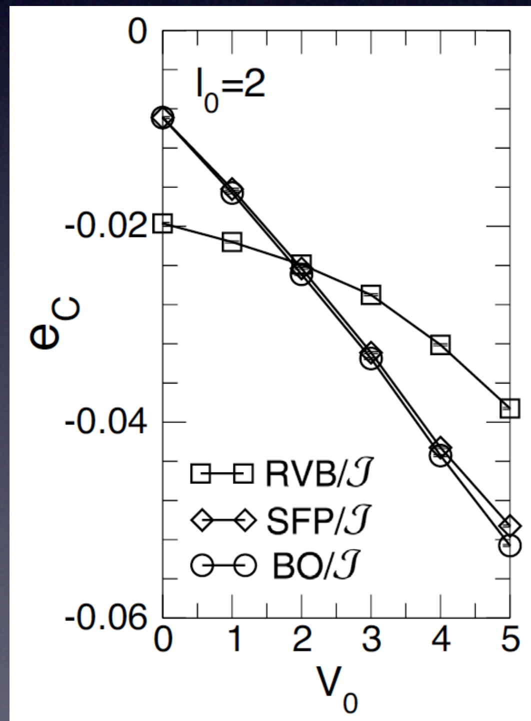
Open issue: magnetism around Zn ? To compare to NMR ...

Competition with orbital-current phases ?





- Motivation from early numerics:
  - scalar-chiral spin correlations (DP, Riera,Dagotto,91)
  - current-curent (Leung, 2000) correlations
- DMRG (White-Scalapino) shows t' destabilizes SDW stripes
- 4x4 "checkerboard" ?



DP, PRB 2005
C.Weber et al., PRB 2006

→ Needs more VMC / DMRG simulations !

Conclusions

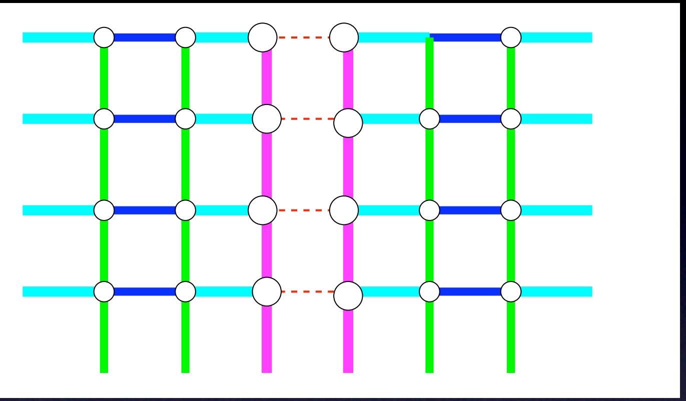
- Striped superconducting states are competitive w.r.t. the uniform RVB but have higher energies within our extended t-J model ...
- Out-of-phase SC domains cost more than in-phase: in agreement with DMRG (S. White et al.)
- Impurities like Zinc induce large domains of modulated SC regions: might have a role in the STM patterns seen
- 4x4 checkerboard charge ordered state seems energetically very competitive: relevant competing non-SC state with TRS breaking ?

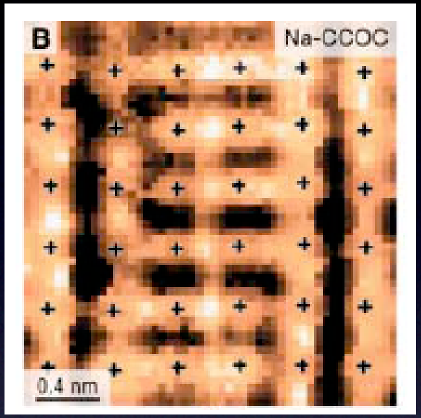
References:

(I) Raczkowski et al., PRB (RC) **76**, 140505 (2007)
(II) Capello et al., PRB **77**, 224502 (2008)
(III) Capello and DP, PRB 79, 224507 (2009)

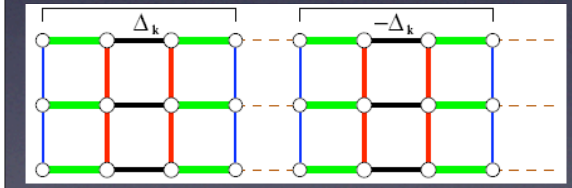
Partial summary

* superconducting RVB hole stripes





* pi-shift RVB hole stripes



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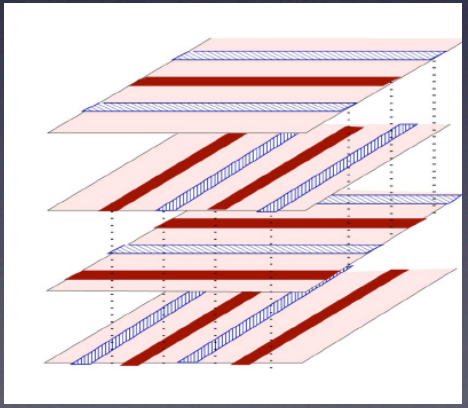
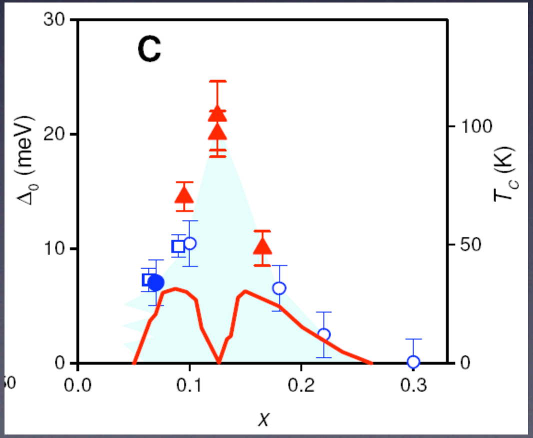
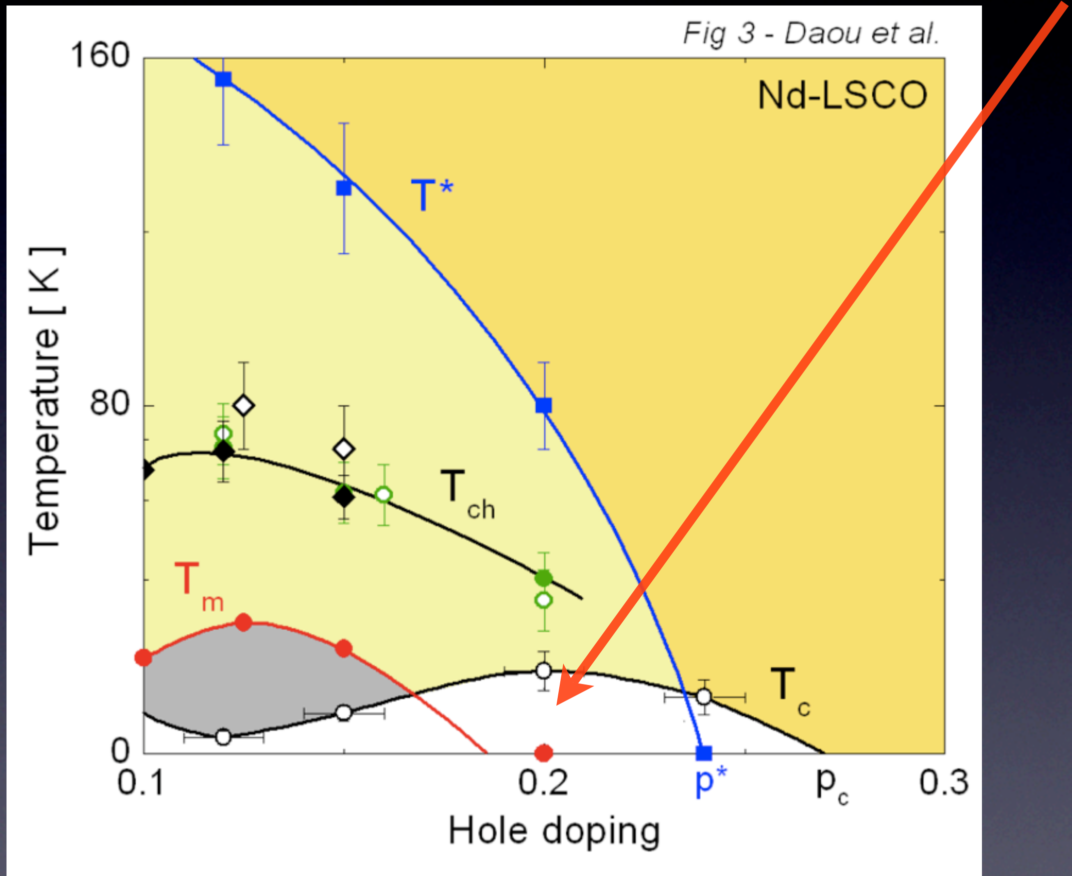


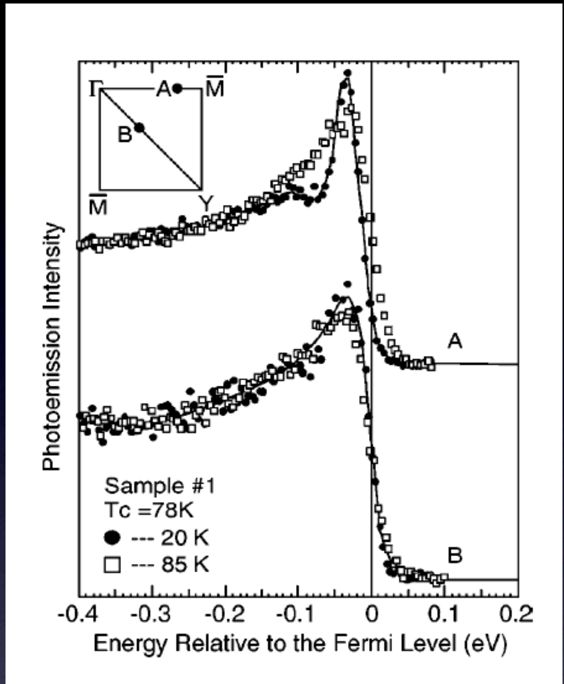


Charge and Superconductivity might coexist even without spin order !

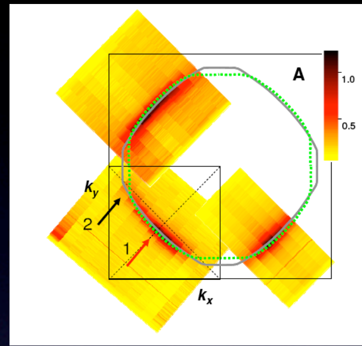


L. Taillefer's group
[arXiv:0806.2881]

ARPES: the d-wave gap

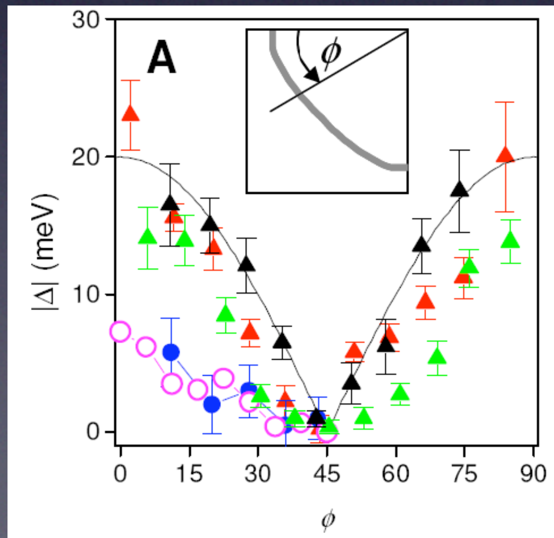


(pi,0) vs (pi/2,pi/2)
Shen 1993
Bi2212
Tc=88K

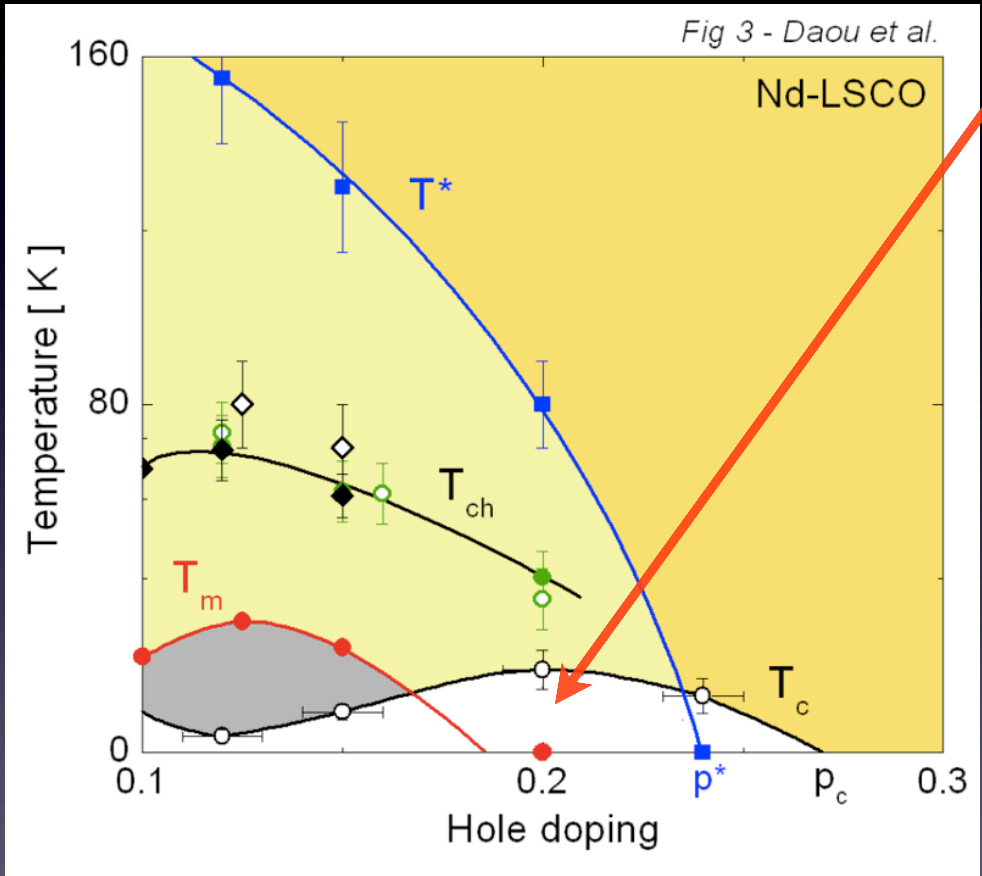


Nodal quasiparticles
at pi/2,pi/2

The gap closes
at pi/2,pi/2



Charge and Superconductivity might coexist even without spin order !



L. Taillefer’s group
[arXiv:0806.2881]

RVB theory: mathematical framework

Correlated wavefunctions
Gutzwiller projected HF d-wave BCS:

$$P\left|\Phi\right\rangle = P\prod_{\vec{k}}\left(u_{\vec{k}} + v_{\vec{k}}c^{\dagger}_{\vec{k}\uparrow}c^{\dagger}_{-\vec{k}\downarrow}\right)\left|0\right\rangle$$

$$P = \prod_i \left(1 - n_{i\uparrow}n_{i\downarrow}\right)$$

→ Variational Monte Carlo

→ Mean field theory

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

Gutwiller approximation

$$\left\langle c^{+}_{i\sigma}c_{j\sigma}\right\rangle = g_t\left\langle c^{+}_{i\sigma}c_{j\sigma}\right\rangle_0$$

$$\left\langle S_i\cdot S_j\right\rangle = g_S\left\langle S_i\cdot S_j\right\rangle_0$$

$$\downarrow$$

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

Competing phases:
d-wave RVB ←→ staggered flux
Affleck-Marston 1988

Meanfield Fermionic theory

Extend RVB picture & formalism to inhomogeneous case

$$H_{\mathrm{MF}} = -t \sum_{\langle ij \rangle \sigma} g^t_{ij} (c^\dagger_{i,\sigma} c_{j,\sigma} + h.c.) - \mu \sum_{i\sigma} n_{i,\sigma}$$
$$-\frac{3}{4} J \sum_{\langle ij \rangle \sigma} g^J_{i,j} (\chi_{ji} c^\dagger_{i,\sigma} c_{j,\sigma} + h.c. - |\chi_{ij}|^2)$$
$$-\frac{3}{4} J \sum_{\langle ij \rangle \sigma} g^J_{i,j} (\Delta_{ji} c^\dagger_{i,\sigma} c^\dagger_{j,-\sigma} + h.c. - |\Delta_{ij}|^2),$$

→ + usual MF self-consistent equations

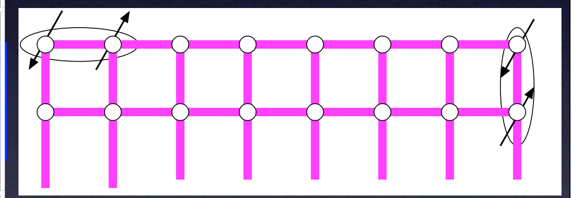
→ Site dependent g's, bond amplitudes and site densities

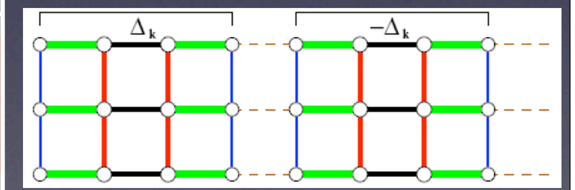
Energetics for the t-J model

$$H_{tJ} = -t \sum_{\langle ij \rangle, \sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + h.c. + J \sum_{\langle ij \rangle} S_i \cdot S_j$$

t/J=3,
doping 1/8
up to
16x16 clusters

WF	E_{RMFT} [t]	E_{VMC} [t]
RVB	-0.4549	-0.45564
SFP	-0.4284	-0.44630
pi-DRVB	-0.4412	-0.44529

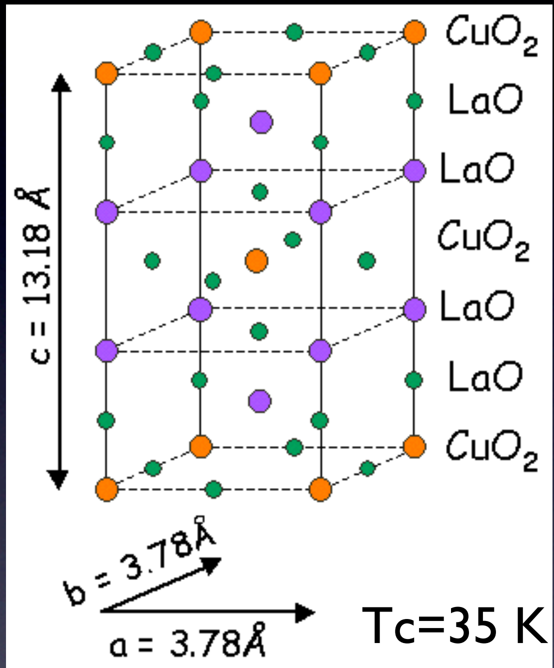




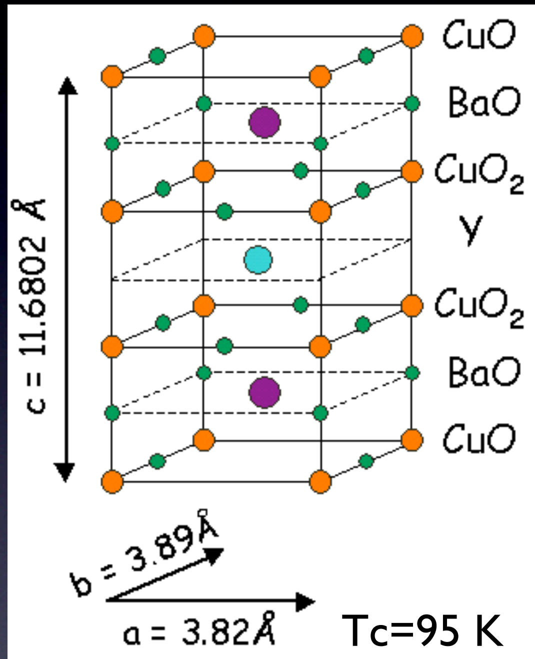
Very close energies but pi-shift in Δ_k has a cost

Cuprates Structure

$La_{2(-x)}\ (Ba_x,Sr_x)\ CuO_4$

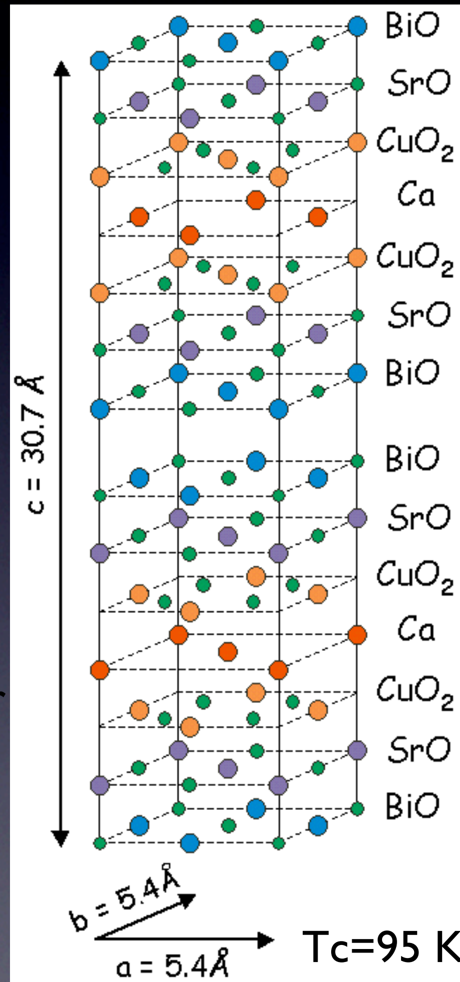


$YBa_2Cu_3O_{7(-x)}$



chains charge reservoir

$Bi_2Sr_2CaCu_2O_{8(+x)}$



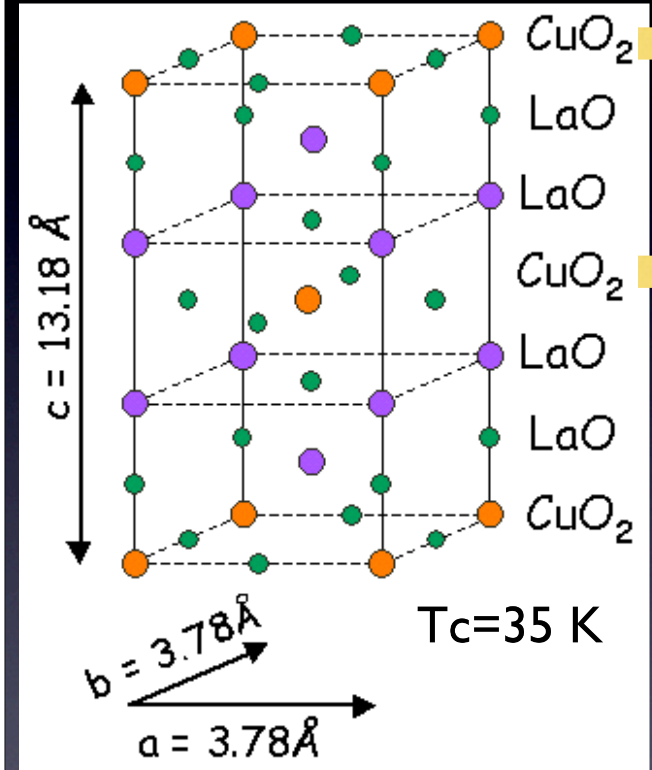
Layered structure with CuO_2 planes

+

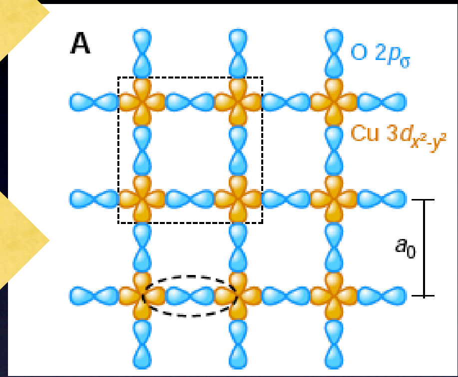
charge reservoirs (La,Y,Ba,Ca,O)

The Cuprates

La_2CuO_4



Layered structure with CuO_2 planes



Cu d-orbitals:
small overlap
strong correlation

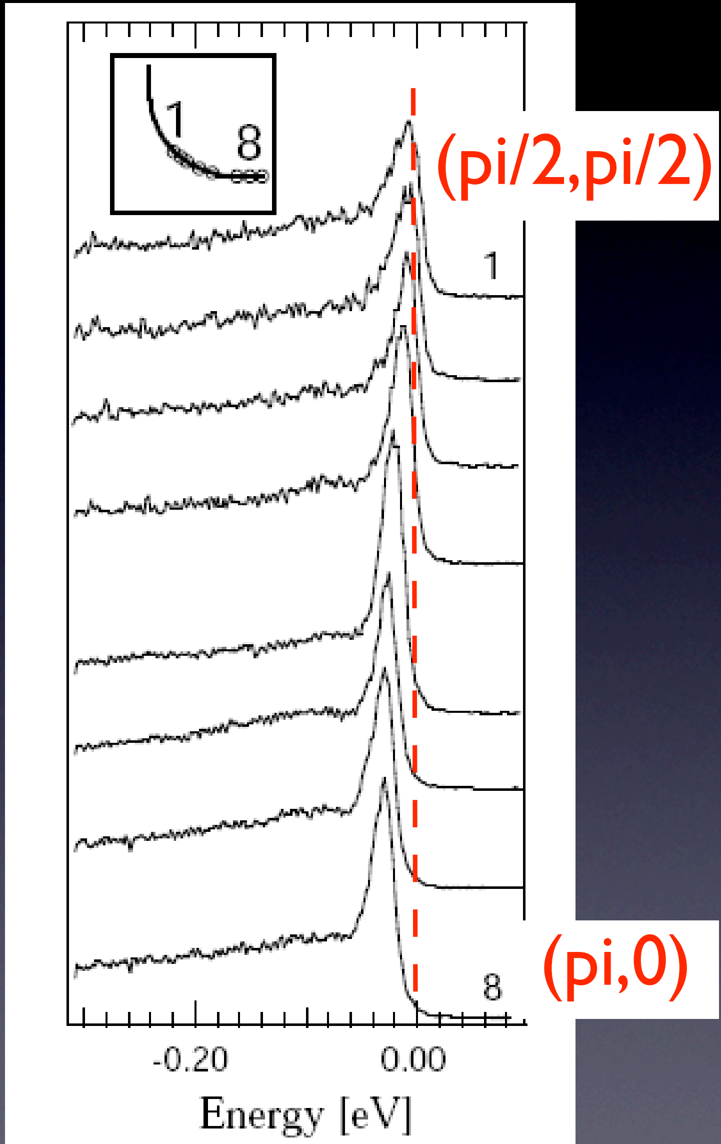
2D square lattice

Interesting Physics upon doping

*Undoped: La_2CuO_4: 1 electron per site

*Doped: La^{3+} substituted with $(Ba,Sr)^{2+}$
introduction of extra carriers (holes)
in the planes

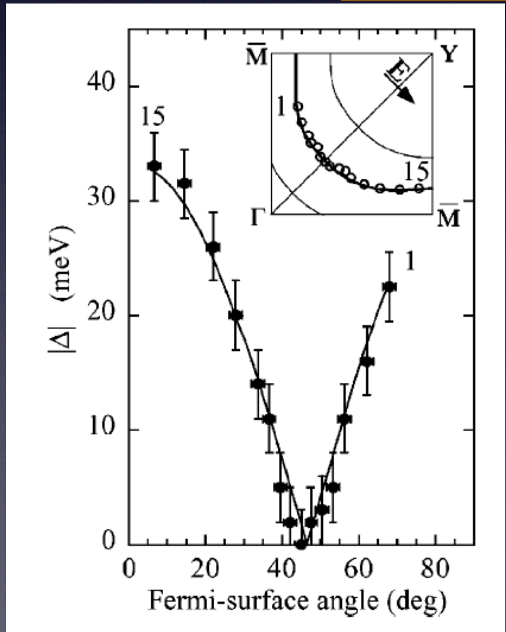
The d-wave superconducting gap



[Bi2212, Kaminski PRL 2001]

Defined quasiparticles
in the superconducting state

d-wave gap:
the gap closes
at (pi/2,pi/2)



[Bi2212, Ding, Norman 1996]