Interplay between charge & pairing modulations in cuprate high-Tc superconductors

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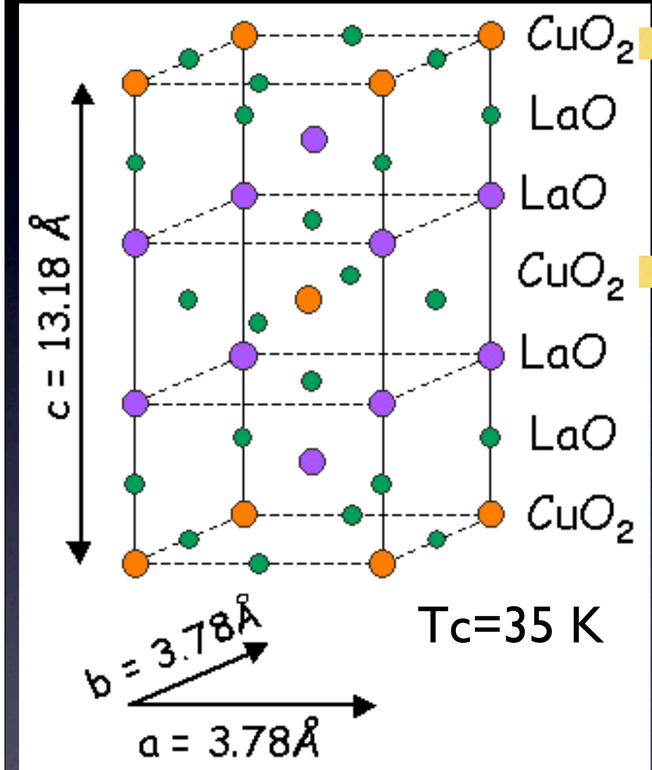
Outline

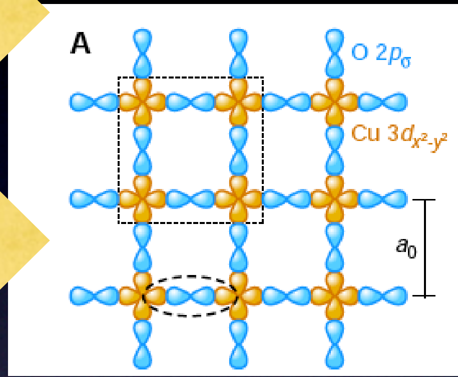
- Motivations: experimental observation of charge ordering in High-Tc materials
- Theoretical framework: t-J model and variational wavefunctions
- Results on superconducting RVB hole stripes

The Cuprates

La_2CuO_4



Layered structure with CuO_2 planes



Cu d-orbitals:
small overlap
strong correlation

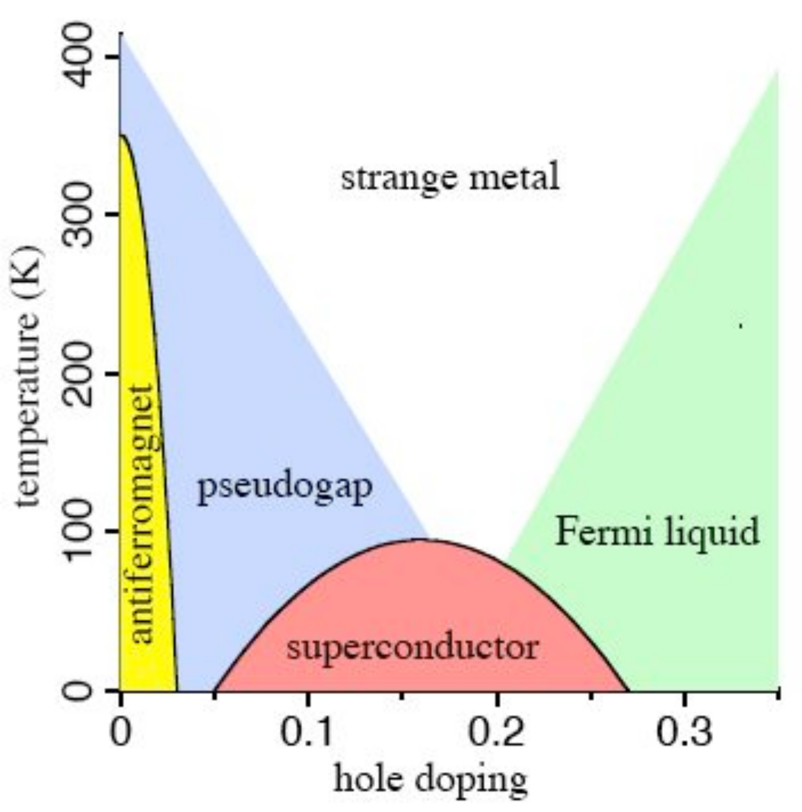
2D square lattice

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

High-Tc Phase diagram



* S=1/2 Mott insulator (AF)

* Pseudogap for underdoped and Non-Fermi liquid

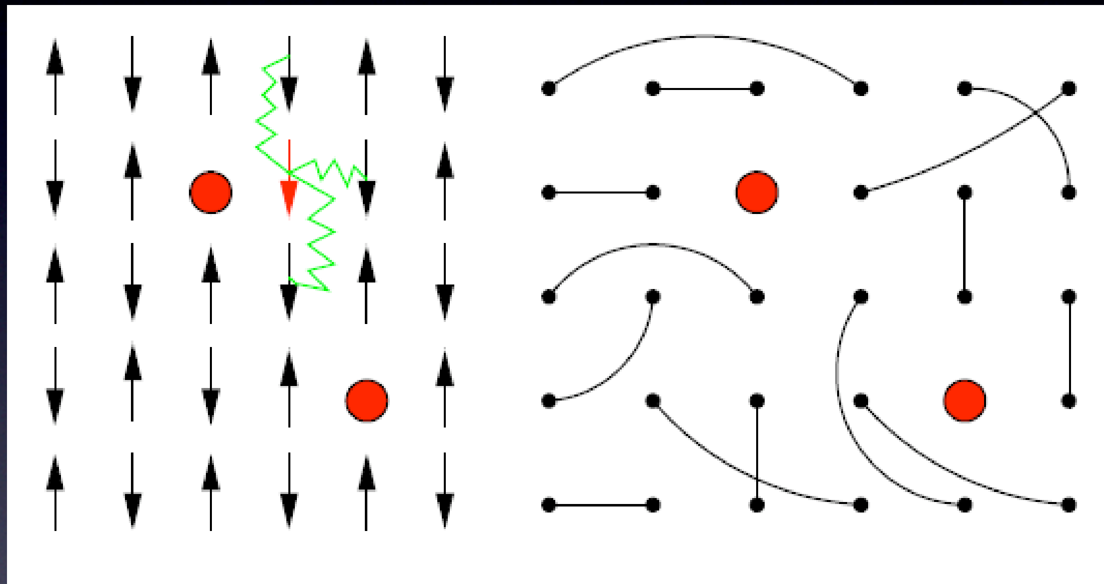
*d-wave superconductivity

* Fermi liquid for overdoped

Strong correlation is ubiquitous in High-Tc
Superconducting state emerges from
doping a Mott insulator

The RVB scenario upon doping

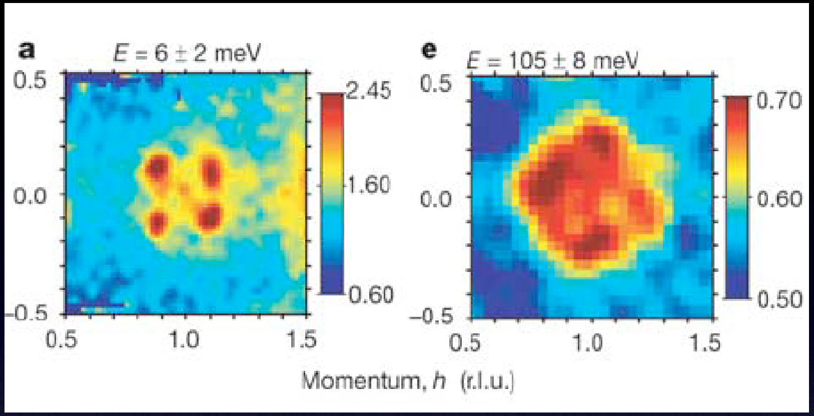
Holes frustrate antiferromagnetism



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

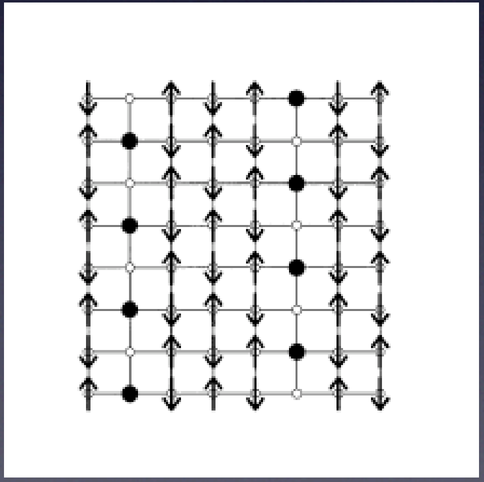
The RVB state naturally becomes a superconductor
since the pairing already exists

Neutron scattering: AF Stripes



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

[Tranquada et al. Nature 1995]

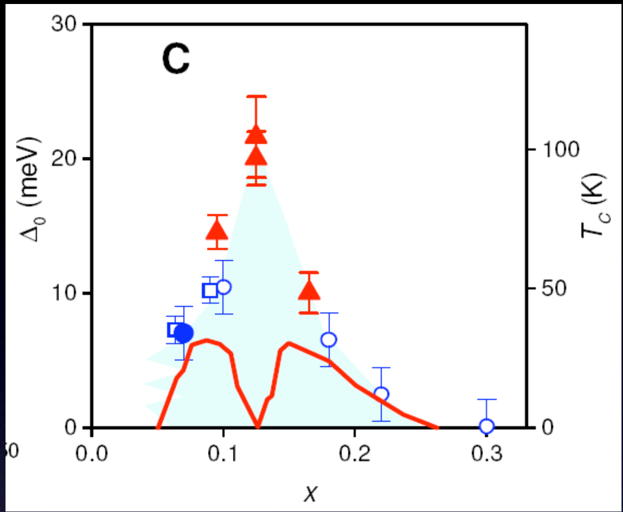


ANTIFERROMAGNETIC STRIPE SCENARIO

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

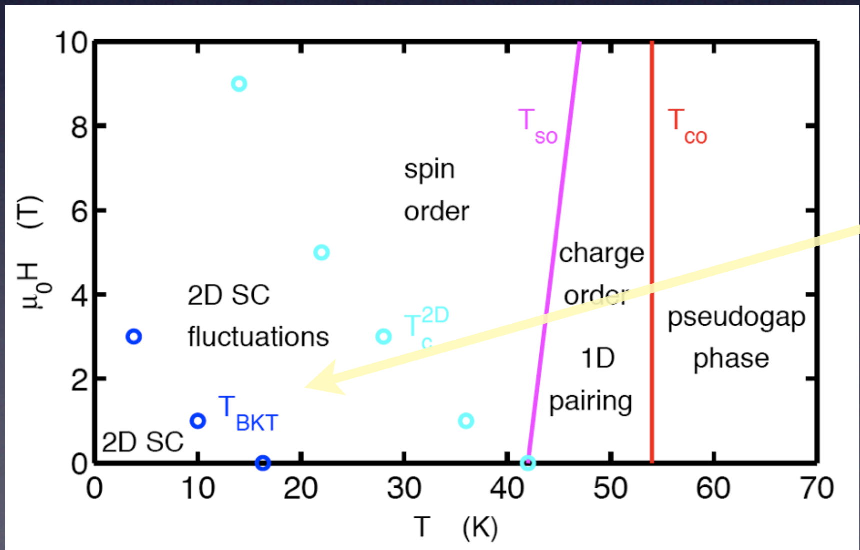
Zaanen et al. PRB 89
Poilblanc-Rice PRB 89

Stripes are compatible with pairing !



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

[Valla et al., Science 2006]



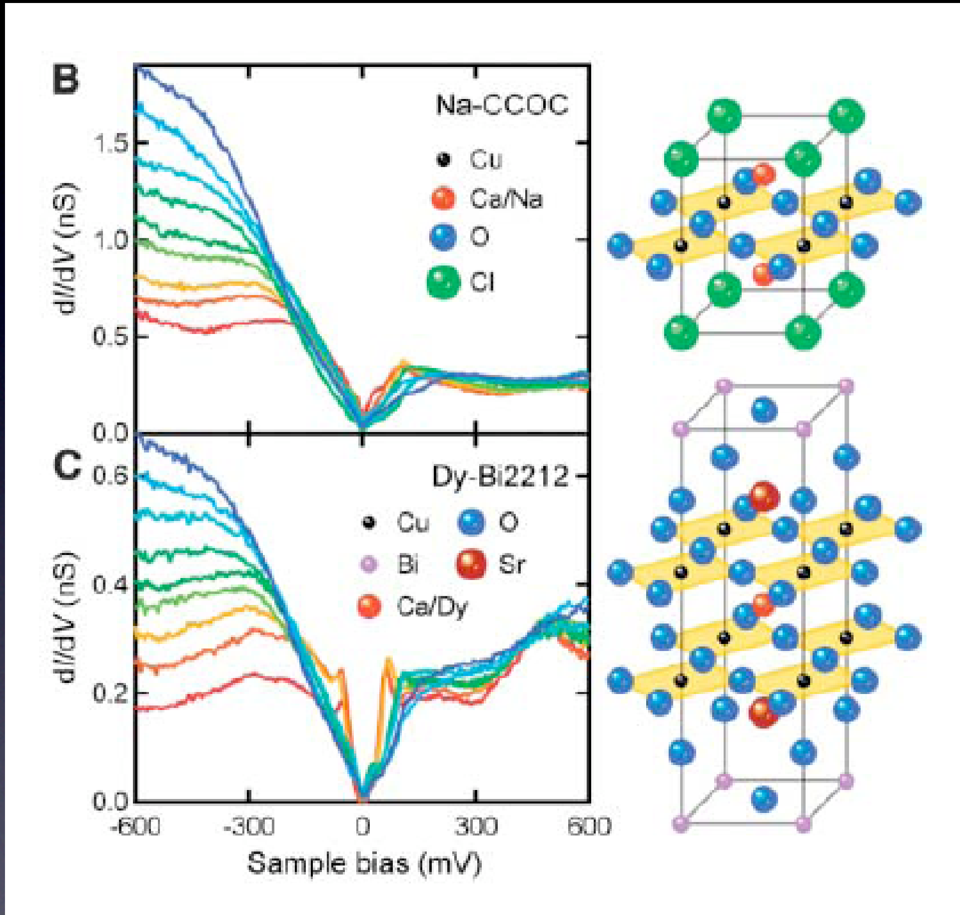
[Li et al., PRL 2007]

Planes are (Josephson) decoupled but pairing exists!

[Berg et al., PRL 2007]

How can one get 2D SC ?

STM Experiments:



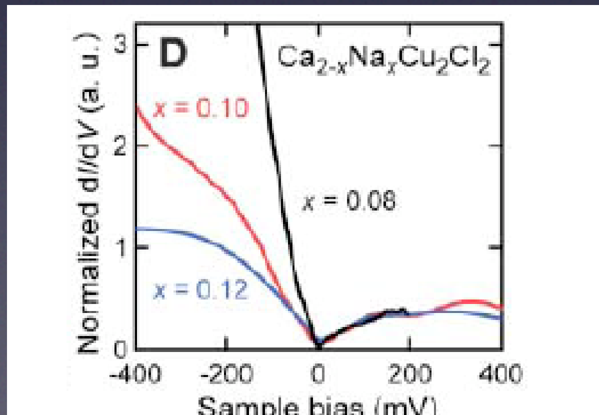
DIFFERENTIAL CURRENT

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

*N(r,E) LOCAL DOS

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

Large spatial dependence of the Tunnelling asymmetry

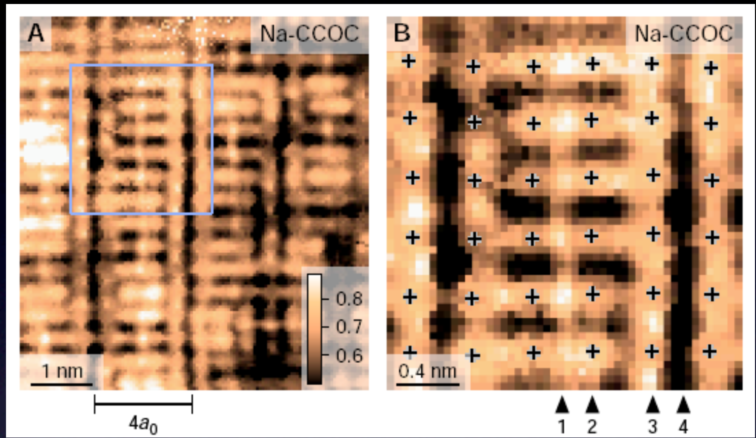


EXTRACT e⁻ INSERT e⁻

STM-experiments: R-maps

$Ca_{2-x}Na_xCuO_2Cl_2$ and Dy-Bi2212 (at T< Tc)

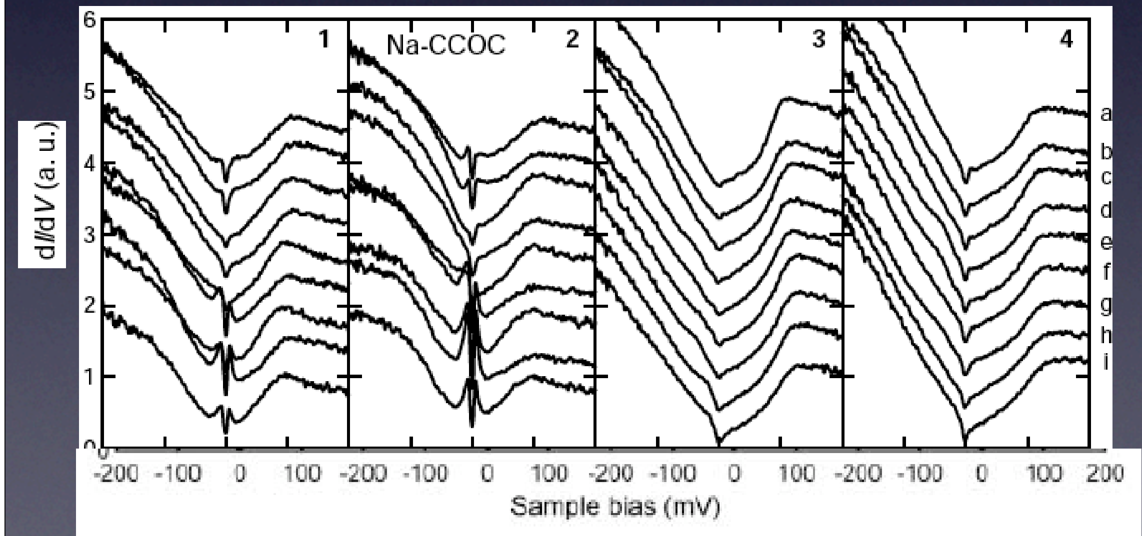
[Kohsaka et al. Science 2007]



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

R≈1 ⇒ more holes

R<1 ⇒ less holes



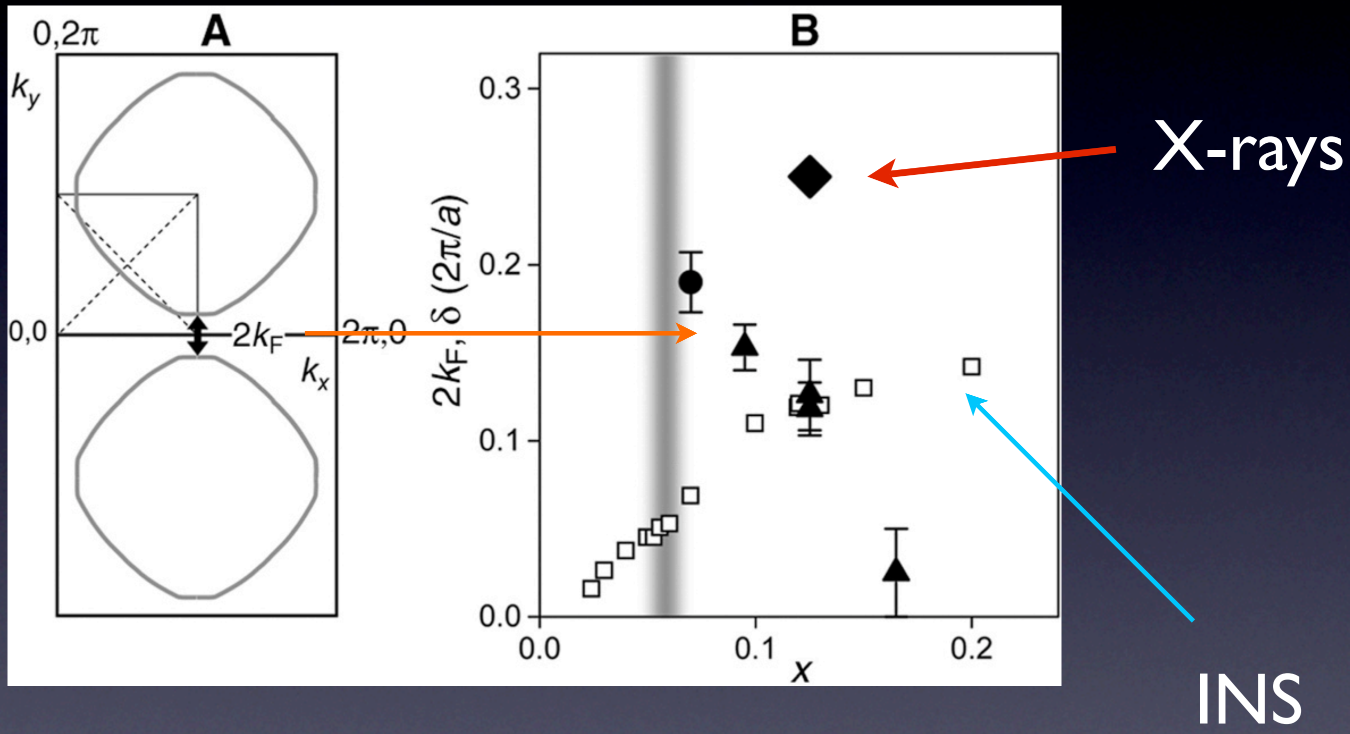
HOLE RICH

HOLE POOR

Bond-centered unidirectional patterns

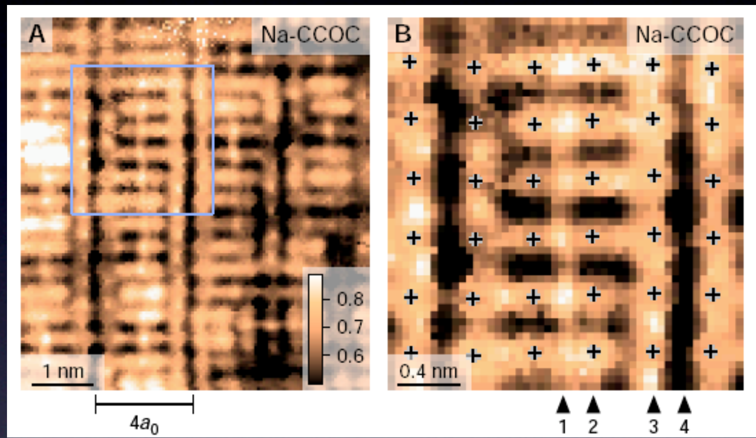
Different low-energy properties

Not a Fermi surface nesting mechanism !



[Valla et al., Science 2006]

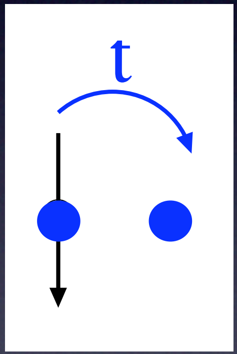
SPATIAL ORDER + SUPERCONDUCTIVITY



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

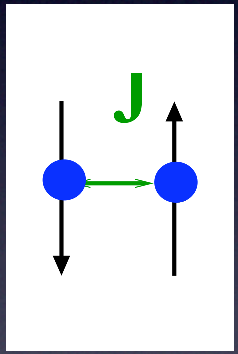
The t-J model

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

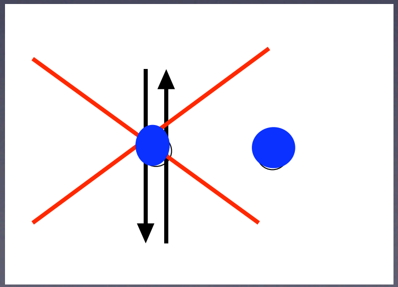


KINETIC
TERM

+



AF
EXCHANGE
TERM



CONSTRAINT of
NO DOUBLE OCCUPANCIES

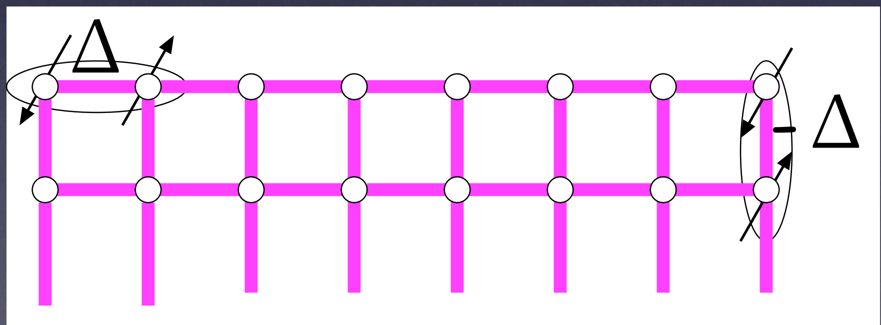
RVB variational state

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

Uncorrelated state $|D\rangle$

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

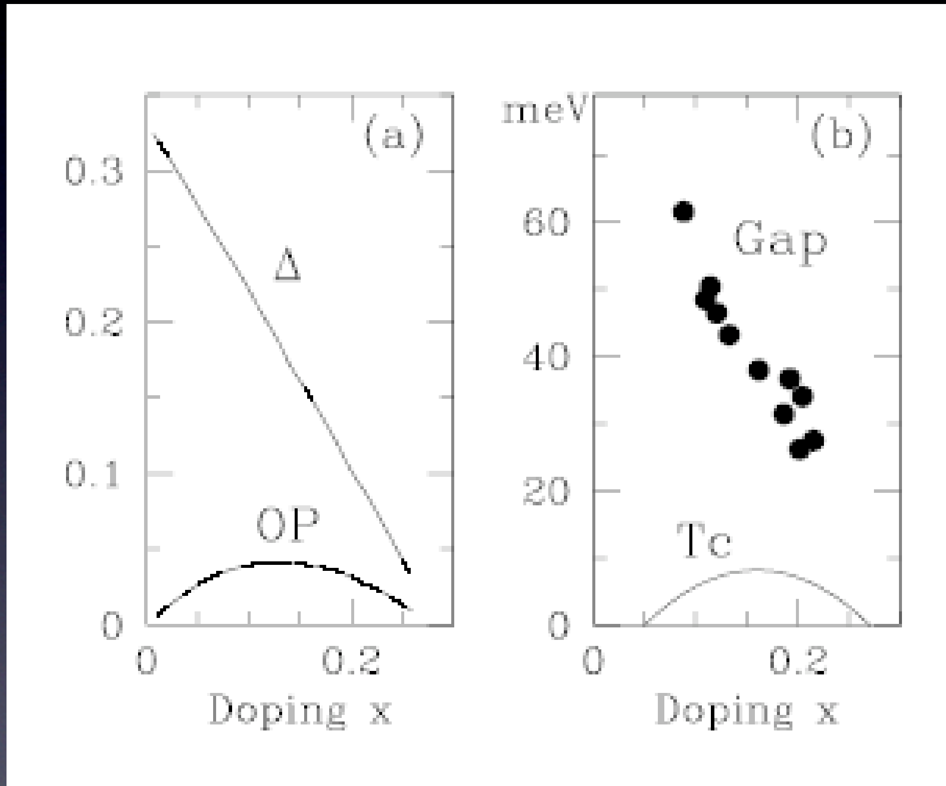
Strongly correlated wavefunction



Δ,μ are variational parameters

All Δ_{ij} uniform with d-wave symmetry

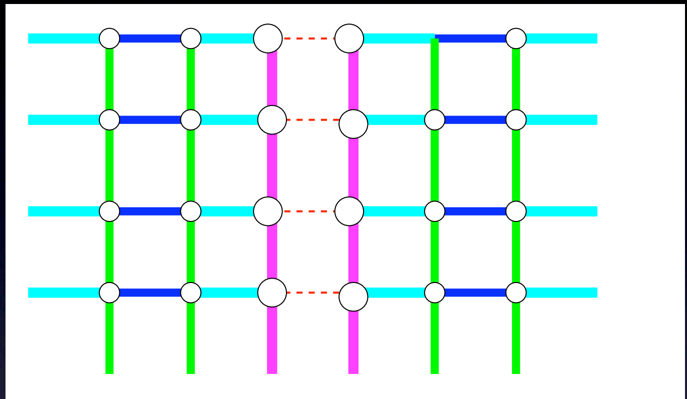
RVB => Correct behavior of pseudo-gap & SC order parameter

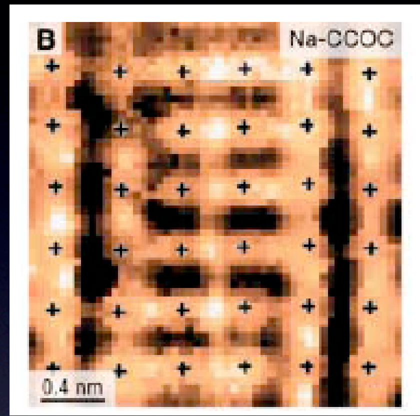


Anderson et al. J.Phys. C 2004

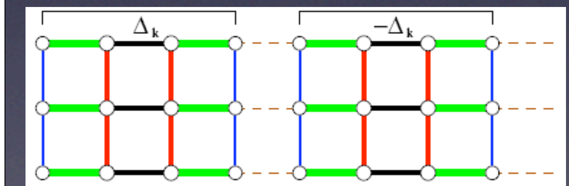
Modulated RVB state ?

* superconducting RVB hole stripes





* pi-shift RVB hole stripes



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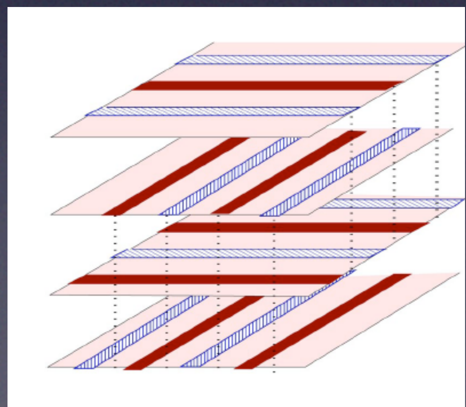
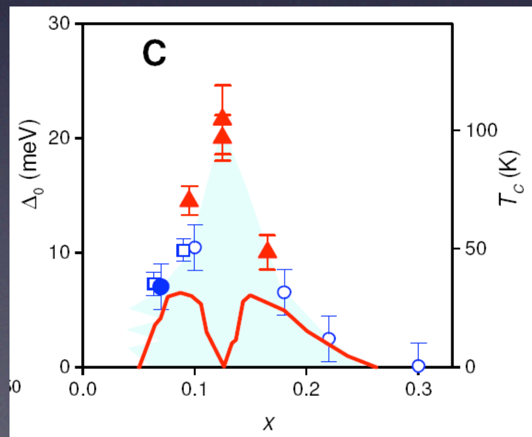


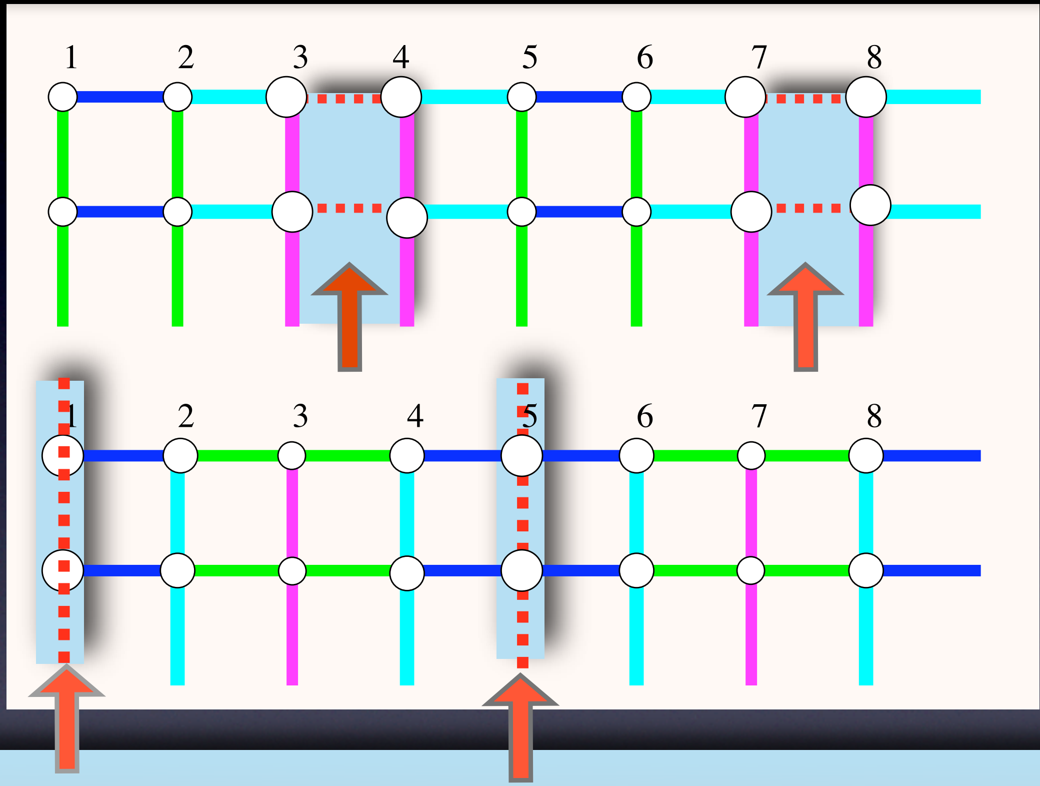


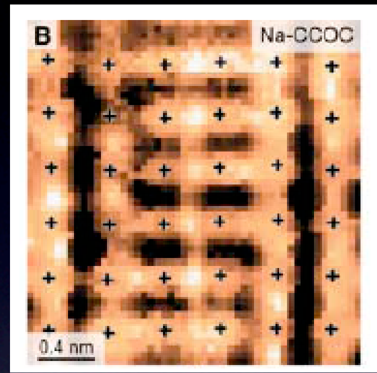
Superconducting stripes

We allow for inhomogeneous Δ_{ij}

Bond centered

Site centered



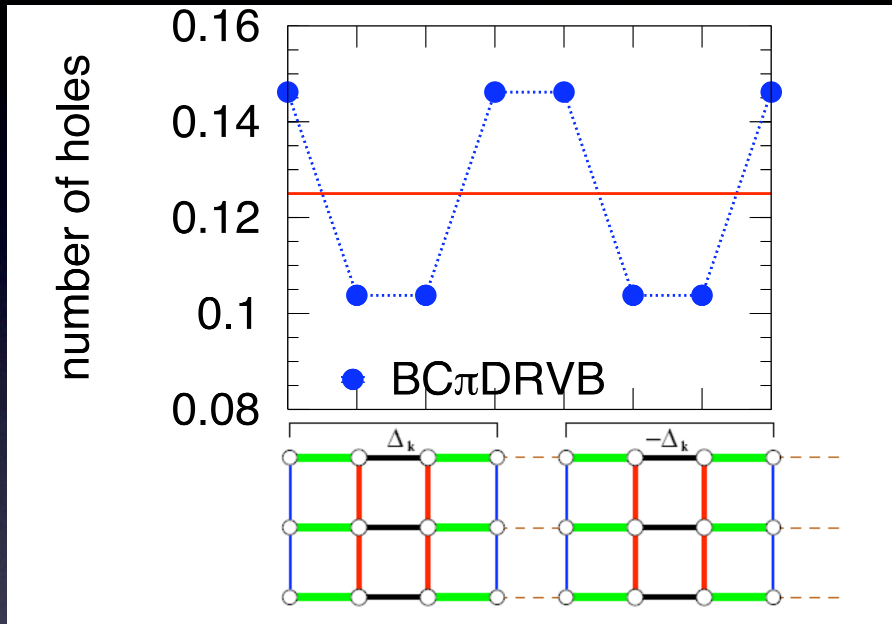


Create line-defects in the RVB state

Impose Δ_{ij}=0 along one direction,

with periodicity 1/2x

Computed charge modulation

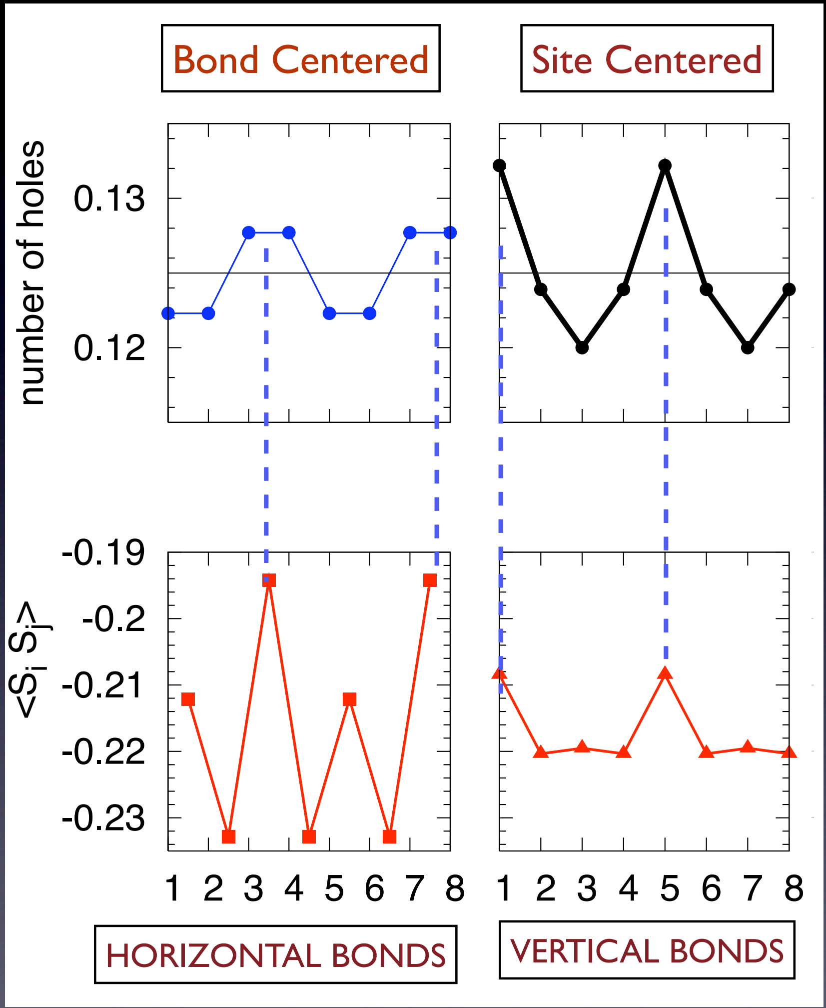


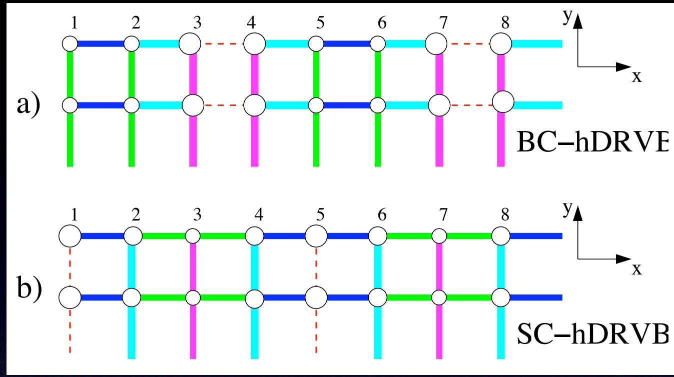
t/J=3,
doping 1/8
up to
16x16 clusters

2 NON-EQUIVALENT SITES

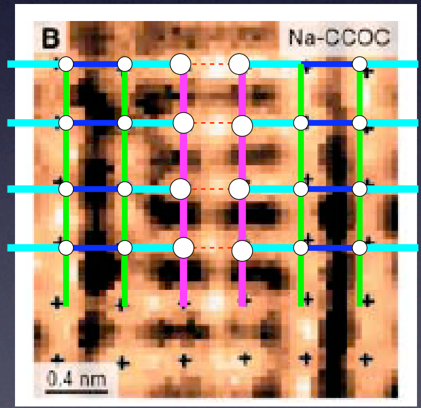
Holes concentrate where spin-pairing is smaller

Bond vs Site centered





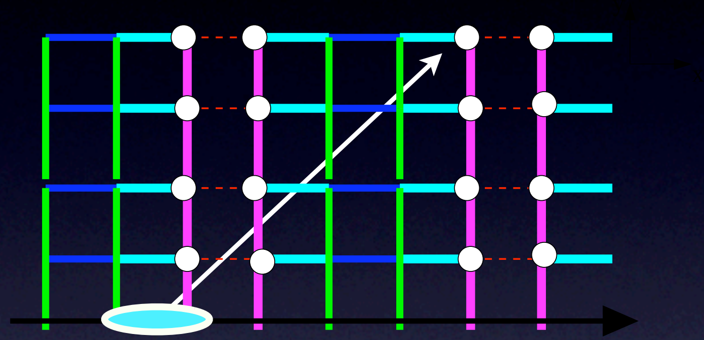
Hole stripes emerge

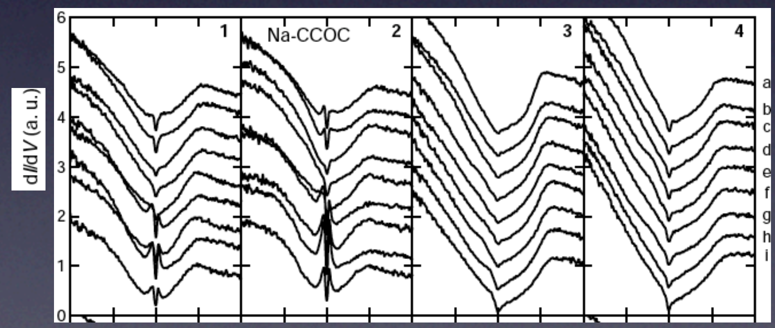


Superconductivity is modulated !

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

$$\tilde{\Delta}^\dagger_s = c^\dagger_{s\uparrow} c^\dagger_{s+a\downarrow} - c^\dagger_{s\downarrow} c^\dagger_{s+a\uparrow}$$

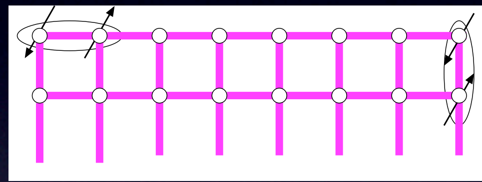


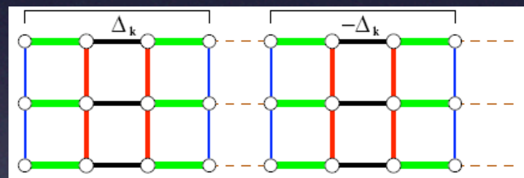


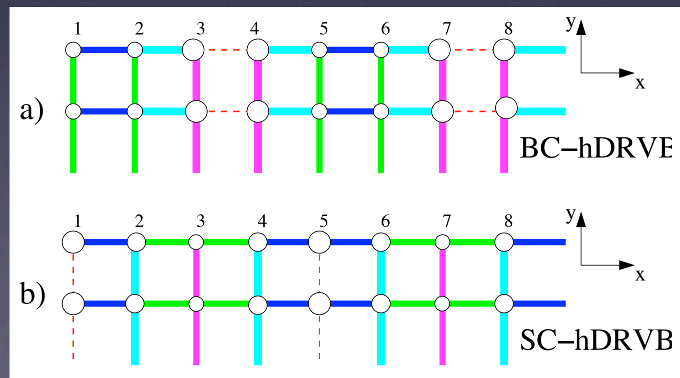
Energies are really close (~10^{-4} t)

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)

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

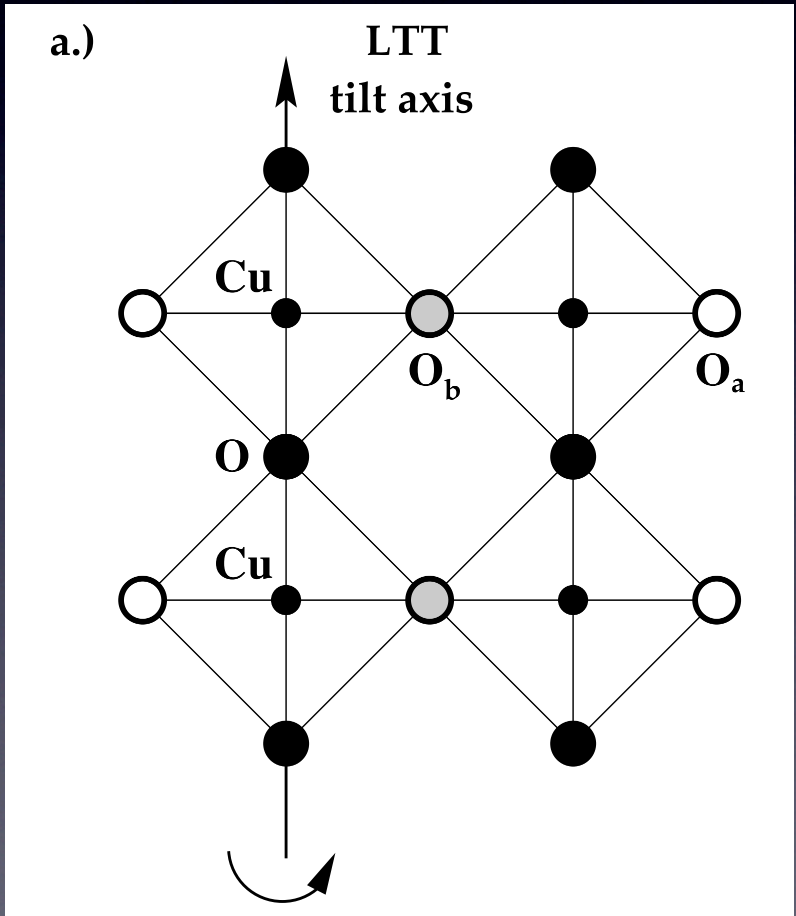






Lattice distortion

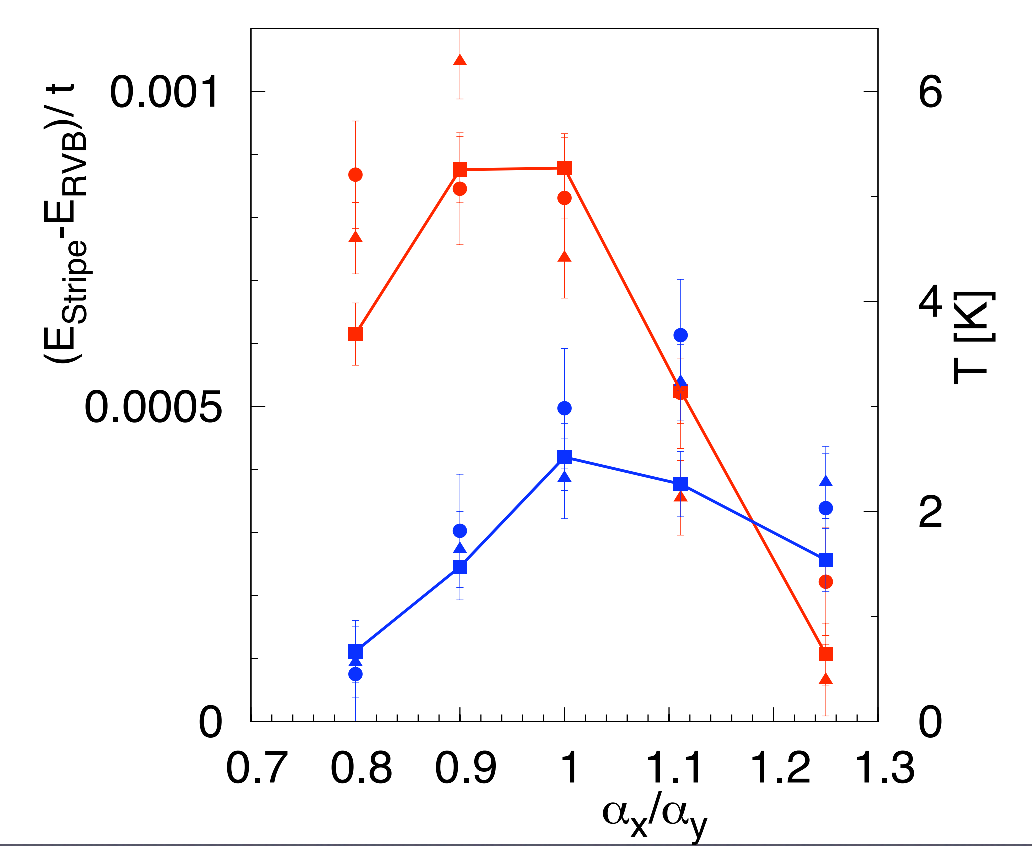
$$H_{tJ}^{\alpha} = -t \sum_{<ij>,\sigma} \alpha_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + h.c. + J \sum_{<ij>} \alpha_{ij}^{2} \, S_i \cdot S_j$$

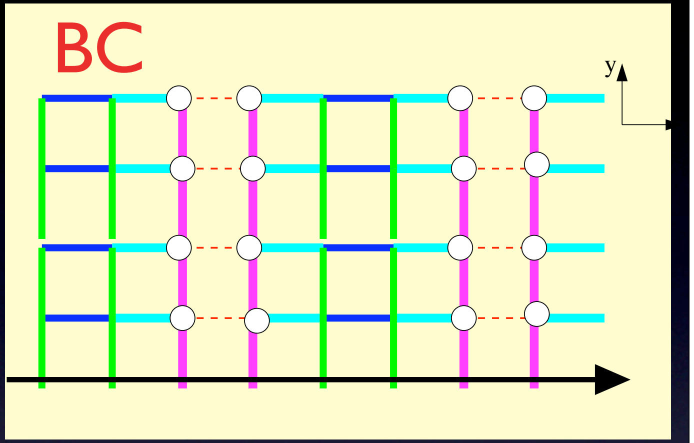


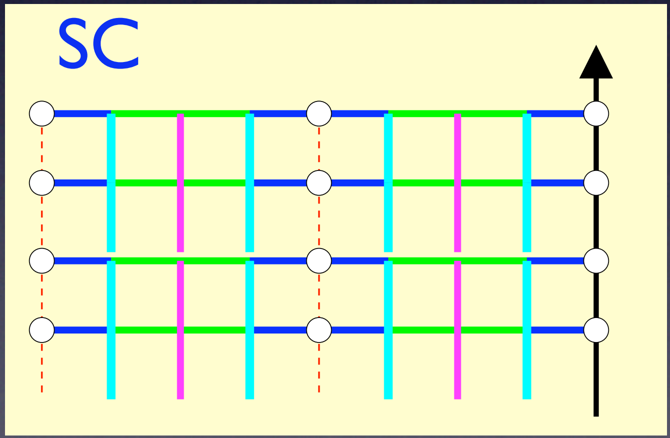
The tilt in the oxygen octahedra induces a different t and J along x and y:

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

Lattice LTT distortion further stabilizes the superconducting stripes







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]

Conclusions

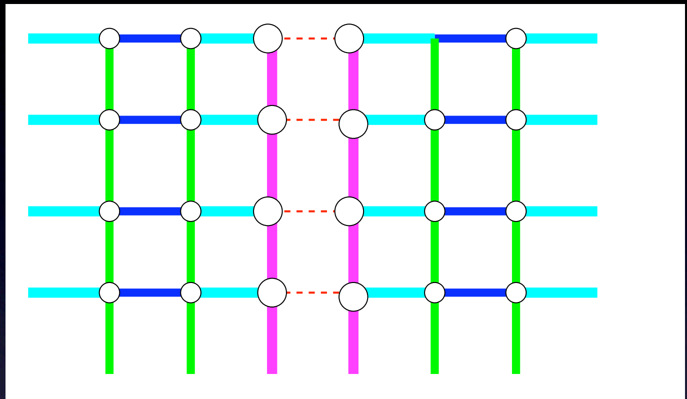
- Evidence that modulated superconducting states are energetically competitive with the uniform RVB.
- Holes patterns/superconducting regions form along unidirectional domains
- Lattice distortion further stabilizes superconducting stripes
- Impurities might also ...

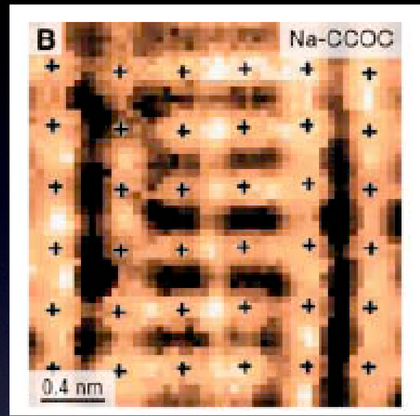
References:

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

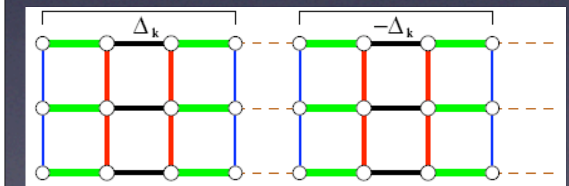
Partial summary

* superconducting RVB hole stripes





* pi-shift RVB hole stripes



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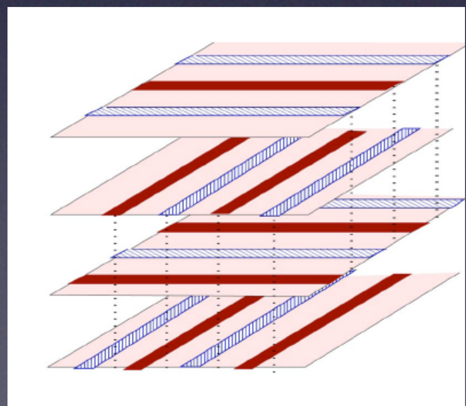
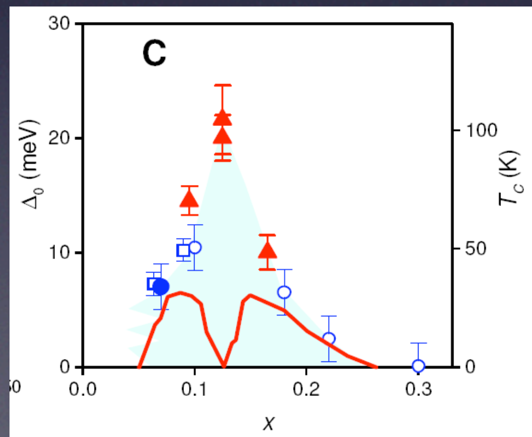


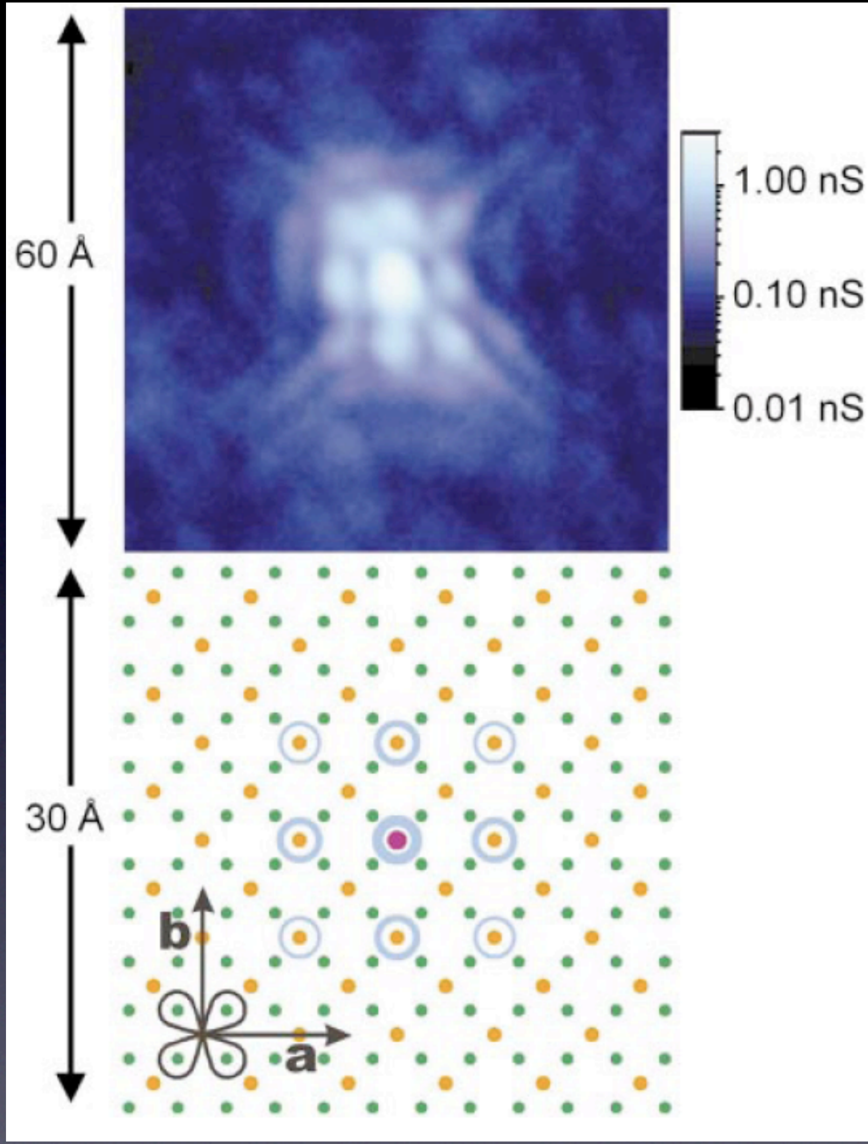


Role of impurities ?

Low-energy DOS around Zinc impurity in SC state

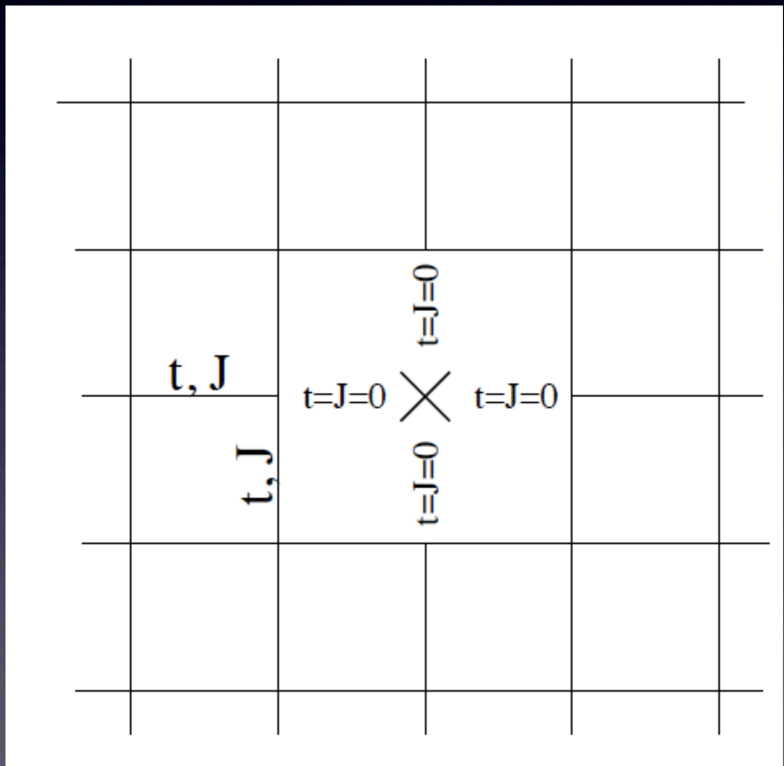
- Large DOS along nodal directions
- Suppression of SC within ~15A from Zn

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 !



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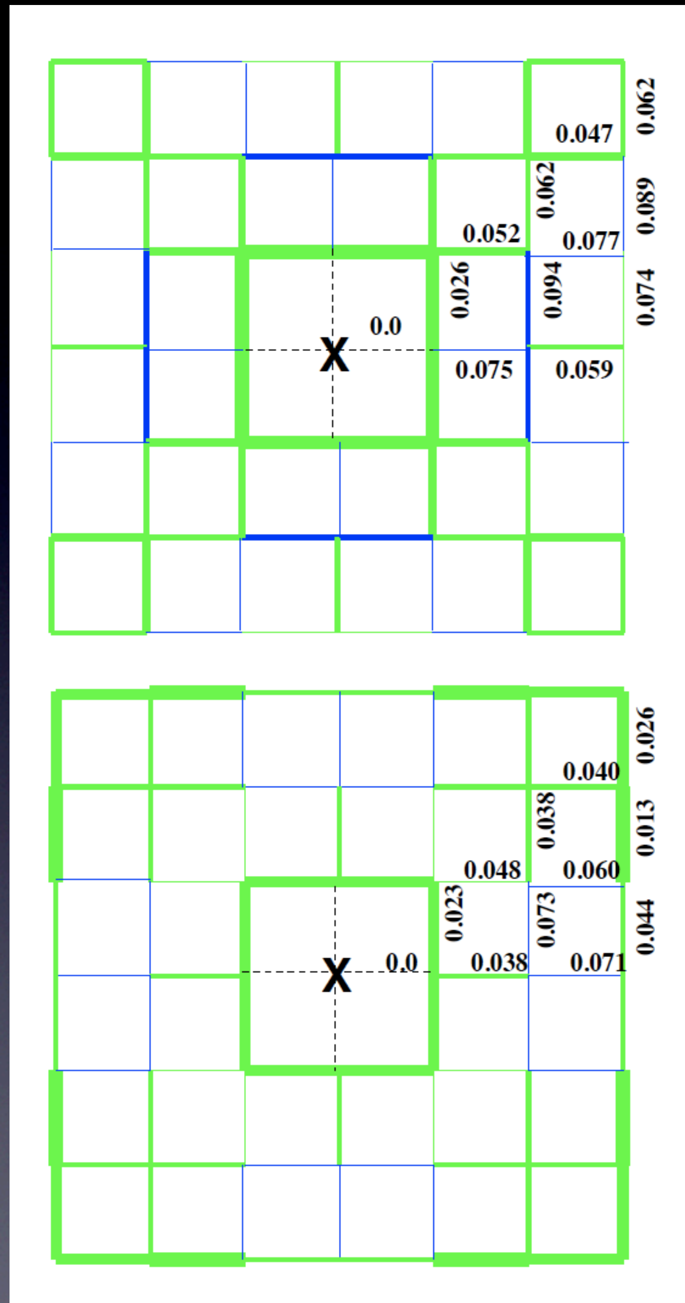
Variational Gutzwiller-projected RVB wavefunction (16x16 clusters) x=12 %

Suppression of pairing correlations over large distances

x=7 %



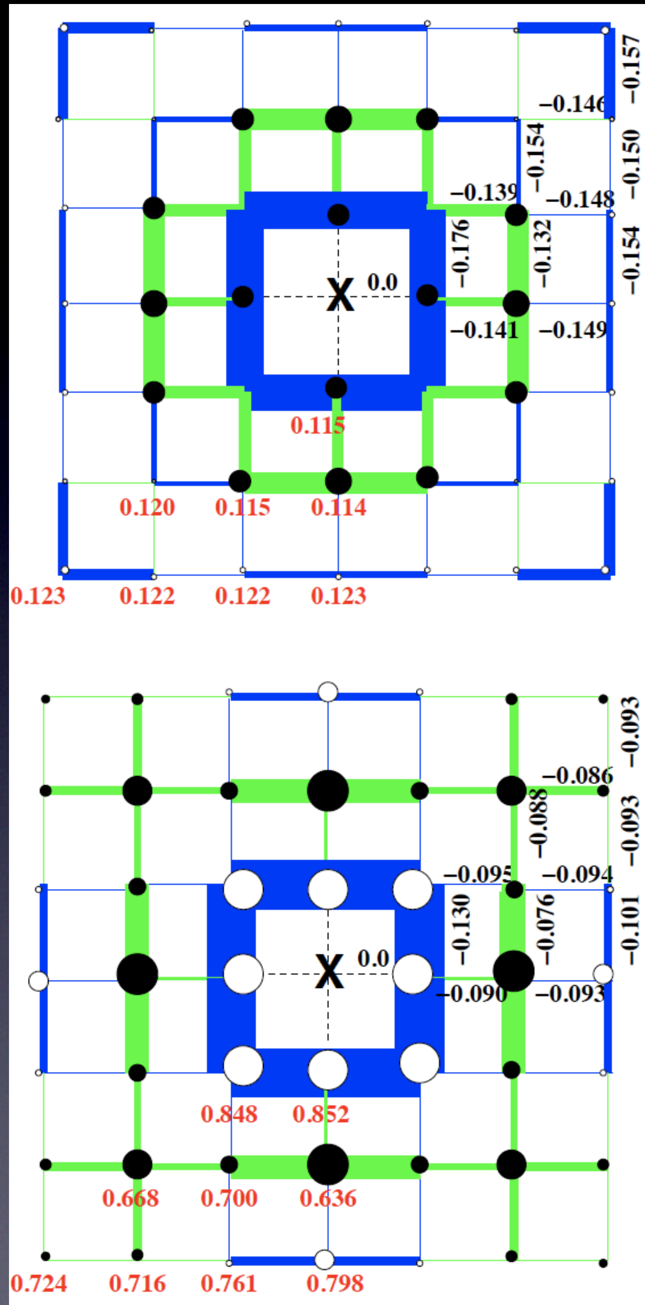
Strong modulation of local hole density

x=12 %

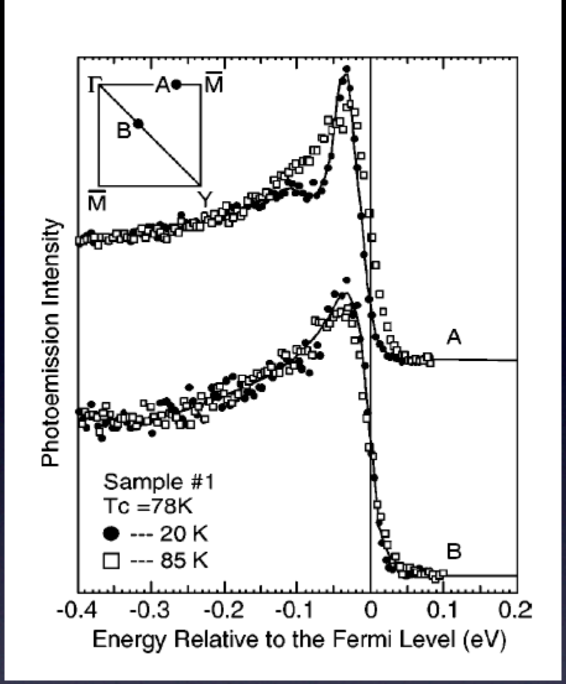
But needs STM R-maps to compare to experiments !!

x=7 %

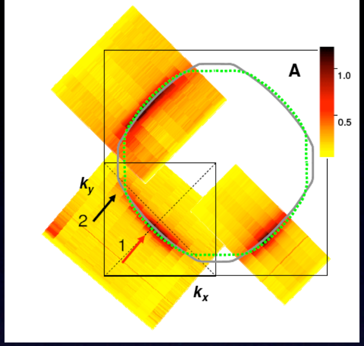
Open issue: magnetism around Zn ?   To compare to NMR ...



ARPES: the d-wave gap

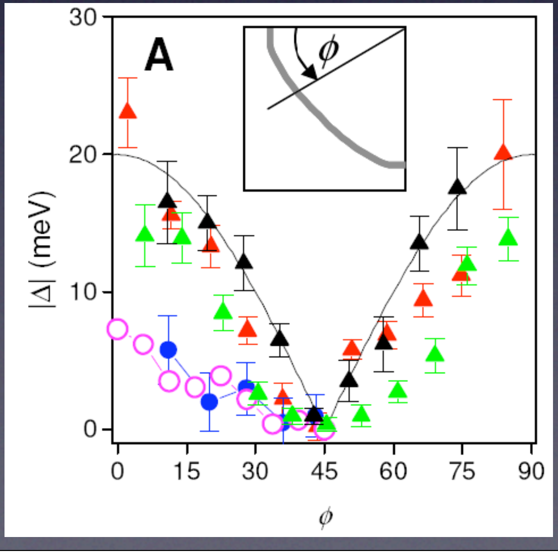


(pi,0) vs (pi/2,pi/2)
Shen 1993
Bi2212
Tc=88K

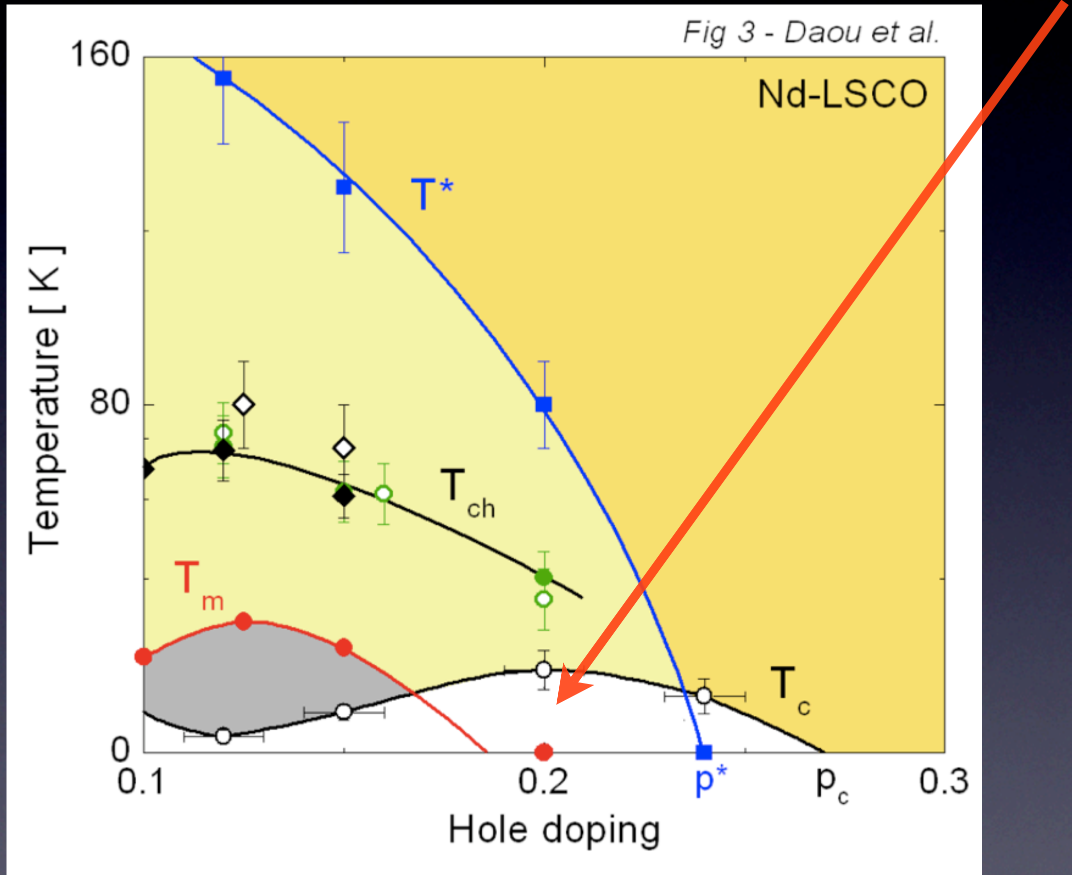


Nodal quasiparticles
at pi/2,pi/2

The gap closes
at pi/2,pi/2



Charge and Superconductivity might coexist even without spin order !



L. Taillefer's group
[arXiv:0806.2881]

Meanfield Fermionic theory

Extend RVB picture & formalism to inhomogeneous case

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

→ + usual MF self-consistent equations

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

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

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

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

↓

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

Competing phases:

d-wave RVB ←→ staggered flux

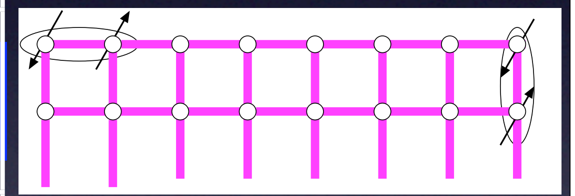
Affleck-Marston 1988

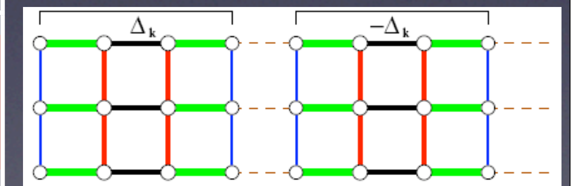
Energetics for the t-J model

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

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

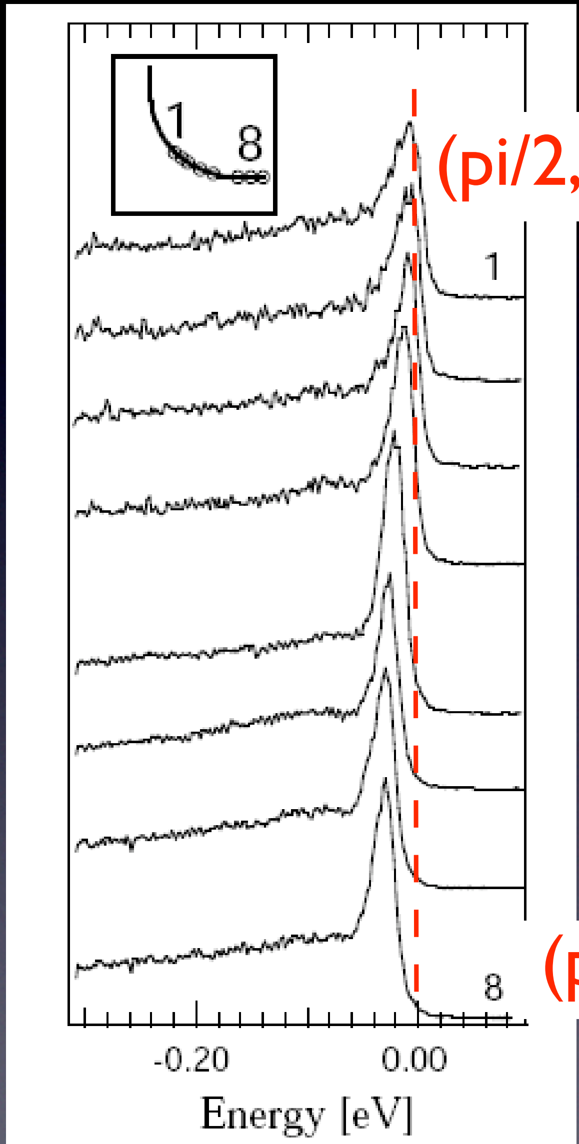
WF	E_{RMFT} [t]	E_{VMC} [t]
RVB	-0.4549	-0.45564
SFP	-0.4284	-0.44630
pi-DRVB	-0.4412	-0.44529





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

The d-wave superconducting gap



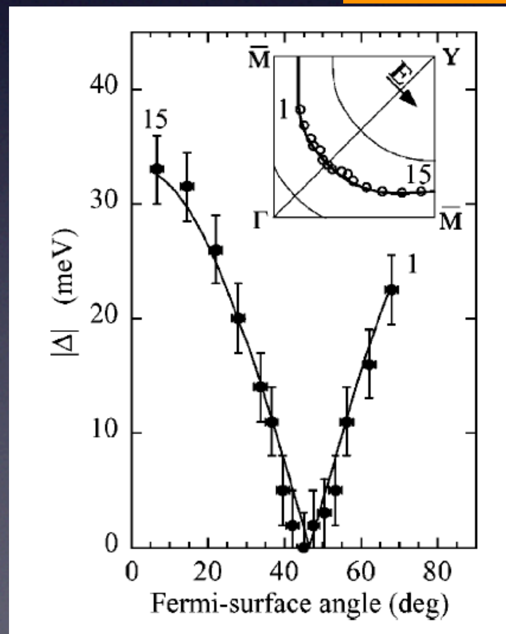
(pi/2,pi/2)

(pi,0)

[Bi2212, Kaminski PRL 2001]

Defined quasiparticles
in the superconducting state

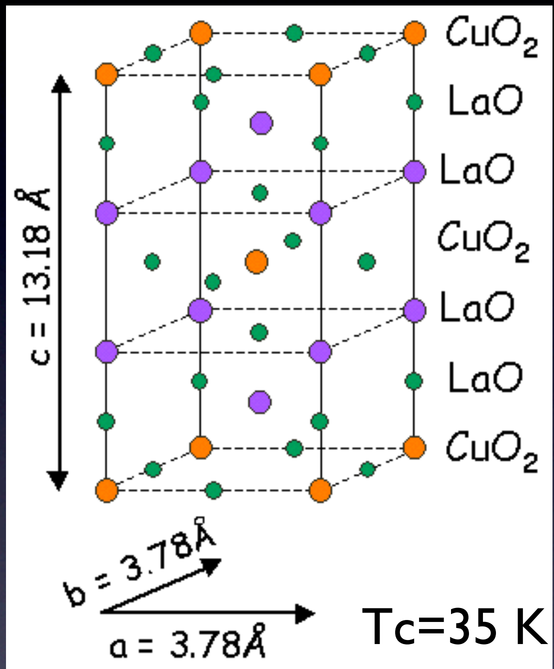
d-wave gap:
the gap closes
at (pi/2,pi/2)



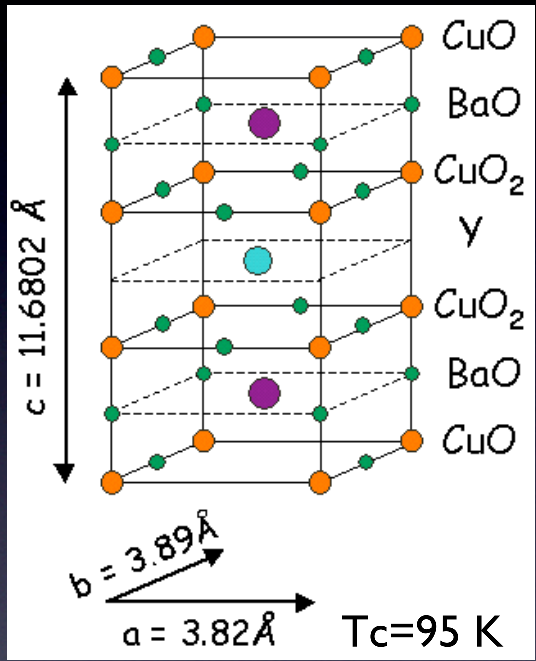
[Bi2212, Ding, Norman 1996]

Cuprates Structure

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

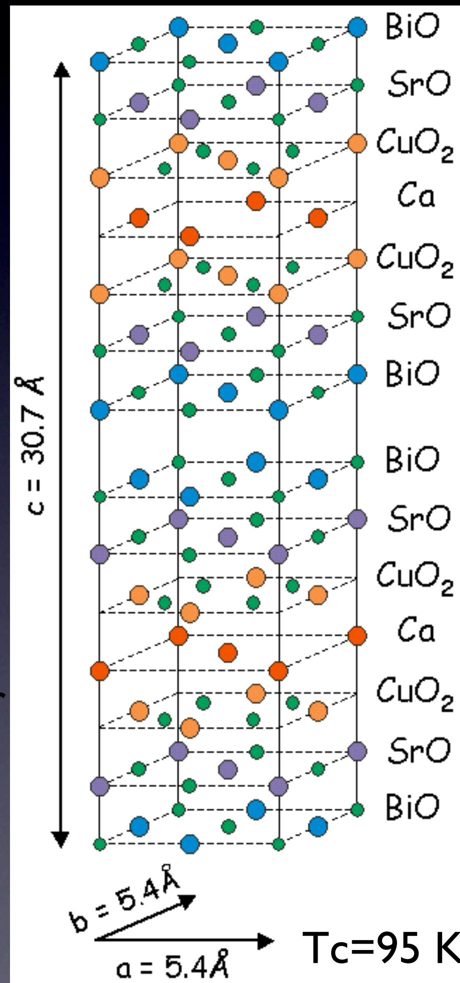


$YBa_2Cu_3O_{7(-x)}$



chains charge reservoir

$Bi_2Sr_2CaCu_2O_{8(+x)}$



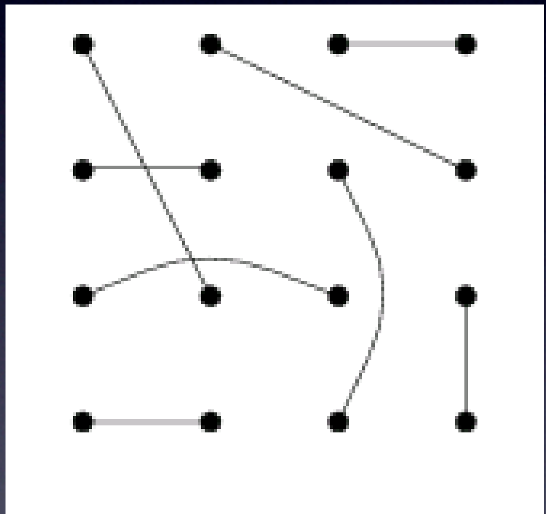
Layered structure with CuO_2 planes

+

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

Resonating Valence Bond state

* Mott physics: no double occupancies
* Antiferromagnetic term important



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

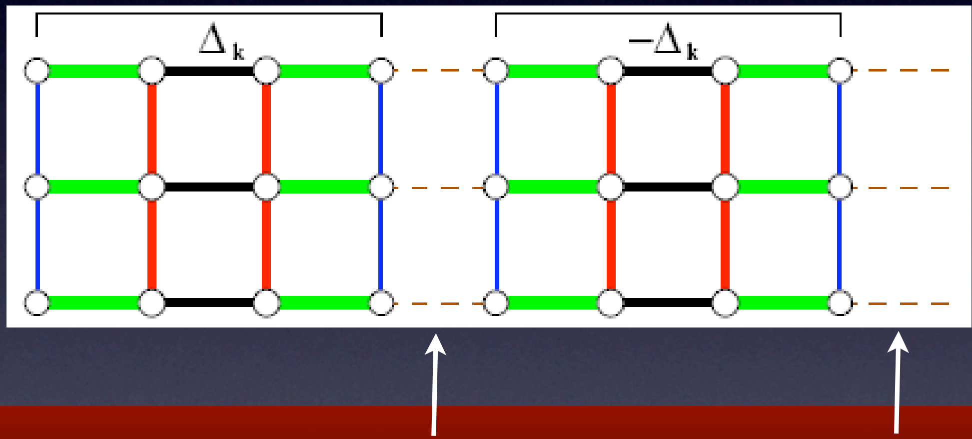
$$\bullet\!\!-\!\!\bullet = \frac{1}{\sqrt{2}}(\uparrow_i\downarrow_j - \downarrow_i\uparrow_j)$$

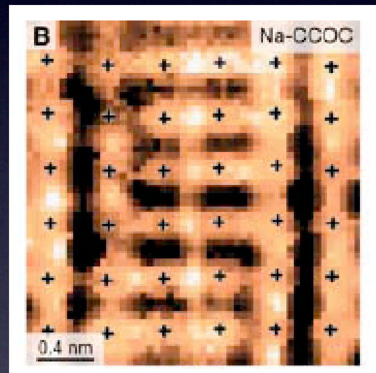
[Anderson, Science 1987]

RVB: liquid of singlets of spins which resonate

Superconducting stripes (I): pi-domain RVB stripes

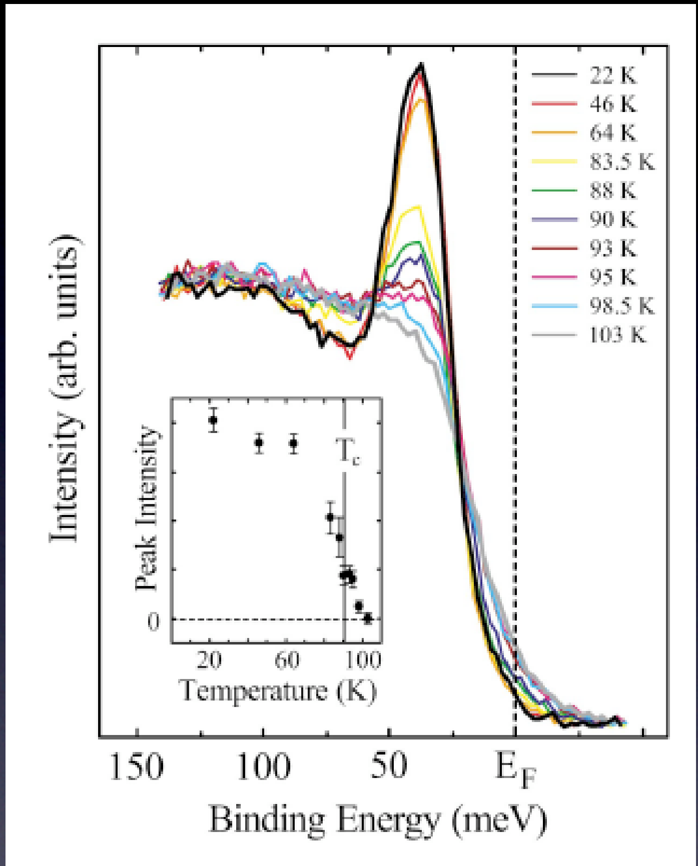
Bond-centered symmetry



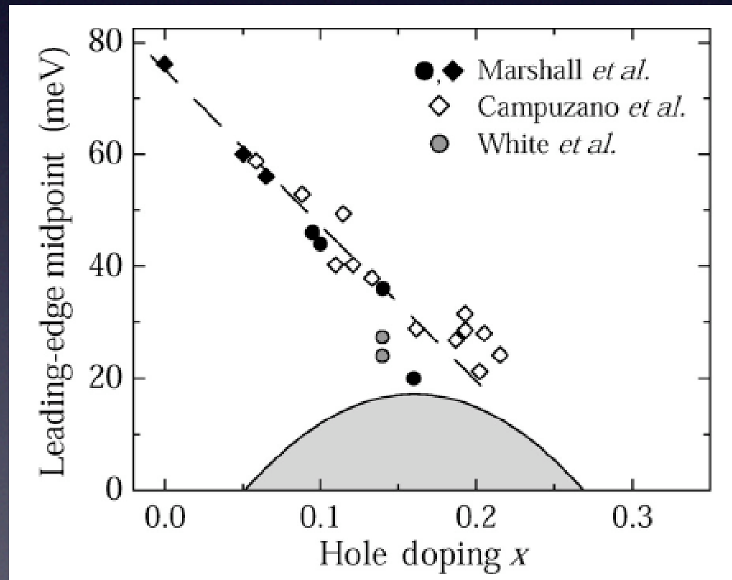


The pi-phase shift in Δ_k implies regions with domain walls in the pairing, with Δ_{ij}=0

The pseudogap phase



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



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