Variational approach to understand high temperature superconductivity

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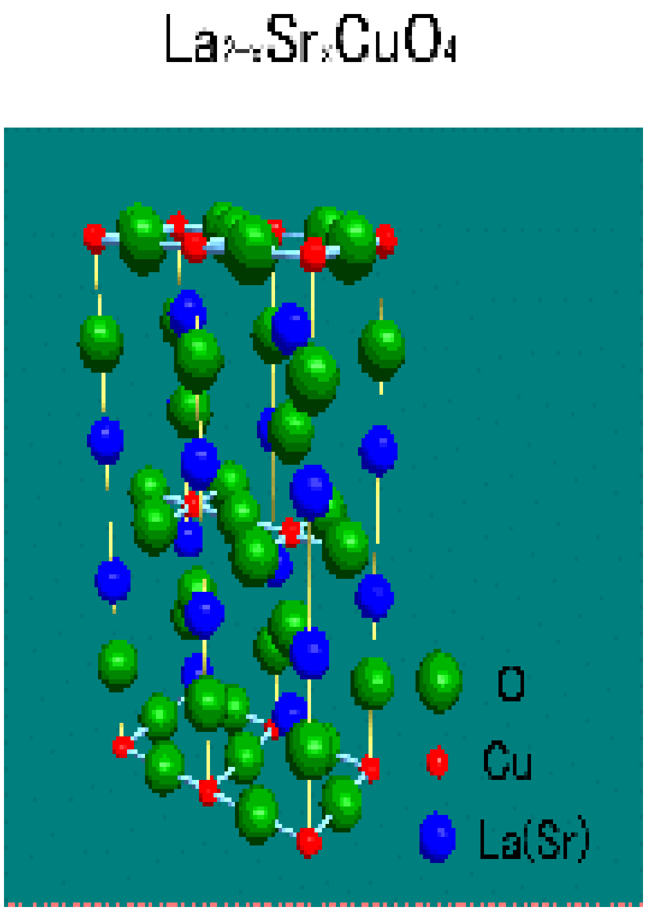
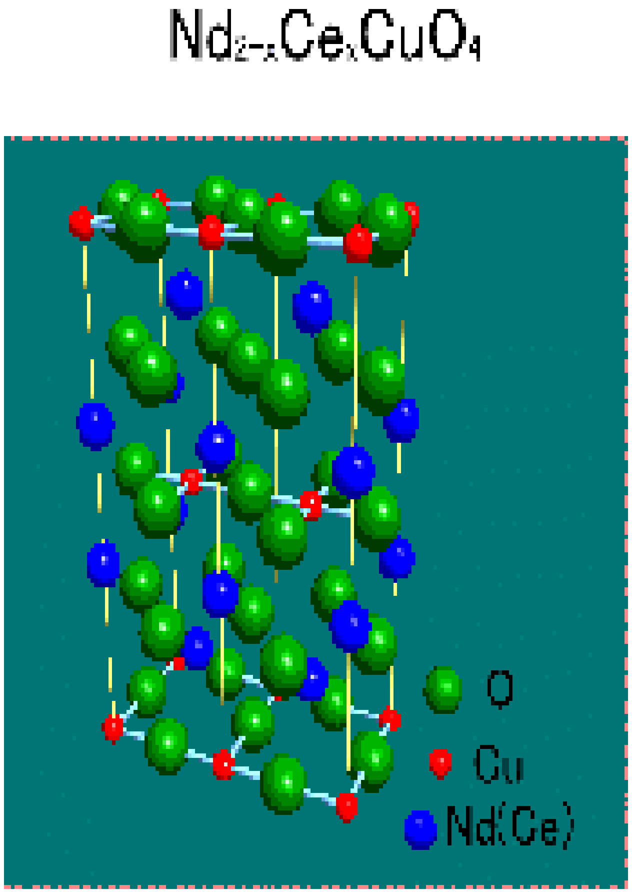
Outline

- Some experimental results of high temperature superconductors
- 2D t-J model – RVB state, consequences
- The extended t-J model
- Recent progress
- conclusions

Hole-doped

Electron-doped

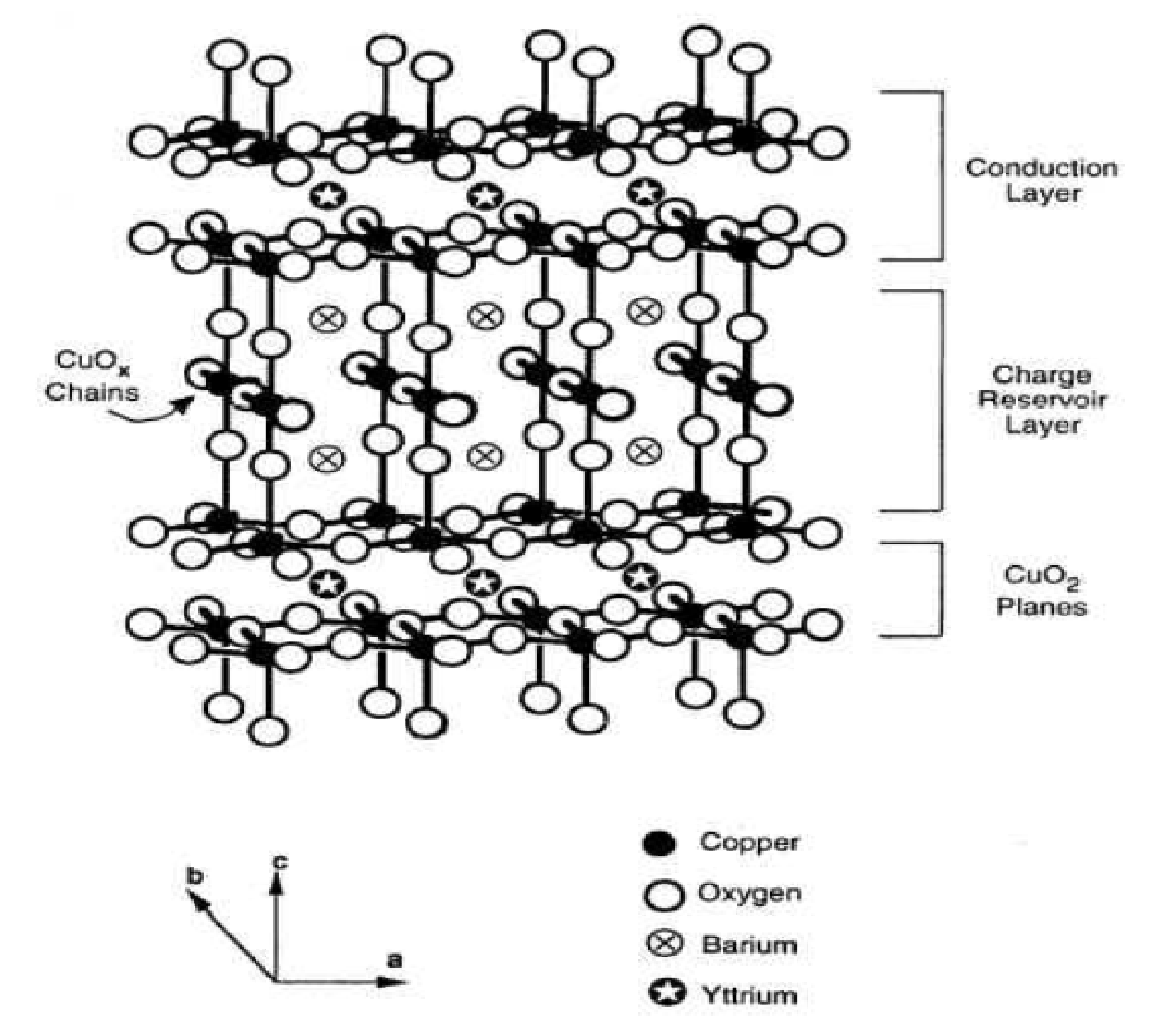




One layer Cu –O plane per unit cell

Cu has no apical O in NCCO

Y $Ba_2 Cu_3 O_{7-x}$



Conduction Layer
Charge Reservoir Layer
CuO_2 Planes
CuO_x Chains
b
c
a
Copper
Oxygen
Barium
Yttrium

Phase diagram

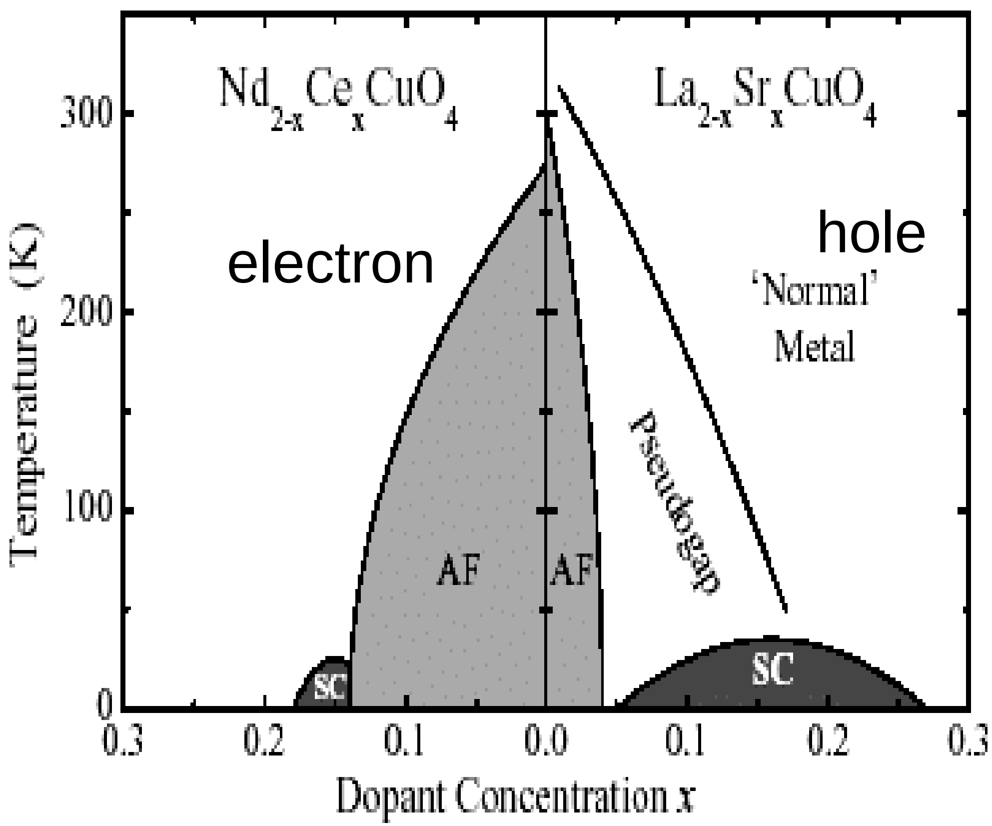


FIG. 1. Phase diagram of n and p-type superconductors.

No particle-hole symmetry! Why?

Coexistence of反鐵磁 AF (antiferromagnetism) and 超導 SC (superconductivity)? --unlikely for p-type

What is Pseudogap?

What is the mechanism of SC?

Damscelli, Shen and Hussain, Review of Modern Phys. 2003

Model proposed by P.W. Anderson in 1987:
t-J model on a two-dimensional square lattice

$$H = -\sum_{i,j\,\sigma} t_{ij}\left(c_{i\sigma}^{+} c_{j\sigma} + H.C.\right) + J\sum_{\langle i,j\rangle}\left(\vec{s}_i \cdot \vec{s}_j - \frac{1}{4} n_i n_j\right)$$

$$\vec{s}_i \rightarrow spin\ ½,$$

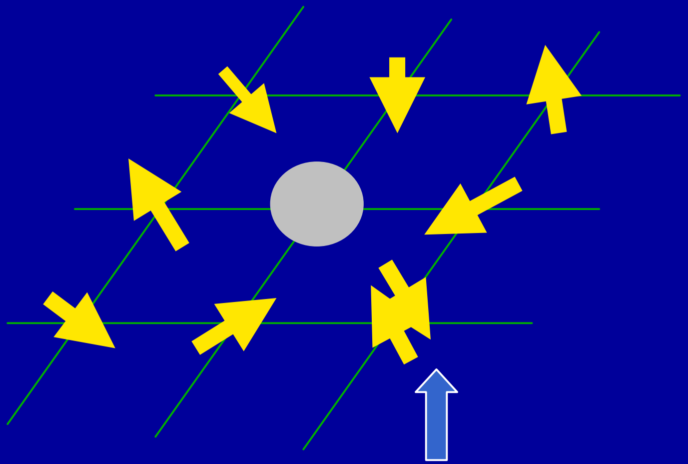
$$n_i = \sum_{\sigma} c_{i\sigma}^{+} c_{i\sigma}$$

t_{ij} = t for nearest neighbor charge hopping

J is for n.n. AF spin-spin interaction

This model is related to the Hubbard model for U/t >>1

$$H = -\sum_{i,j\,\sigma} t_{ij}\left(c_{i\sigma}^{+} c_{j\sigma} + H.C.\right) + U\sum_{i} n_{i\uparrow} n_{i\downarrow}$$



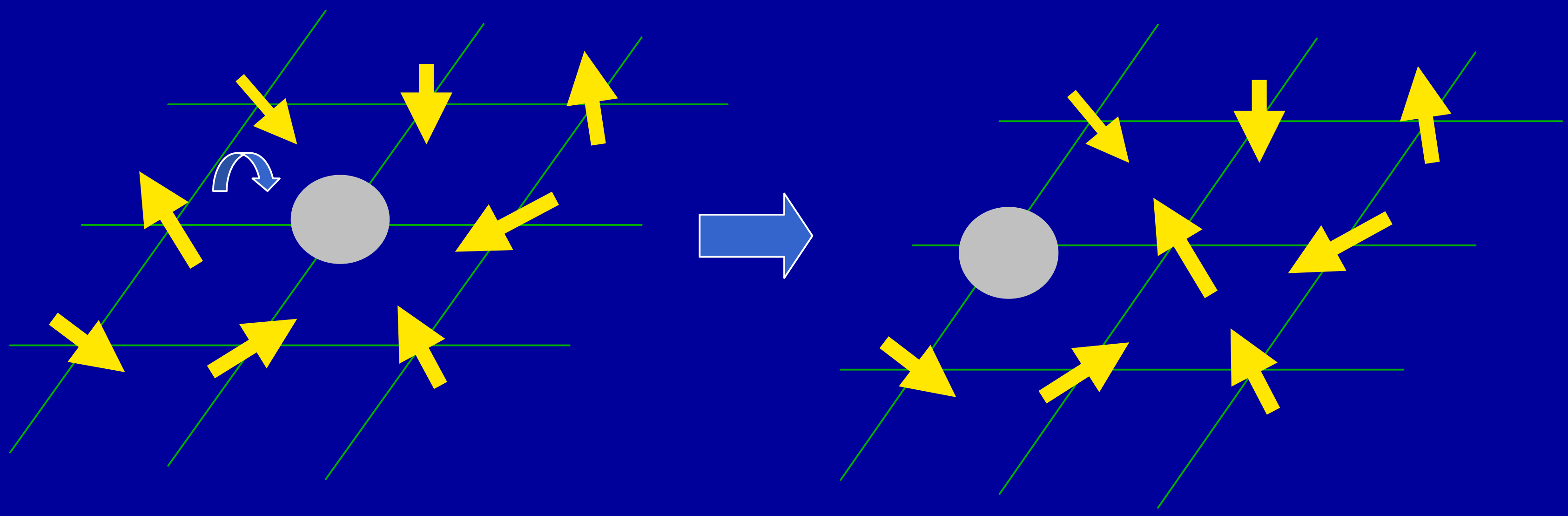
Cost energy U

Constraint:

For hole-doped systems

Two electrons are not allowed on the same lattice site

Three possibilities: an up spin, a down spin or an empty site or "no-fermion hole"



$$H_J = J\sum_{\langle i,j\rangle}\left(\vec{s}_i\cdot\vec{s}_j - \frac{1}{4}n_i n_j\right)$$

$$= -\frac{J}{2}\sum_{\langle i,j\rangle}(C^+_{i,\uparrow}C^+_{j,\downarrow} - C^+_{i,\downarrow}C^+_{j,\uparrow})(C_{i,\downarrow}C_{j,\uparrow} - C_{i,\uparrow}C_{j,\downarrow})$$

$$= -\frac{J}{2}\sum_{\langle i,j\rangle}\Delta^+_{i,j}\Delta_{i,j}$$

This provides the pairing mechanism!

The resonating-valence-bond (RVB) variational wave function proposed by Anderson,

$$\left| RVB \right\rangle = \mathrm{P_d} \left[\prod_k \left(u_k + v_k C^+_{k,\uparrow} C^+_{-k,\downarrow} \right) \right] \left| 0 \right\rangle$$

The constraint operator $\mathrm{P_d}$ enforces no doubly occupied sites for hole-doped systems

$$v_k / u_k = \frac{E_k - \xi_k}{\Delta_k}, \Delta_k = \Delta(\cos k_x - \cos k_y)$$

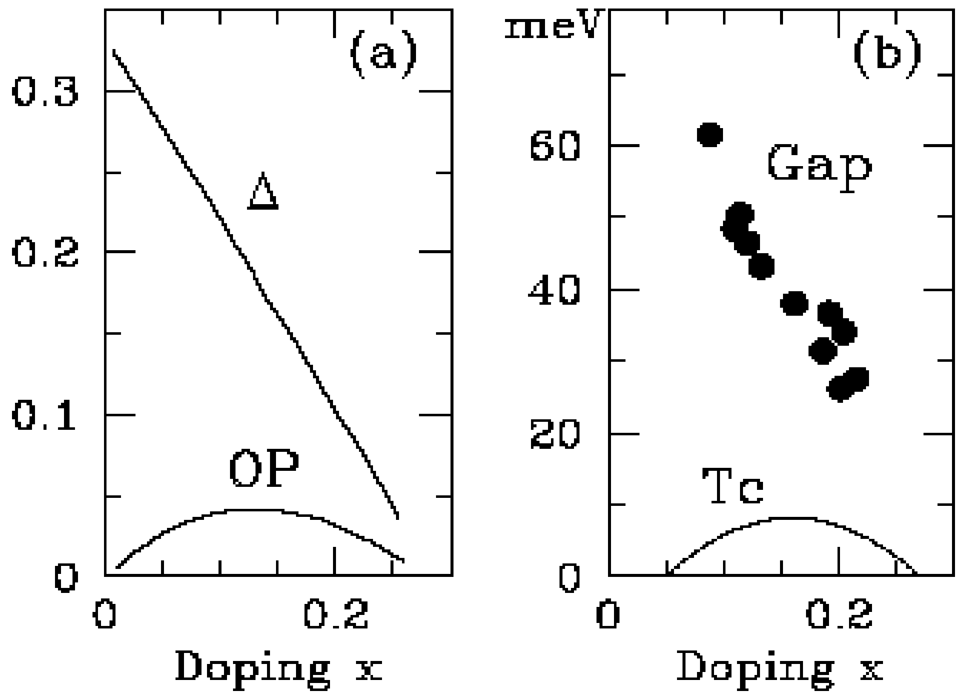
$$\xi_k = -2(\cos k_x + \cos k_y) - \mu, E_k = \sqrt{\xi_k^2 + \Delta_k^2}$$

s-wave pairing was proposed in 1987. It should have been d-wave!

RVB = A projected d-wave BCS state!

Two of the most important predictions of RVB are d-wave SC and the pseudogap

Excitation gap (renormalized mean-field theory)



ARPES
For BSCO

What about antiferromagnetism (AF) at very low doping?

To include AF, besides d-wave RVB pairing

$$\pm\Delta = \left\langle c_{i\uparrow} c_{j\downarrow} - c_{i\downarrow} c_{j\uparrow} \right\rangle \qquad \begin{cases} +, \ if \ \ i - j = \hat{x} \\ -, \ if \ \ i - j = \hat{y} \end{cases}$$

Assume AF order parameters:

staggered magnetization $$m = \left\langle s_A^z \right\rangle = -\left\langle s_B^z \right\rangle$$

And uniform bond order $$\chi = \left\langle \sum_{\sigma} c_{i\sigma}^{+} c_{j\sigma} \right\rangle$$

Two sublattices and two bands – upper and lower spin-density-wave (SDW) bands

RVB + AF for the half-filled ground state

$$\left|\psi_0\right\rangle = P_d \left[\sum_k{}' \left(A_k a^+_{k\uparrow} a^+_{-k\downarrow} + B_k b^+_{k\uparrow} b^+_{-k\downarrow}\right)\right]^{Ne/2} \left|0\right\rangle$$

Ne= # of sites

$$a_{k\sigma} - lower \quad SDW \quad \& \; b_{k\sigma} - upper \quad SDW \quad bands$$

$$A_k = \frac{E_k + \xi_k}{\Delta_k}$$ & $$B_k = -\frac{E_k - \xi_k}{\Delta_k}$$

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

$$E_k = \left(\xi_k^2 + \Delta_k^2\right)^{1/2}$$

$$\xi_k = \left[\left(\tfrac{3}{4} J\chi\right)^2 \left(\cos k_x + \cos k_y\right)^2 + \left(Jm\right)^2\right]^{1/2}$$

Variational results	"best" results	
$\langle \vec{s}_i \cdot \vec{s}_j \rangle = -0.3324(1)$	-0.3344	Liang, Doucot And Anderson
staggered moment m = 0.367	$0.375 \sim 0.3$	

Phase diagram

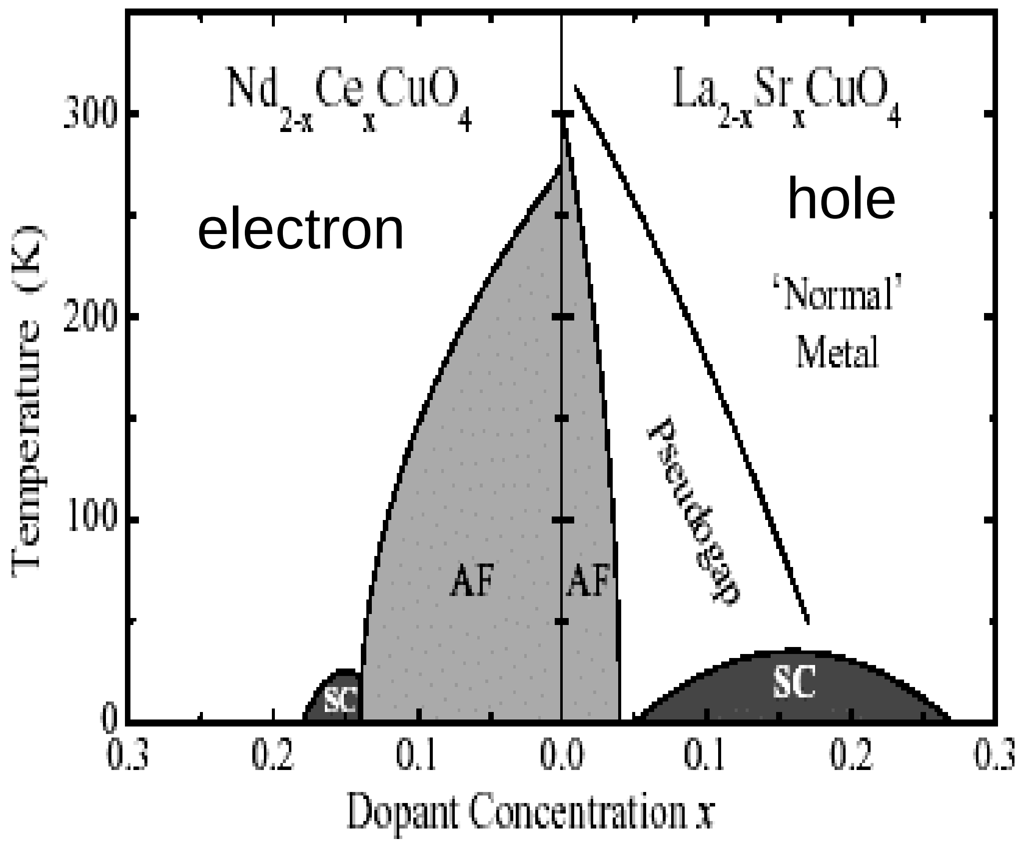


FIG. 1. Phase diagram of n and p-type superconductors.

$$H = -\sum_{i,j\,\sigma} t_{ij}\left(c_{i\sigma}^{+} c_{j\sigma} + H.C.\right) + J\sum_{\langle i,j\rangle}\left(\vec{s}_i \cdot \vec{s}_j - \frac{1}{4} n_i n_j\right)$$

T-J model has particle -hole symmetry, but not for real HTS! Why?

Damscelli, Shen and Hussain, Review of Modern Phys. 2003

After doping, t-J model is not enough.
It has the particle-hole symmetry, unlike HTS(高溫超導體)!

Consider t-t'-t"-J model or the extended t-J model

$$H = -\sum_{i,j\,\sigma} t_{ij}\left(c_{i\sigma}^{+} c_{j\sigma} + H.C.\right) + J\sum_{\langle i,j\rangle}\left(\vec{s}_i \cdot \vec{s}_j - \frac{1}{4} n_i n_j\right)$$

t for n.n., t' for 2nd n.n., and t" for 3rd n.n.

t' and t" breaks the equivalence between doping electrons and doping holes!

From hole-doped to electron-doped, just change
$t'/t \rightarrow -t'/t$ and $t''/t \rightarrow -t''/t$
Different Hamiltonians!

Two possibilities for wave functions of hole-doped systems:

1. Including chemical potential in RVB+AF (for 4 holes)

$$|\psi\rangle = \mathrm{P_d}\left[\sum_q{}' \left(A'_q a^+_{q\uparrow} a^+_{-q\downarrow} + B'_q b^+_{q\uparrow} b^+_{-q\downarrow}\right)\right]^{Ne/2-2} |0\rangle$$

Chemical potential μ is inlcuded in A_k' and B_k' --- large fermi surface

$$A_k = \frac{E_k + \xi_k}{\Delta_k} \qquad B_k = -\frac{E_k - \xi_k}{\Delta_k}$$

2. Holes created from the Mott insulator vacuum as charge excitations

Lee and Shih, PRB55, 5983(1997); Lee, Ho, Nagaosa, PRL 90 (2003); Lee et al. PRL 91 (2003).

$$|\psi_{4h}\rangle = \mathrm{P_d}\left[\sum_{q\neq k_1,k_2}{}' \left(A_q a^+_{q\uparrow} a^+_{-q\downarrow} + B_q b^+_{q\uparrow} b^+_{-q\downarrow}\right)\right]^{Ne/2-2} |0\rangle$$

No chemical potential, A_k and B_k same as half-filling ---small fermi surface

Create charge excitations in the Mott Insulator “vacuum”.

$$|\psi_0\rangle = P_d \left[\sum_k{}' \left(A_k a^+_{k\uparrow} a^+_{-k\downarrow} + B_k b^+_{k\uparrow} b^+_{-k\downarrow} \right) \right]^{Ne/2} |0\rangle$$

The state with one hole

$$|\psi_{1h}(k, S_z = 1/2)\rangle \propto c_{-k\downarrow} |\psi_0\rangle$$

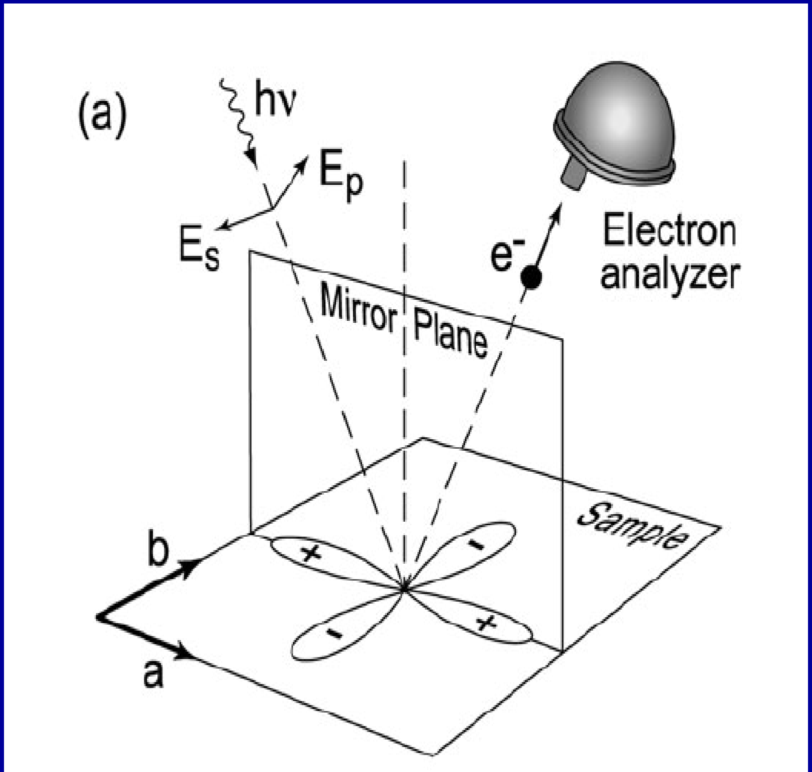
$$= \mathrm{P_d}\; c^+_{k\uparrow} \left[\sum_{q \neq k}{}' \left(A_q a^+_{q\uparrow} a^+_{-q\downarrow} + B_q b^+_{q\uparrow} b^+_{-q\downarrow} \right) \right]^{Ne/2 - 1} |0\rangle$$

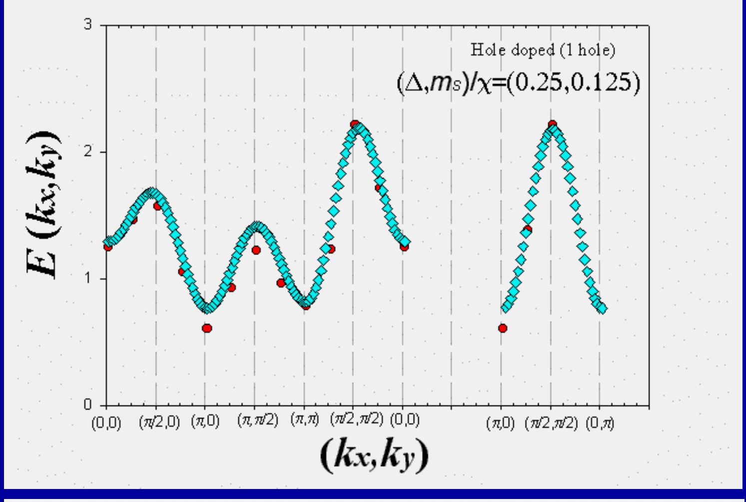
A down spin with momentum –k (& – k + (π, π)) is removed from the half-filled ground state. --- This is different from all previous wave functions studied.

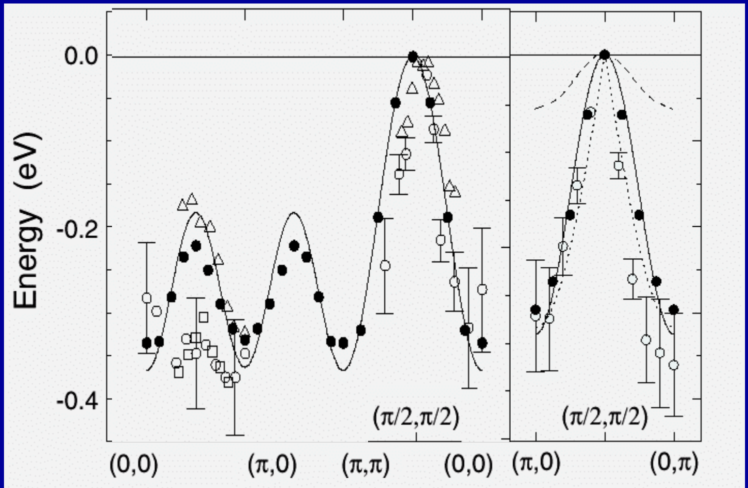
J/t=0.3

Dispersion for a single hole. t'/t= - 0.3, t"/t= 0.2

Angle-resolved photoemission spectroscopy (ARPES)



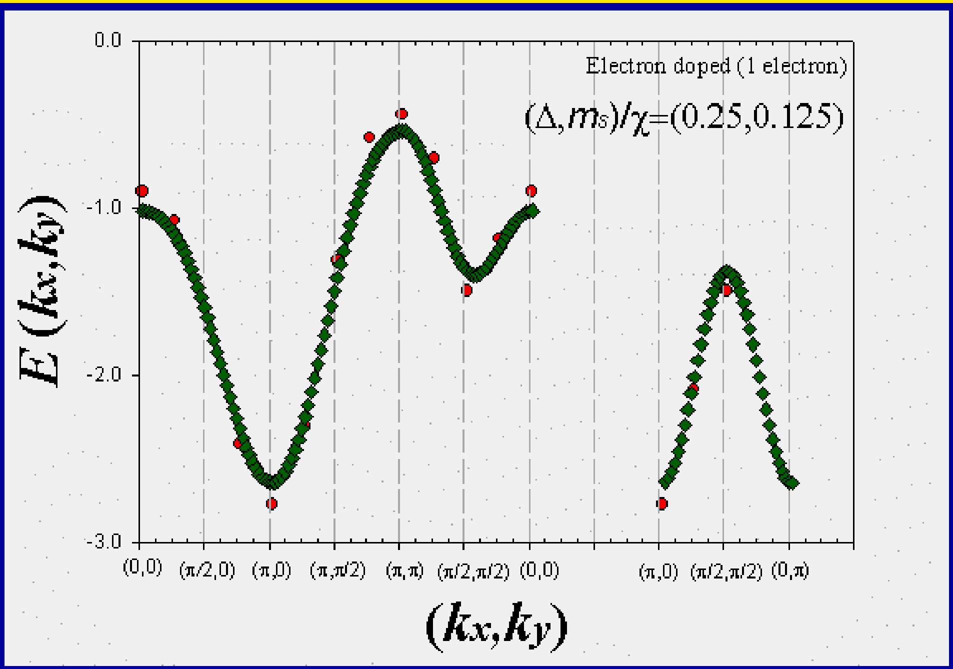




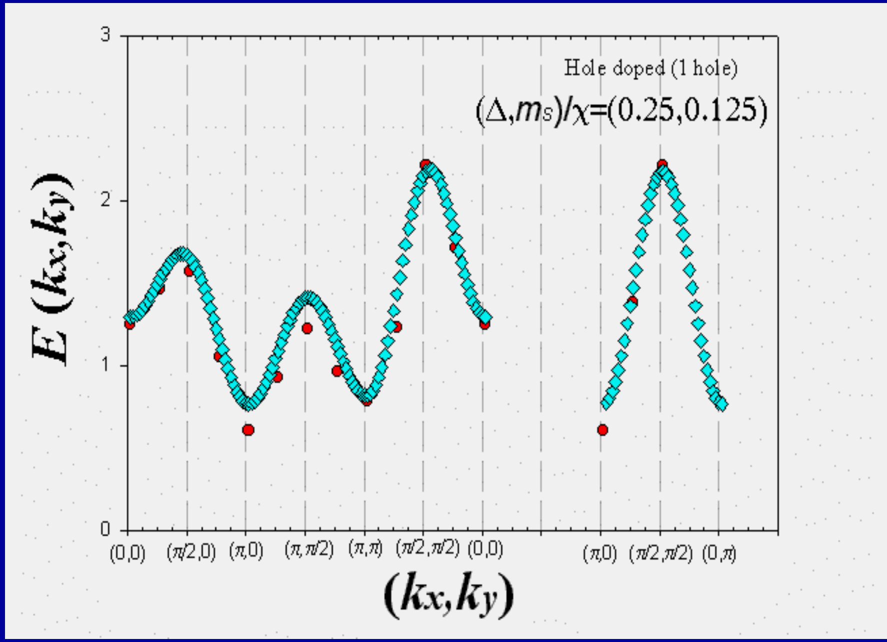
□ Kim et. al. , PRL80, 4245 (1998); ○ Wells et. al.. PRL74, 964(1995); Δ LaRosa et. al. PRB56, R525(1997).
● SCBA for t-t'-t''-J model

J/t=0.3

Energy dispersion after one electron is doped. The minimum is at (π, 0). t'/t= 0.3, t"/t= - 0.2



Dispersion for a single hole. t'/t= - 0.3, t"/t= 0.2



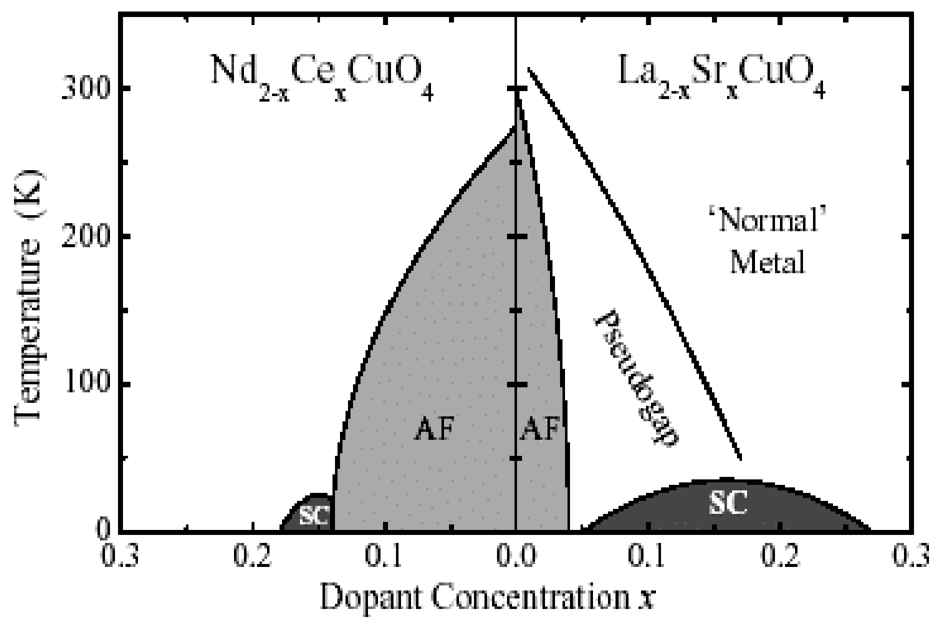
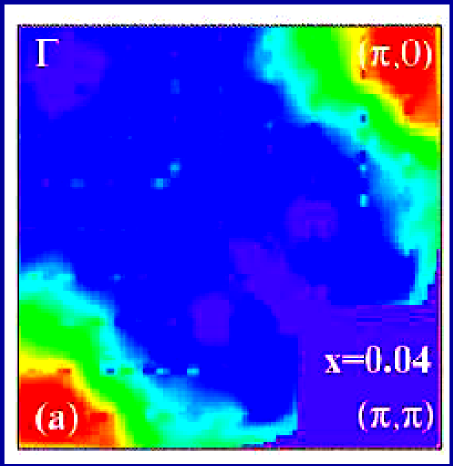


FIG. 1. Phase diagram of n and p-type superconductors.

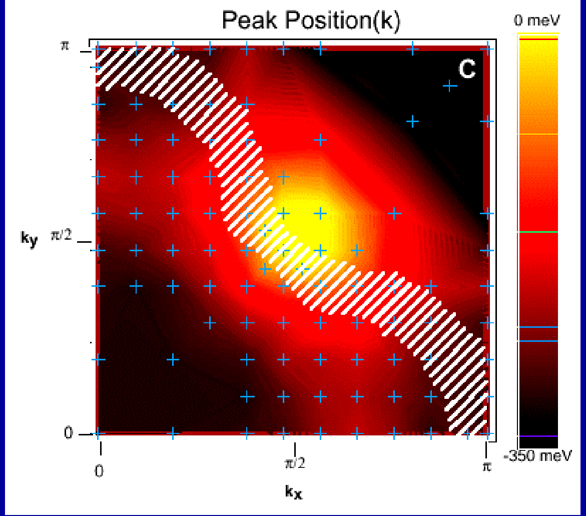
Same wave function for hole- and electron-doped materials.

$Nd_{2-x}Ce_x CuO_4$ -- with 4% extra electrons



Fermi surface around (π ,0) and (0, π)!

ARPES for $Ca_2CuO_2Cl_2$



The lowest energy is at

$k = (\pi/2, \pi/2)$

Armitage *et al*., PRL (2002)

Ronning, Kim and Shen, PRB67 (2003)

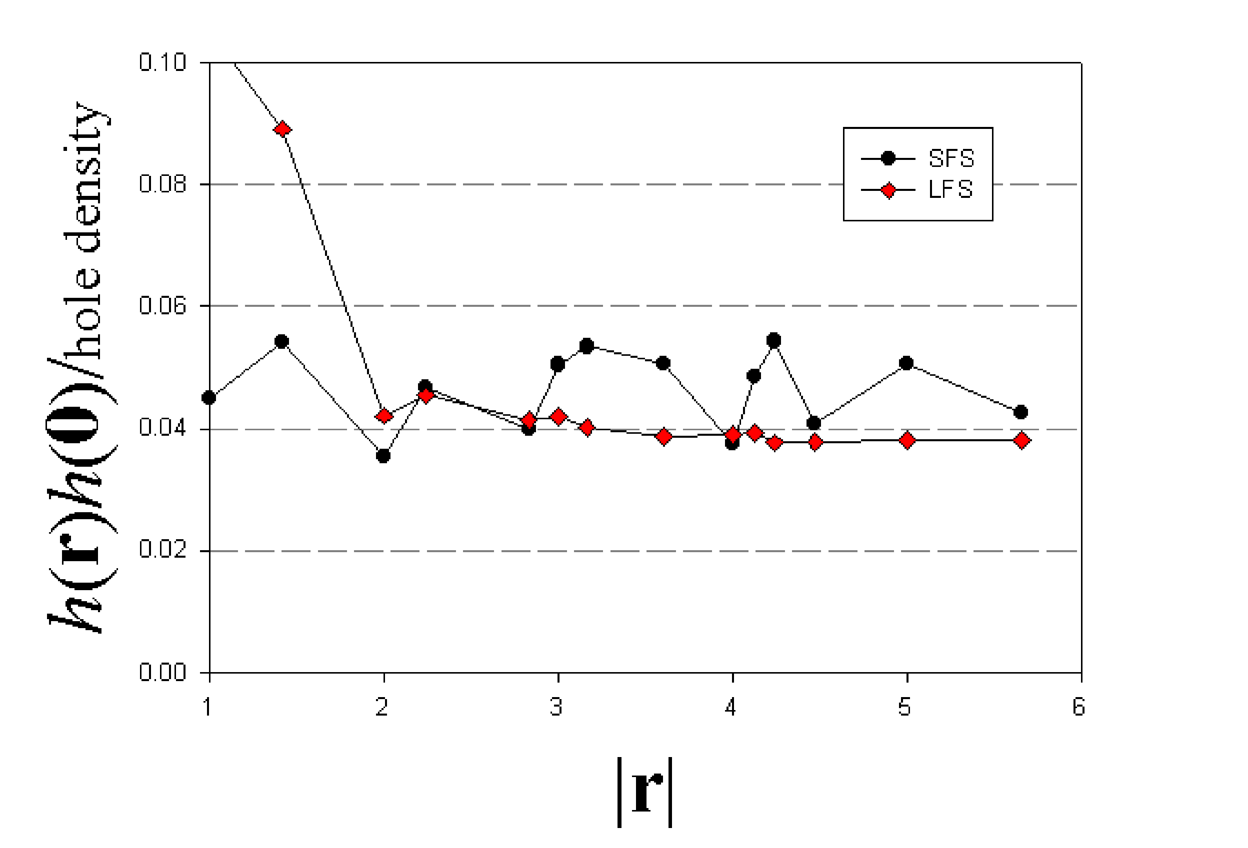
$$\left|\psi_{4h}\right\rangle = \mathrm{P_d}\left[\sum_{q\neq k_1,k_2}{}^{/}\left(A_q a^+_{q\uparrow}a^+_{-q\downarrow} + B_q b^+_{q\uparrow}b^+_{-q\downarrow}\right)\right]^{Ne/2-2}\left|0\right\rangle$$

---small fermi surface

$$\left|\psi\right\rangle = \mathrm{P_d}\left[\sum_{q}{}^{/}\left(A'_q a^+_{q\uparrow}a^+_{-q\downarrow} + B'_q b^+_{q\uparrow}b^+_{-q\downarrow}\right)\right]^{Ne/2-2}\left|0\right\rangle$$

Chemical potential μ is inlcuded in A_k' and B_k'

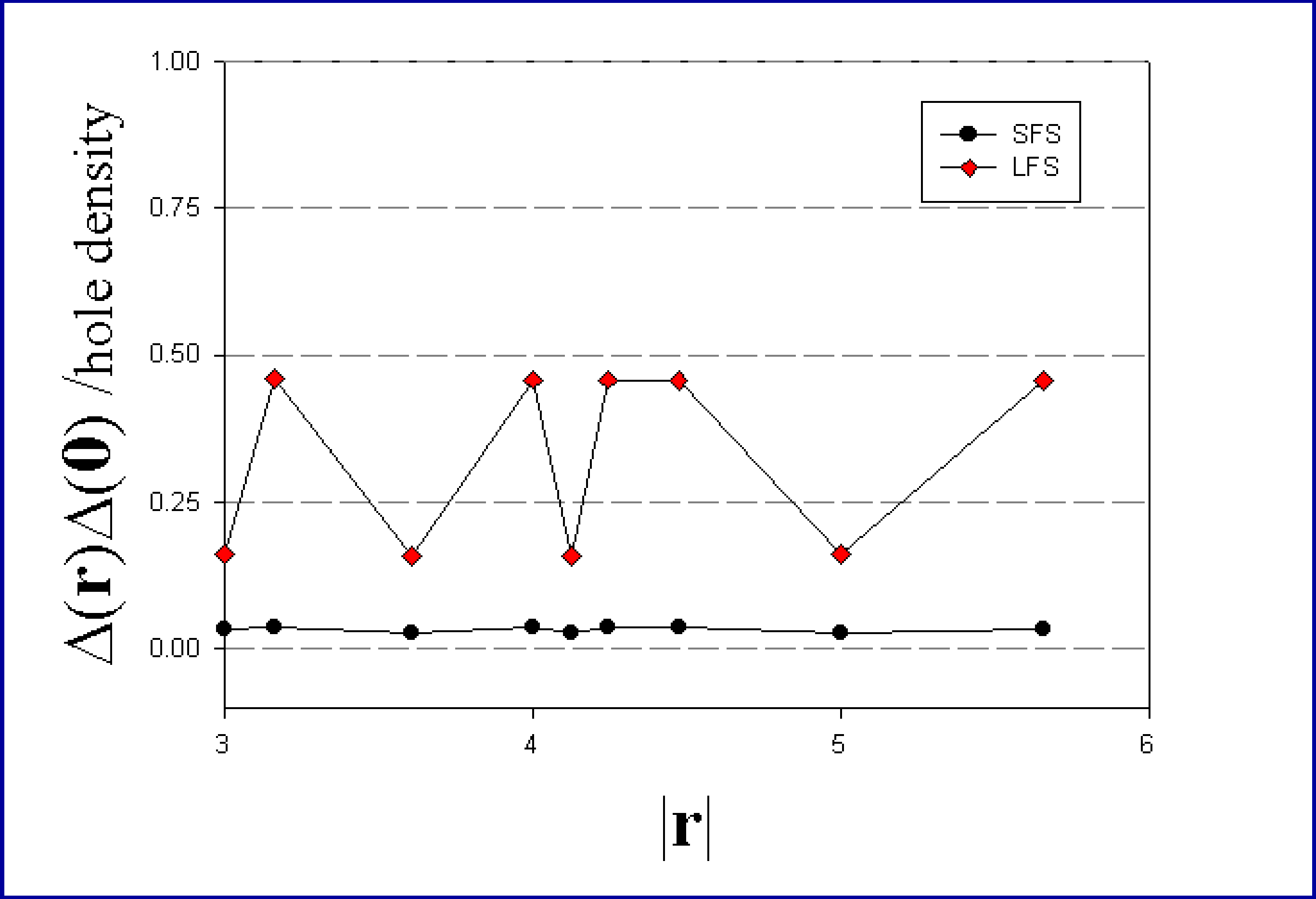
--- large fermi surface



4 holes in 64 sites

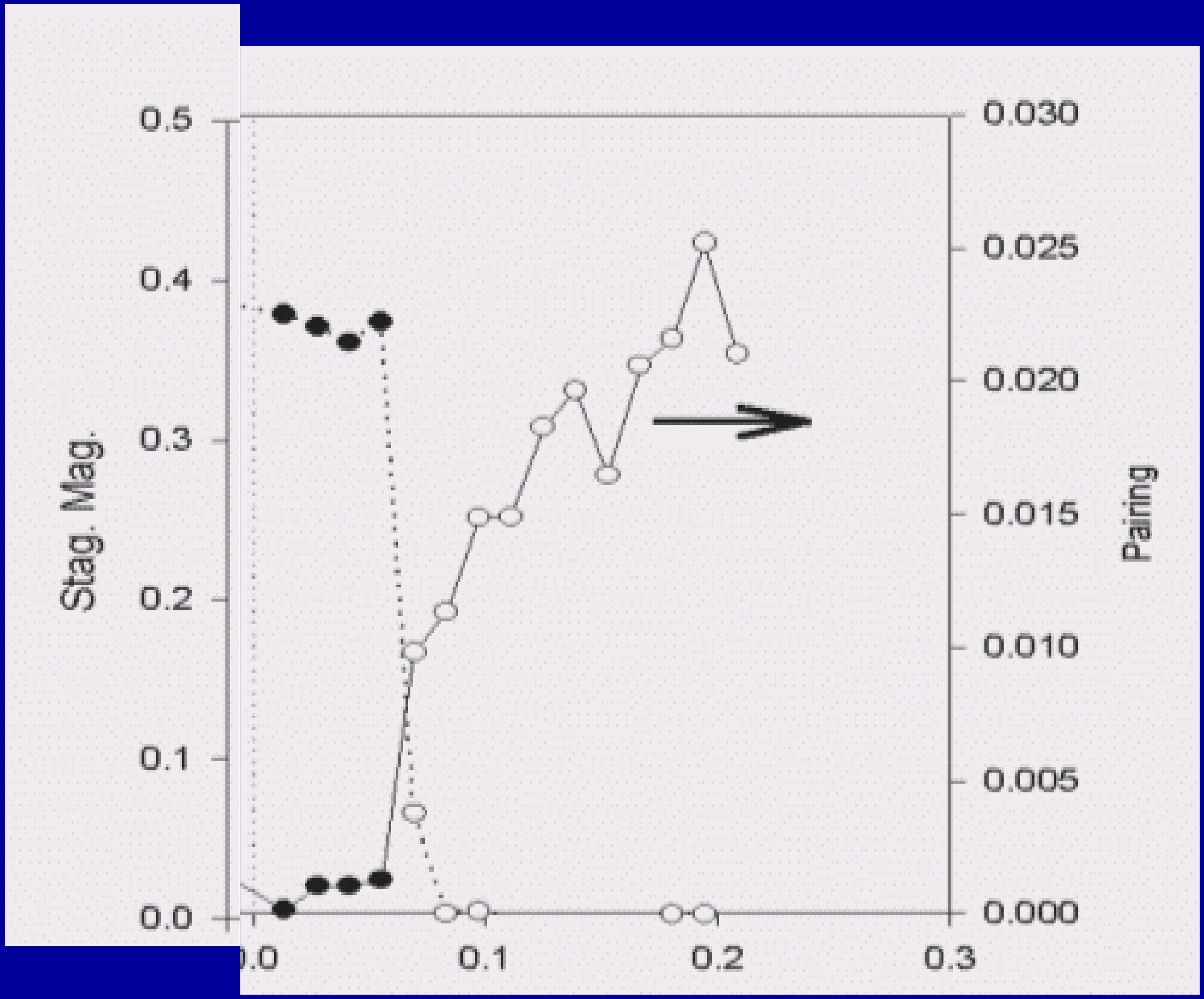
d-wave pairing correlation function

$$P_{s \text{ or } d}(R) = \frac{1}{N_s} \sum_i \langle \Delta_i^\dagger \Delta_{i+R} \rangle \qquad \Delta_i = c_{i\uparrow}(c_{i+\hat{x}\downarrow} + c_{i-\hat{x}\downarrow} \pm c_{i+\hat{y}\downarrow} \pm c_{i-\hat{y}\downarrow})$$



Our (SFS) new wave function has AF but negligible pairing.

AF (without SC) below 7% hole density



Hole density

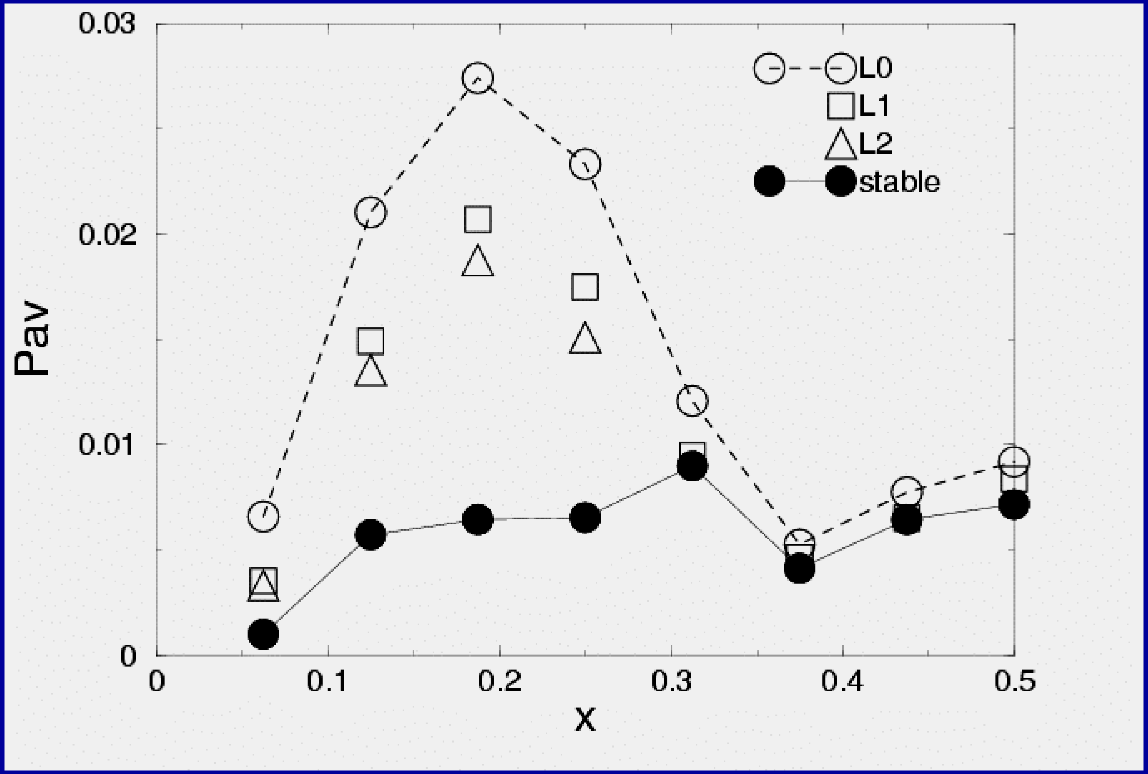
Controversies about pairing

Is t-J sufficient to explain high Tc?

No! --- Shih,Chen, Lin and Lee, PRL 81, 1294 (1997)

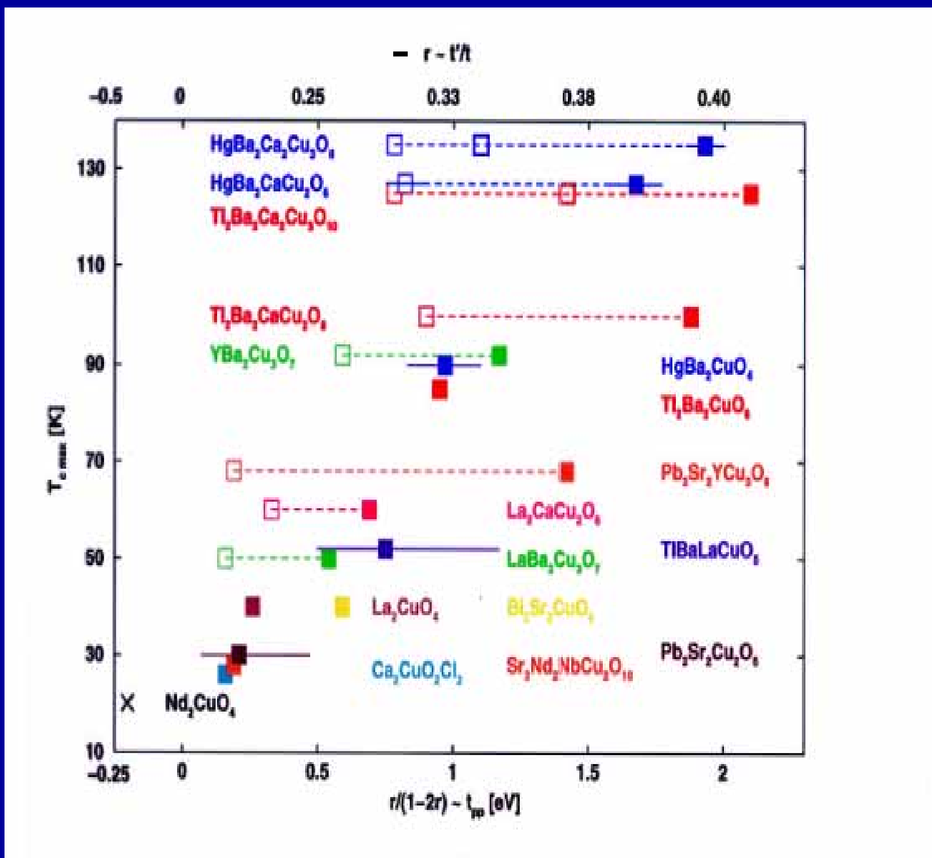
64 sites, J=0.4, PL0=VMC of d-RVB

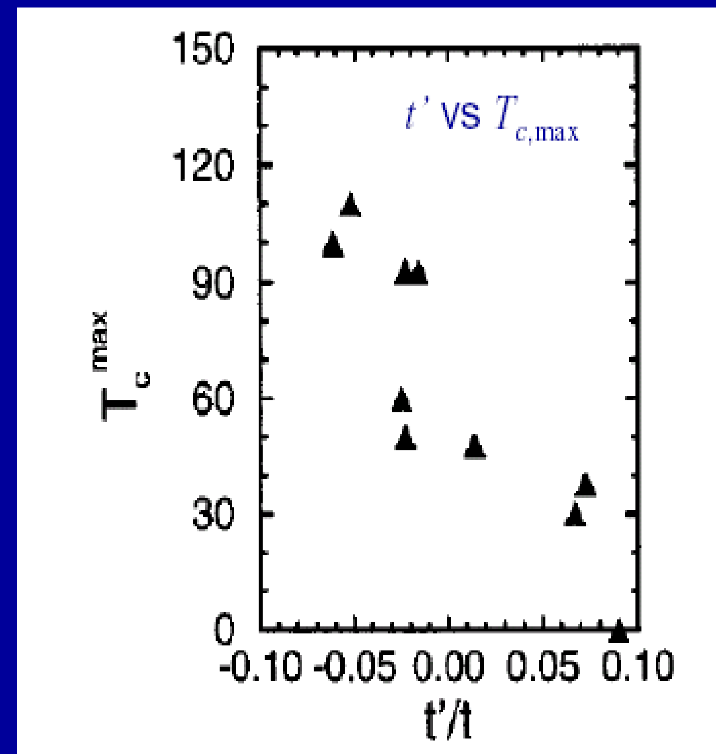
PL1-1st order Lanczos, PL2-2nd order



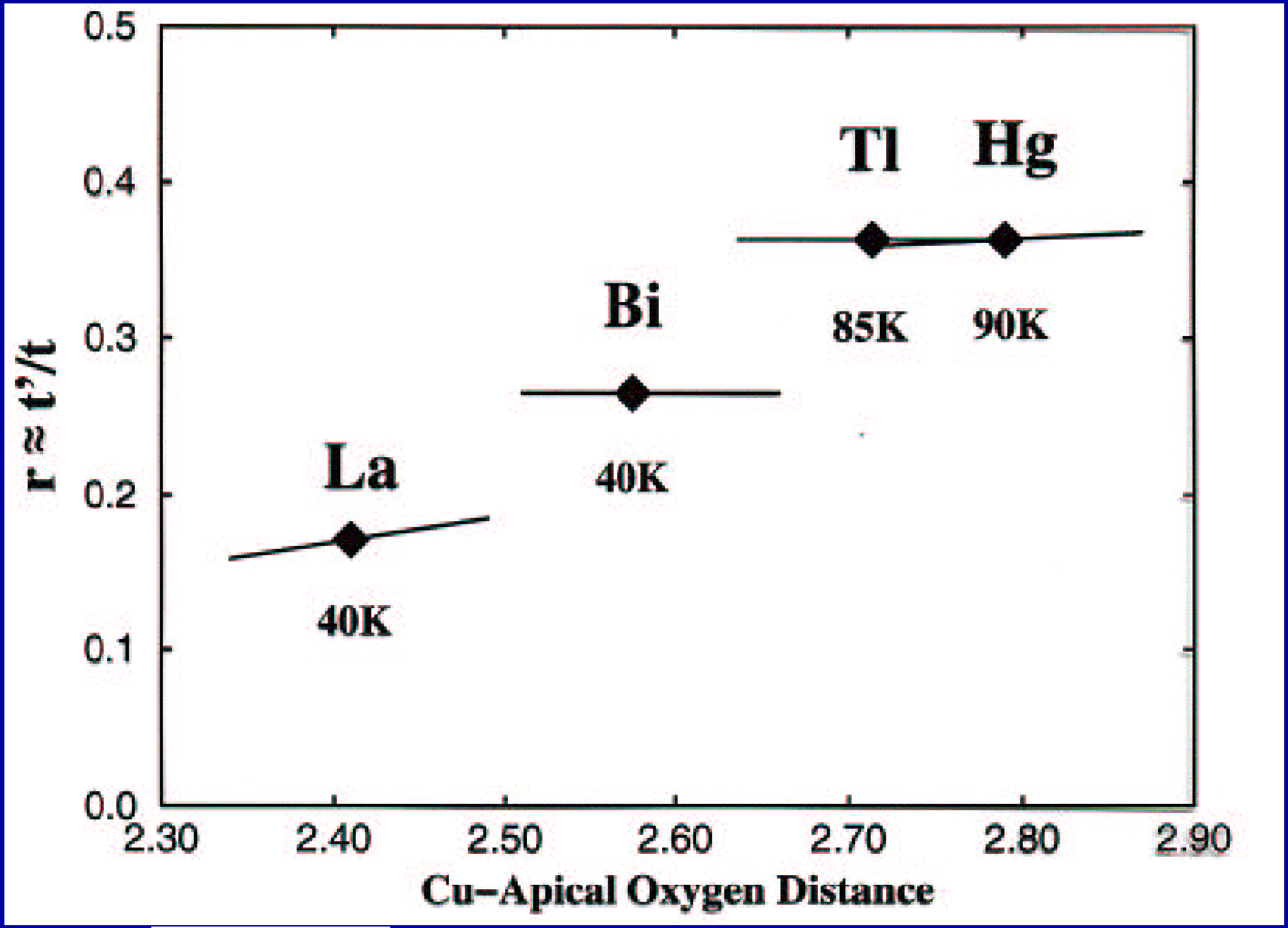
E. Pavarini, O.K. Andersen and co-workers, PRL 87, 047003 (2001)

R. Raimondi, *et al*., PRB53, 8774 (1996)





Tc,max correlates strongly with the value of t'/t (t''/t'=-0.5)

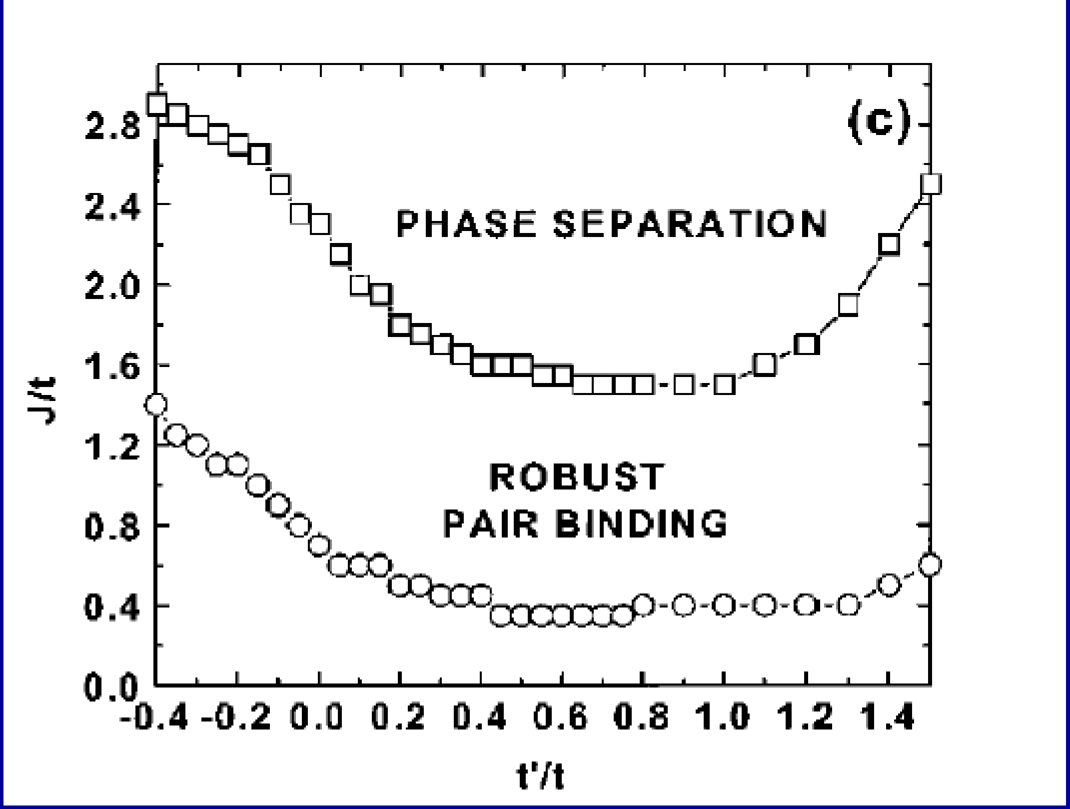


t'' ~ -t'/2

Why t' enhances Tc?

Steven R. White and D.J. Scalapino, PRB 60, R753 (1999),
Martins, Xavier, Arrachea and Dagotto, PRB 64, 180513 (2001).
Shih, Chen and Lee, Physica C341-348, 113(2000).

-- t'/t <0 (for hole-doped cases) suppresses pairing.



2 holes on a 2x8 ladder

A completely opposite conclusion from Andersen's results and experiments!

Re-do the VMC calculation for the extended t-J model, RVB-t' state

$$\left|RVB\right\rangle_{t'} = \mathrm{P_d}\left[\prod_k (u_k + v_k C^+_{k,\uparrow} C^+_{-k,\downarrow})\right]\left|0\right\rangle$$

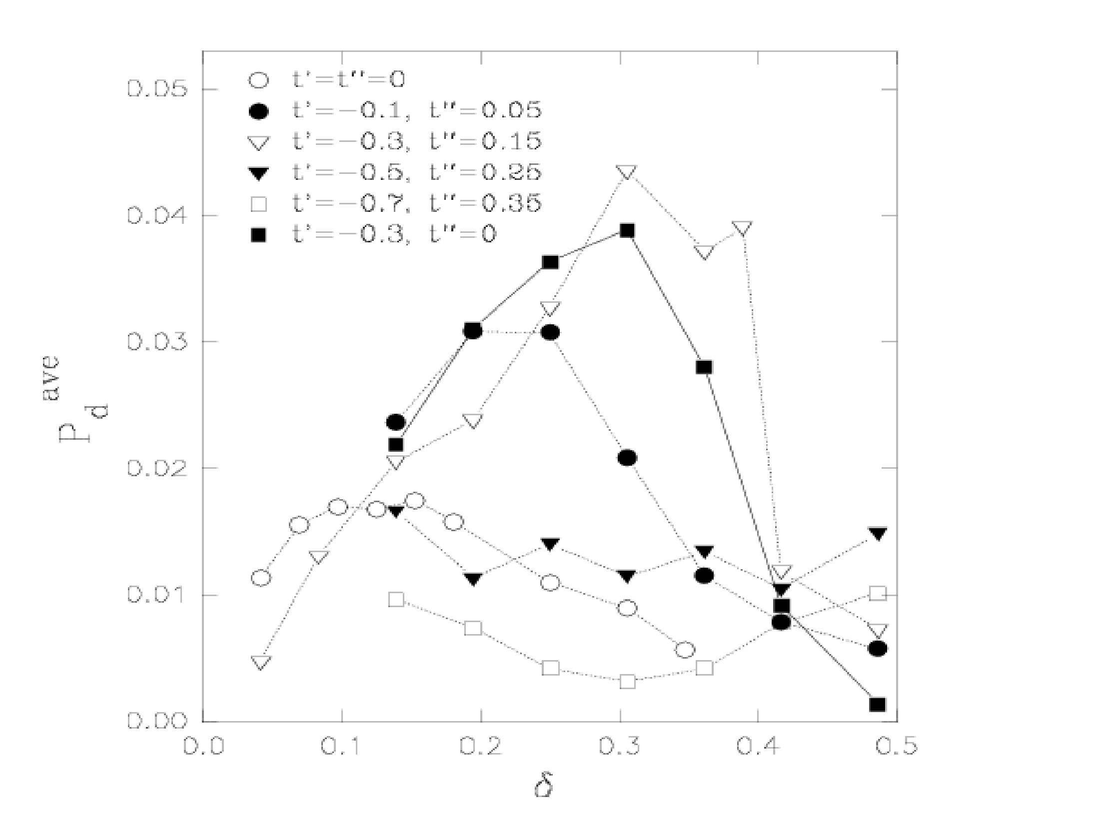
$$v_k / u_k = \frac{E_k - \varepsilon_k}{\Delta_k}, \Delta_k = \Delta(\cos k_x - \cos k_y)$$

$$\varepsilon_k = -2(\cos k_x + \cos k_y) - 4t'_v \cos k_x \cos k_y - 2t''_v (\cos 2k_x + \cos 2k_y) - \mu,$$

$$E_k = \sqrt{\varepsilon_k^2 + \Delta_k^2}$$

four variational parameters, t_v’ t_v’’ Δ, and μ

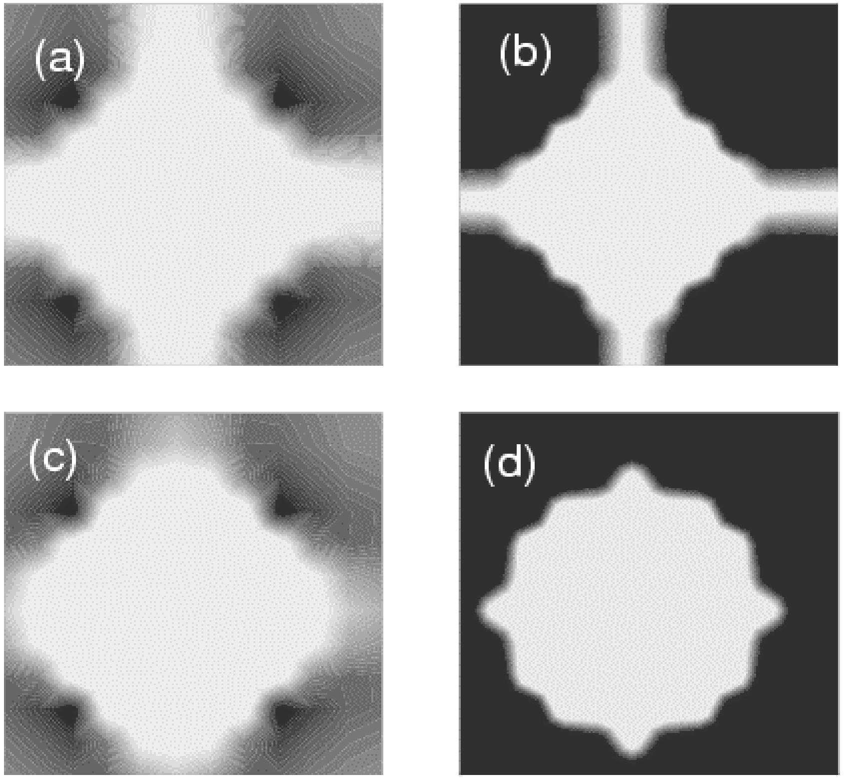
Long range d-wave pairing correlation
t''= - t'/2, 144 sites, J=0.3, t=1



At underdoping, t' suppresses pairing slightly, in agreement with White and Scalapino, Martins et al. But for higher doping, t' enhances pairing strongly.

Fermi surface topology is important for pairing in the overdoped region.

n(k)



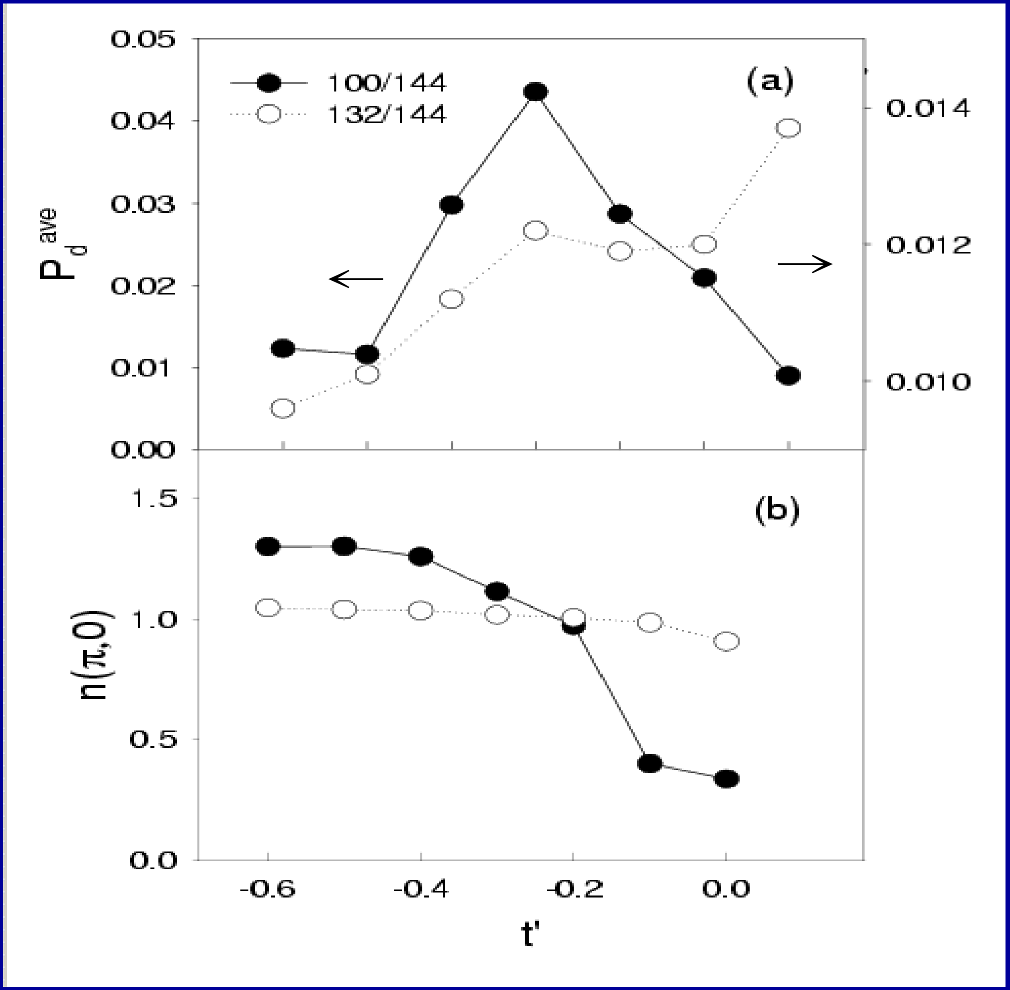
132/144, δ =0.08, t'=-0.3

100/144, δ =0.31, t'=-0.3

δ =0.08, t'=0

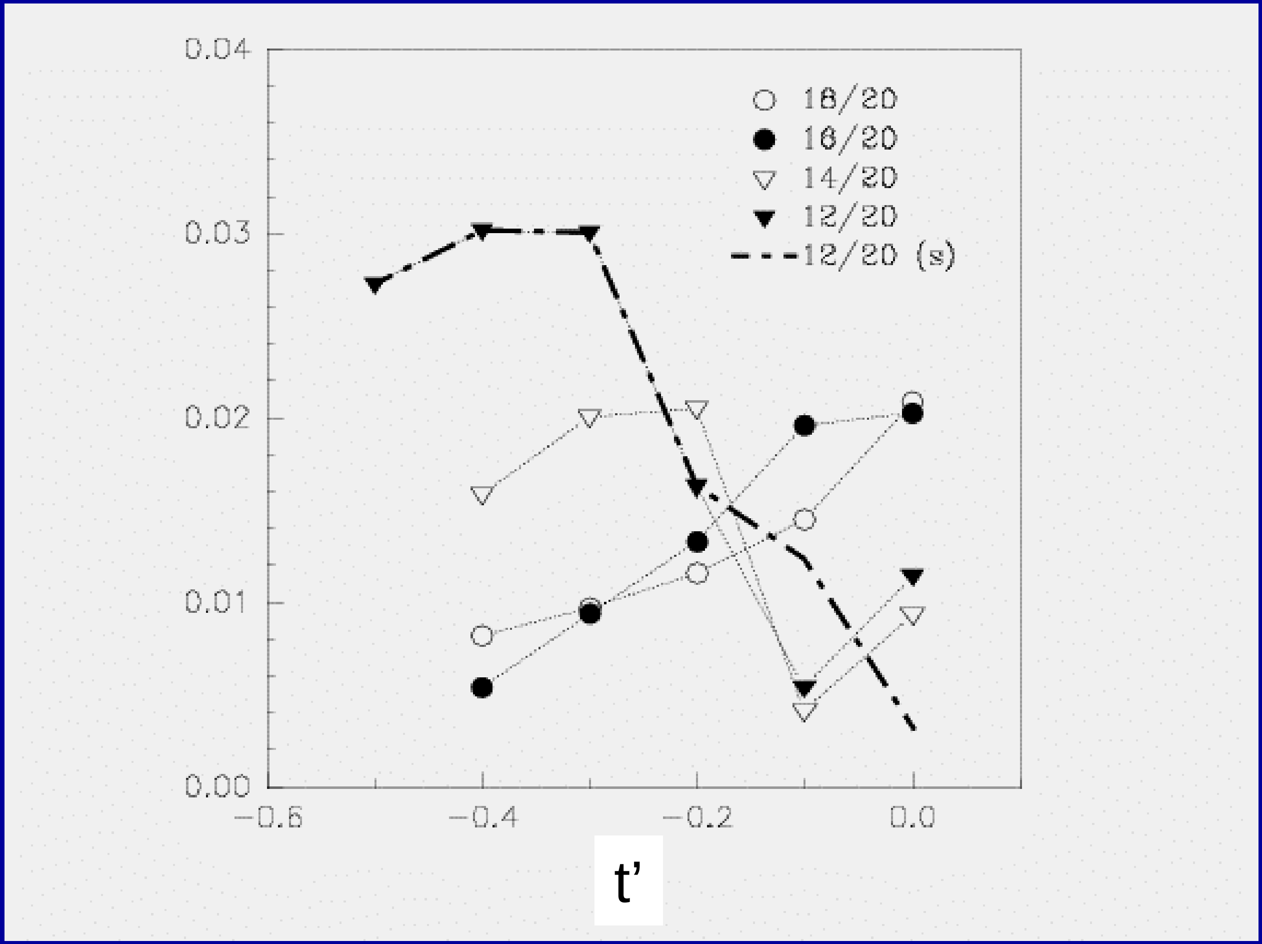
δ =0.31, t'=0

In addition to the effect of van Hove singularity, d-wave order parameter, Δ_k , is largest near (π, 0) or (0,π) . Hence occupation of electrons in these regions contributes significantly to pairing.



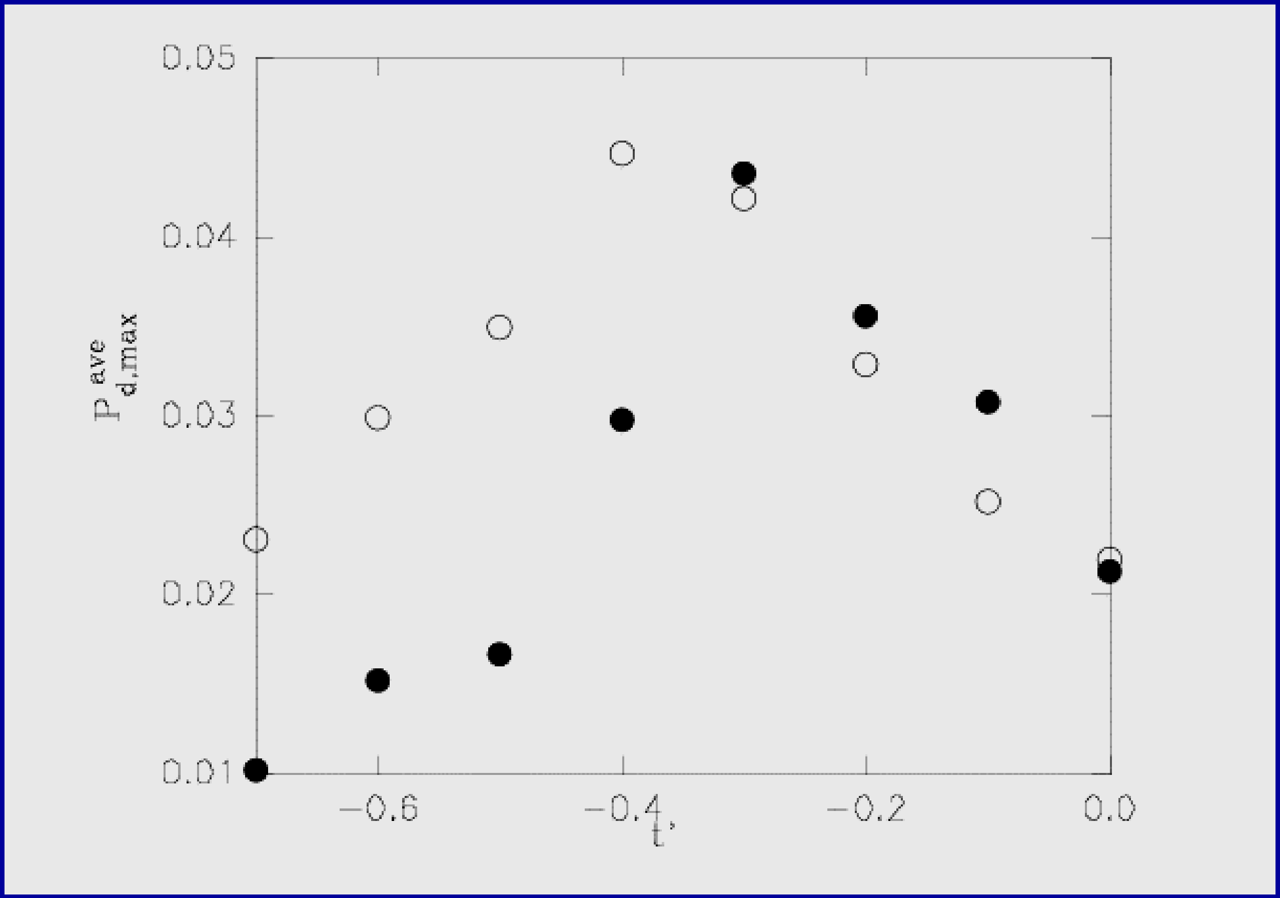
d-wave order parameter, Δ_k , is largest near (π, 0) or (0,π) . Hence occupation of electrons in these regions contribute significantly to pairing.

Exact Pd (R=(1,3)) results for 20 sites for t''=-t'/2



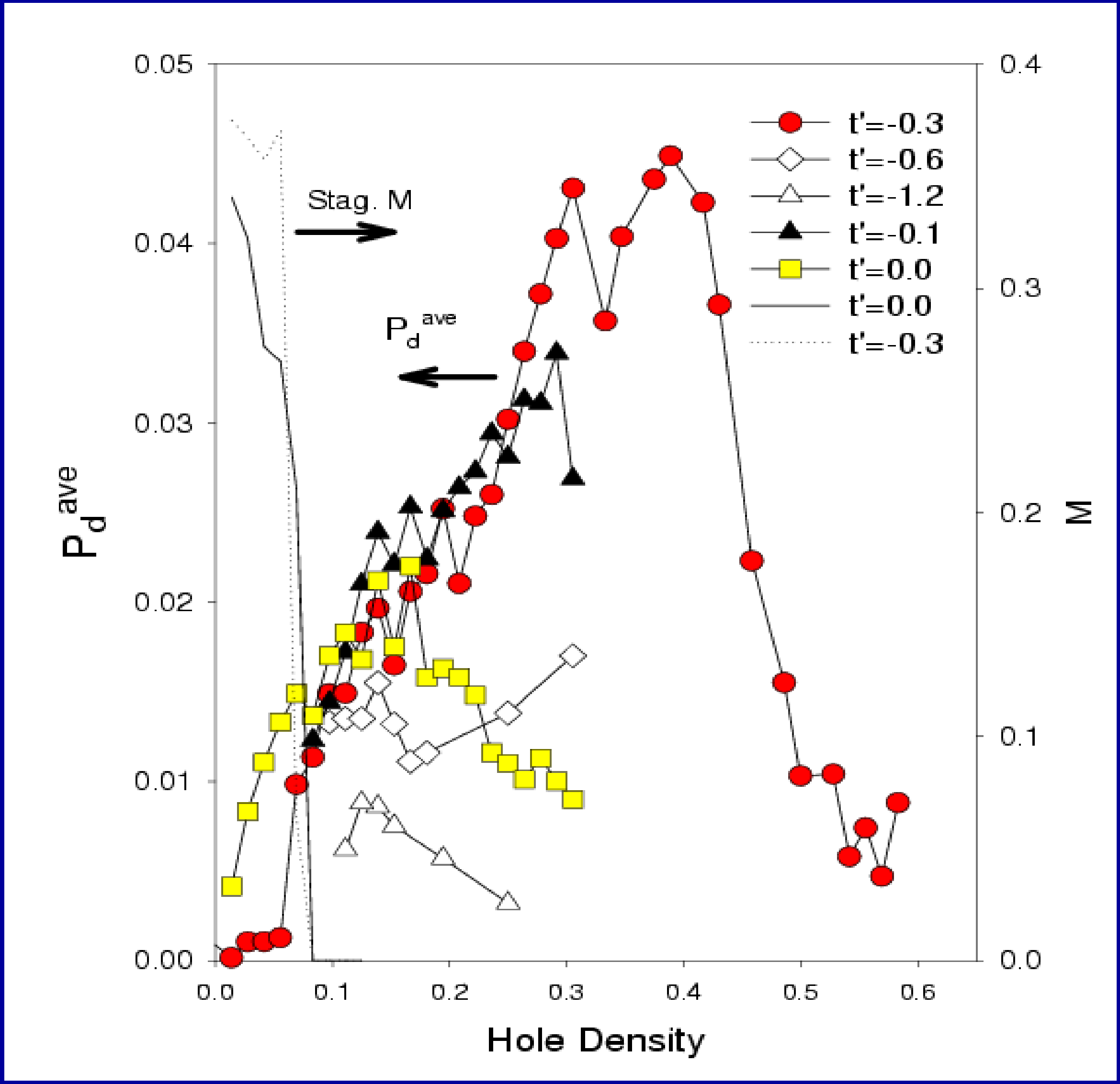
Phys. Rev. Lett. 92, 227002 (2004)

The maximum value of long-range d-wave pairing correlation scales with - t'/t , agrees with Andersen et al.



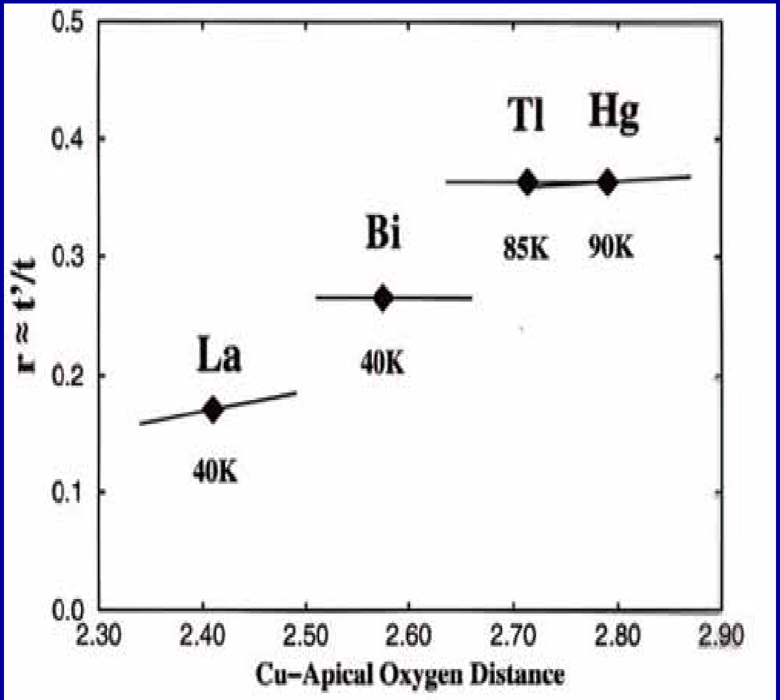
Bad news: it seems for –t'/t larger than 0.3~0.4, Tc will not get higher.

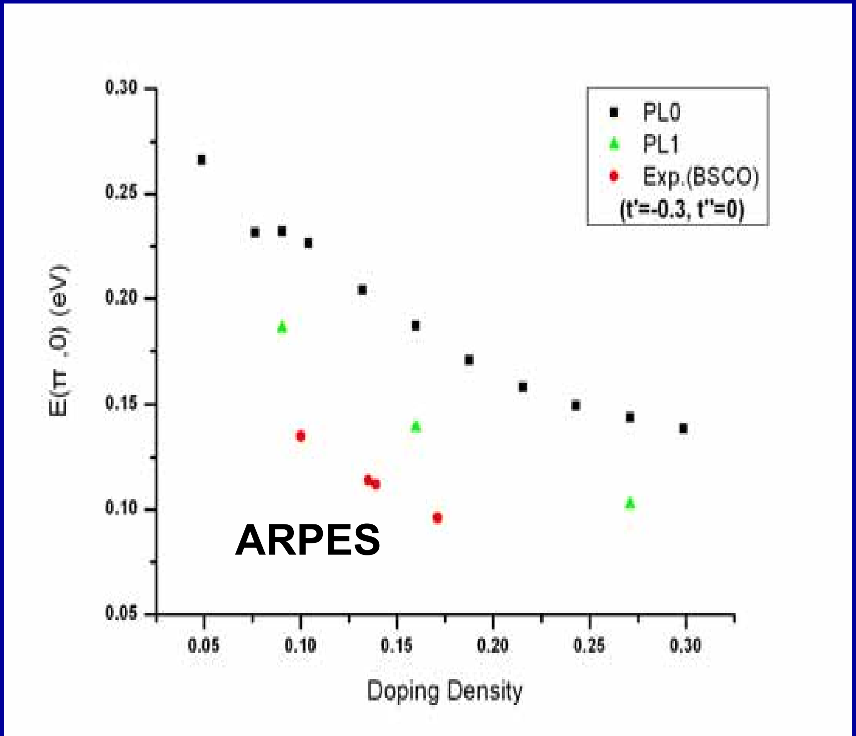
Phase diagram predicted by extended t-J model



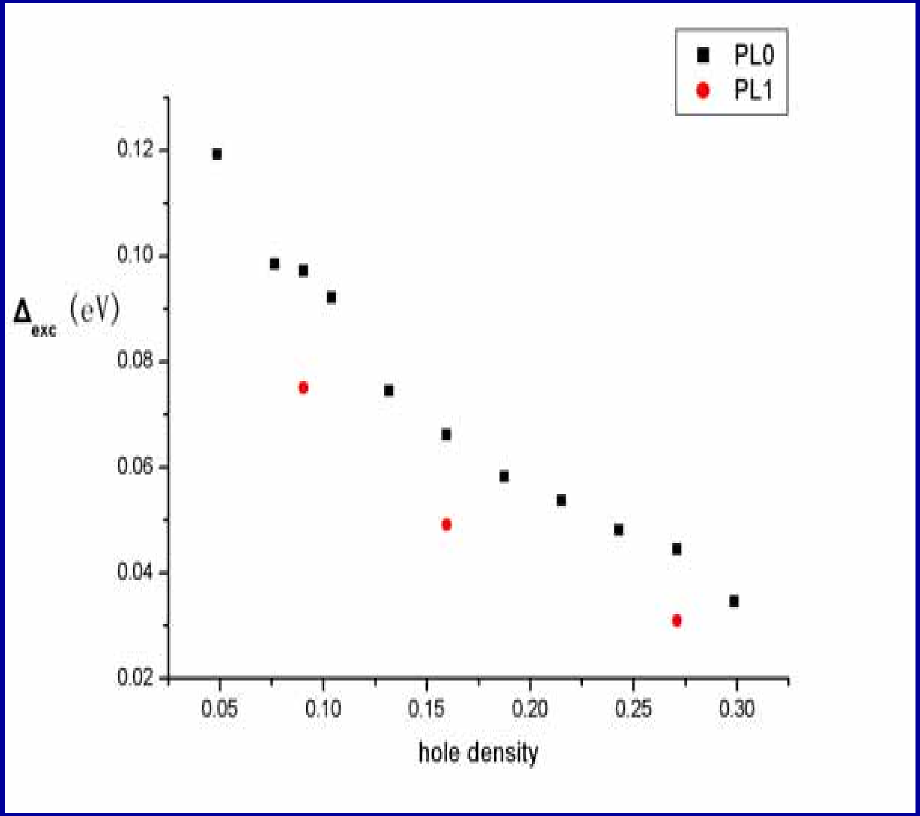
- Low energy excitations in the SC phase

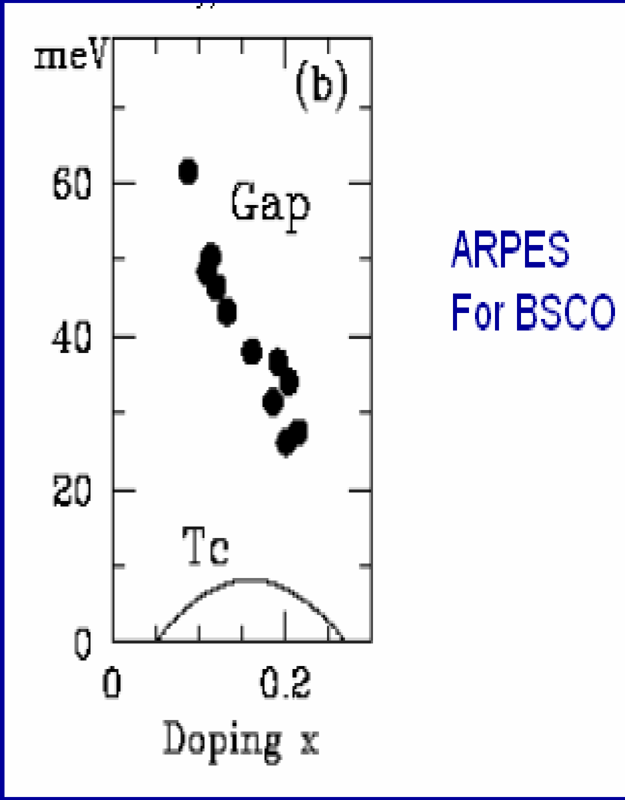
t'/t=-0.3, t''/t=0.2





Excitation gap calc. by t-t'-t''-J model,
J/t=0.3, t'/t=-0.3, t''/t=0.2, t=0.3 eV





ARPES
For BSCO

Summary

- **AF phase diagram of HTS is explained.**
- **No coexistence of AF and SC for t'/t=-0.3.**
- **A first order transition between AF and SC.**
- **Enhancement of Tc,max by t' is explained.**
- **d-SC and pseudogap are obtained by RVB.**
- **Semi-quantitative agreement with experiments for several physical quantities.**
- **Questions remained:**

➢ **k-dependence of pseudogap, it's relation with SC?**

➢ **stripes?**

➢ **SC symmetry for electron-doped?**

➢ **quantum critical point?**

Collaborators:

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Naoto Nagaosa, University of Tokyo, Japan

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Chung-Pin Chou and Shinn-Ming Huang, NTHU

Thank you for your attention!