Extended t-J model – the variational approach

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Outline

- Background and motivation

- Variational Monte Carlo method
  -- basic approach
  -- improve trial wave functions
    -- increase variational parameters
    -- power Lanczos method

- Hole- (and electron-) doped cases, antiferromagnetic (AFM) and superconducting states.
  -- ground state
  -- excitations – ARPES and STM..

- Summary

Phase diagram

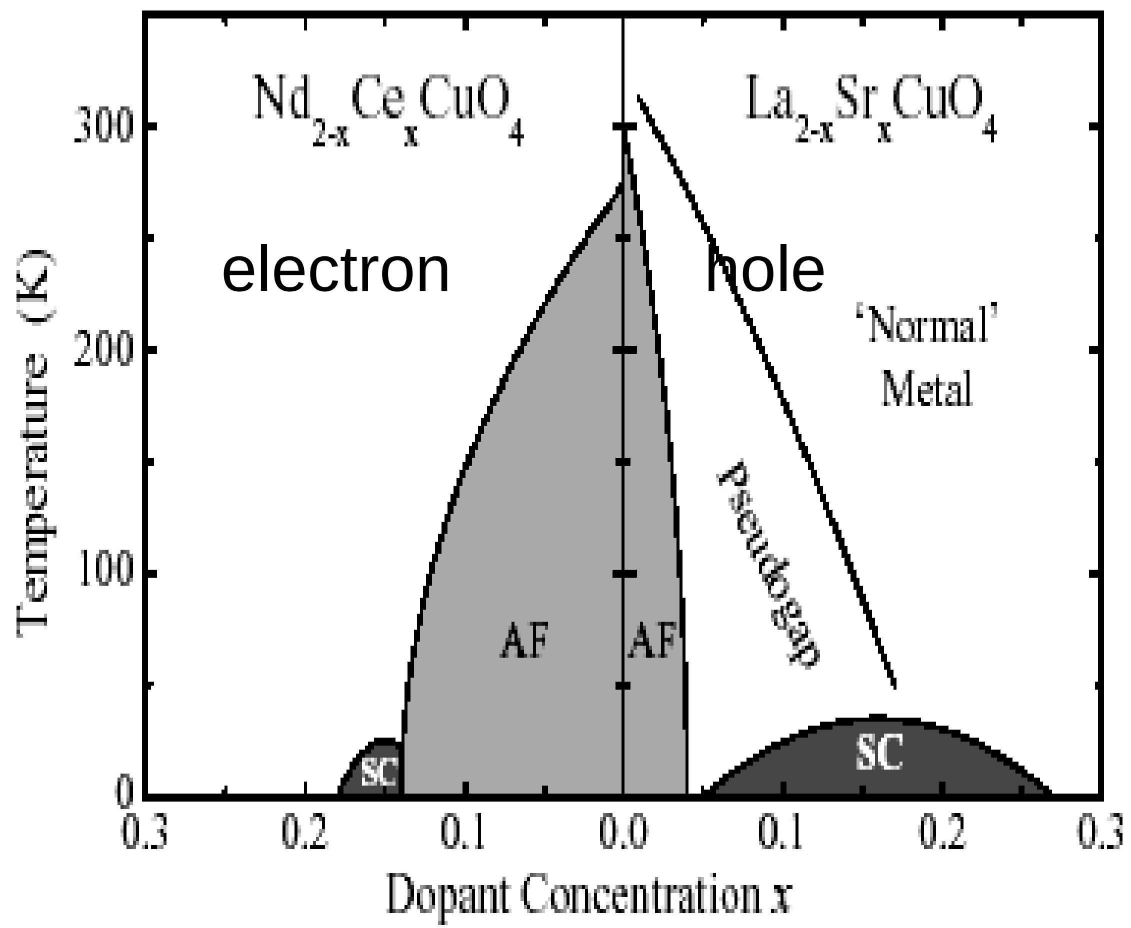
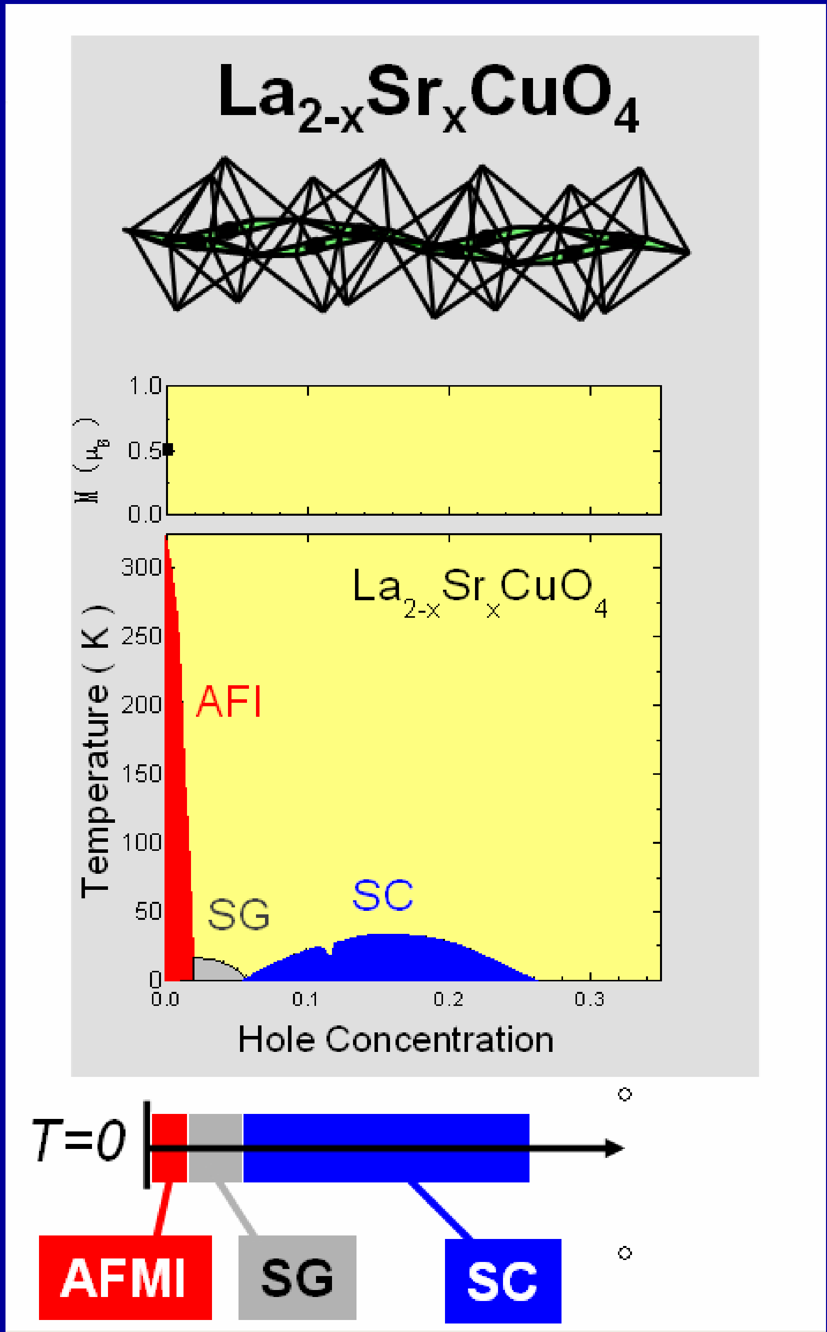


FIG. 1. Phase diagram of n and p-type superconductors.

Damscelli, Hussain, and Shen, Rev. Mod. Phys. 2003



Only AFM insulator (AFMI)?
How about metal (AFMM),
if no disorder?

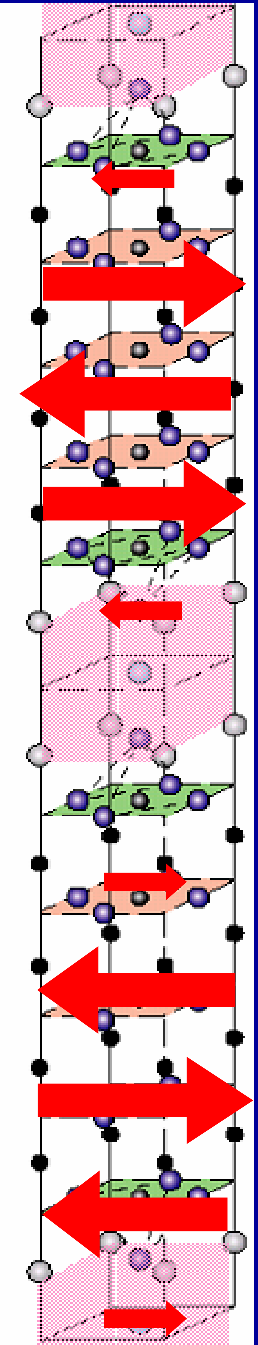
Coexistence of
AF and SC?

Related to the
mechanism of SC?

UD Hg-1245

Phase diagram for multi-layer systems

(T_c=72K, T_N~290K)



SC(72K)+AFM(0.1 μ_B)

AFM (0.67 μ_B)

AFM (0.69 μ_B)

AFM (0.67 μ_B)

SC(72K)+AFM(0.1 μ_B)

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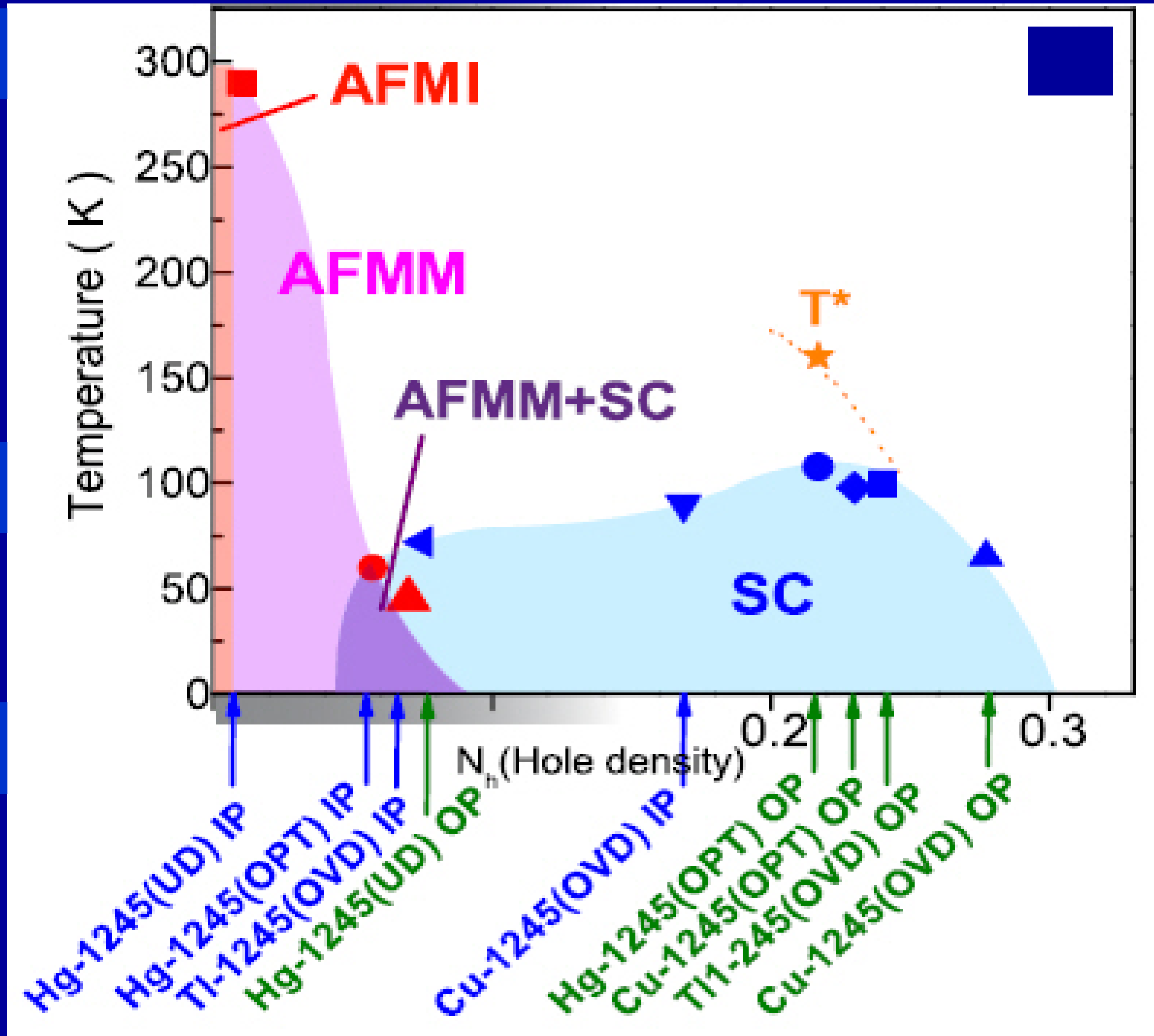
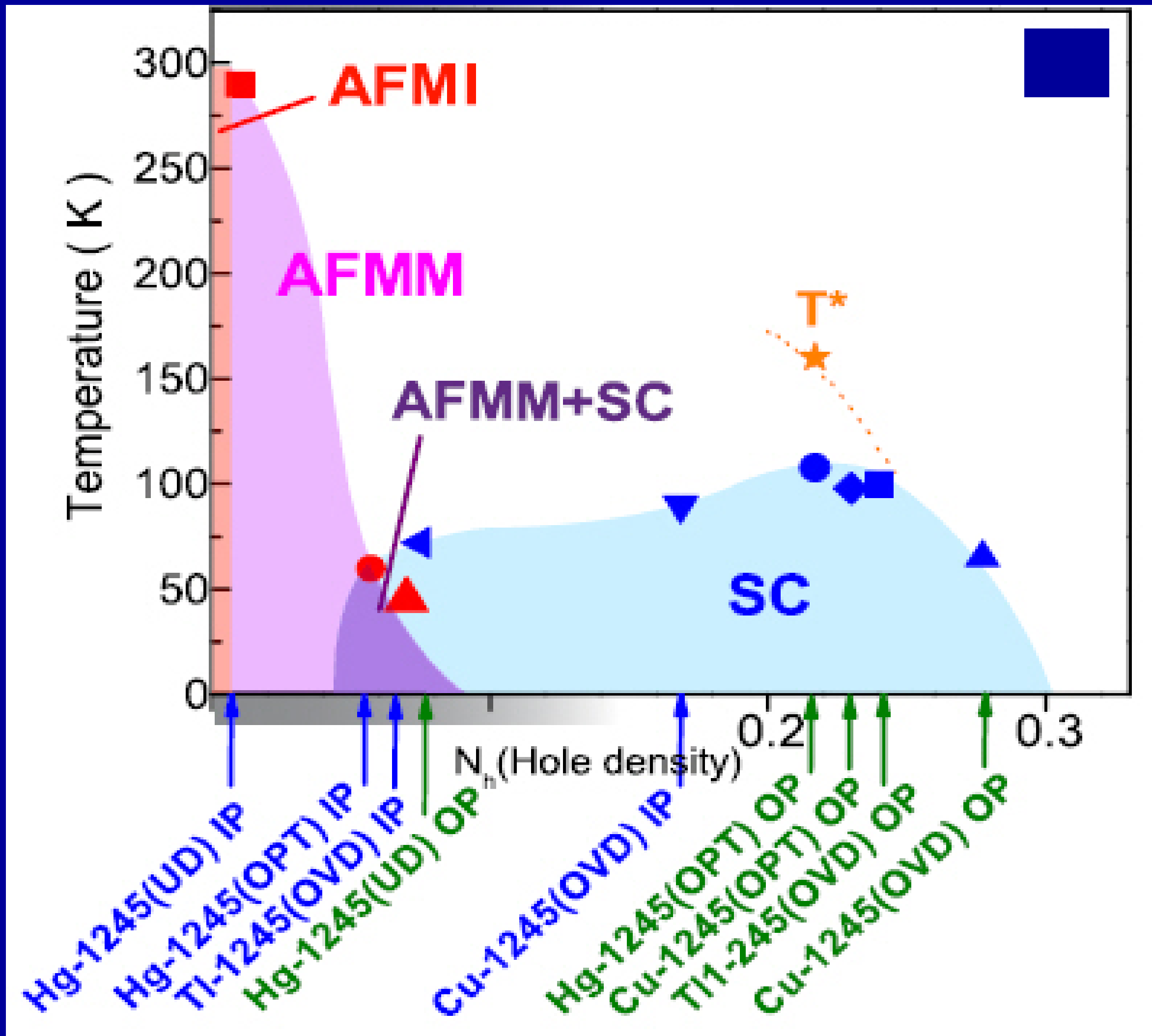
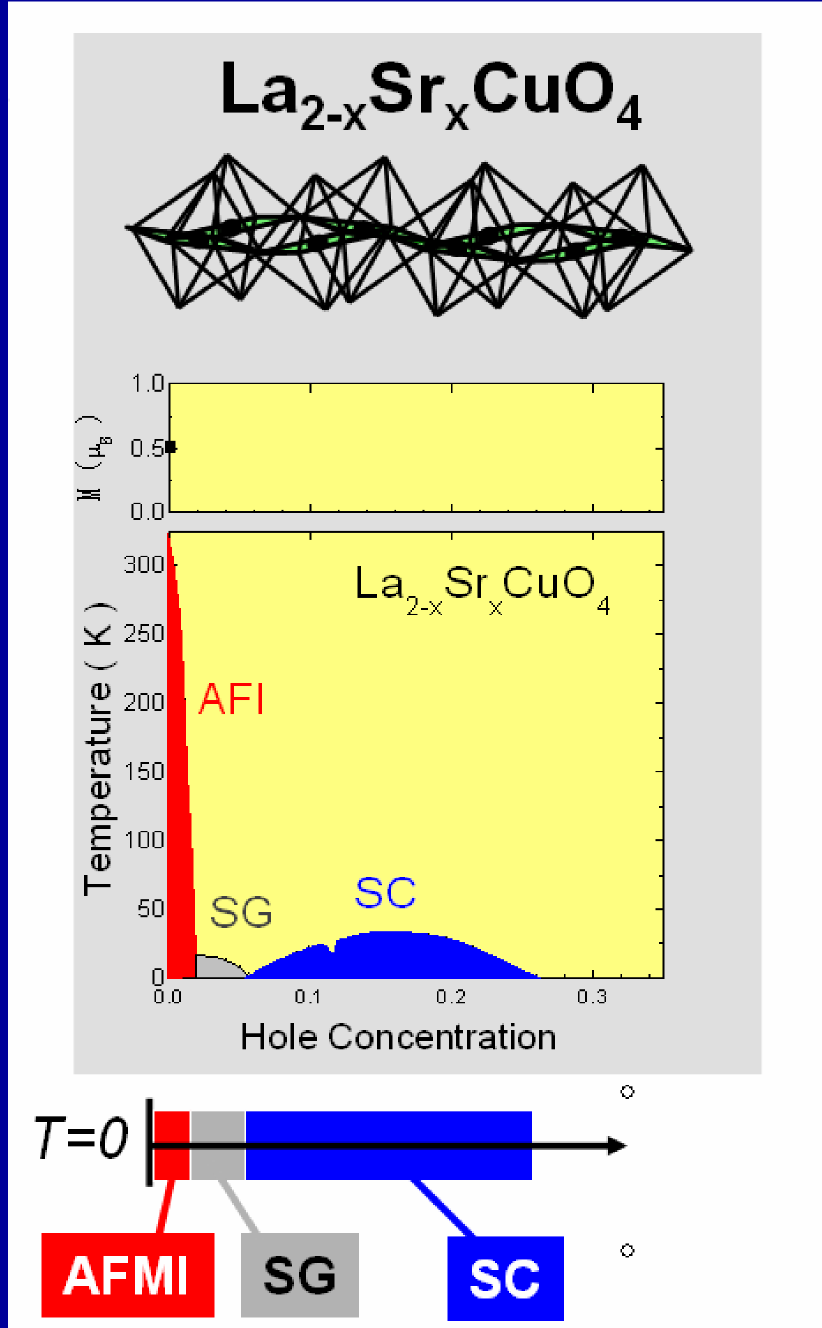


H Mukuda et al., PRL ('06)

"ideal" Phase diagram for hole-doped cupartes?





Basic info from experiments

- 5 possible phases:
  AFMI, AFMM, d-wave SC, and AFM+d-SC, normal metal.
- e-doped system is different from hole-doped.
- Broken symmetries: particle and hole; AFM, SC…

Theoretical challenge:

the simplest model to account for all these properties?

To start, only consider the homogeneous solution.

Minimal theoretical models

- 2D Hubbard model – U and t differ by almost an order of magnitude, reliable numerical approaches:

  exact diagonalization (ED) for 18 sites with 2 holes (Becca et al, PRB 2000)

  finite temp. quantum Monte Carlo (QMC) , fermion sign problem (Bulut, Adv. in Phys. 2002)

  2D t-J type models –

Model proposed by P.W. Anderson in 1987:
t-J model on a two-dimensional square lattice, generalized to include long range hopping

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

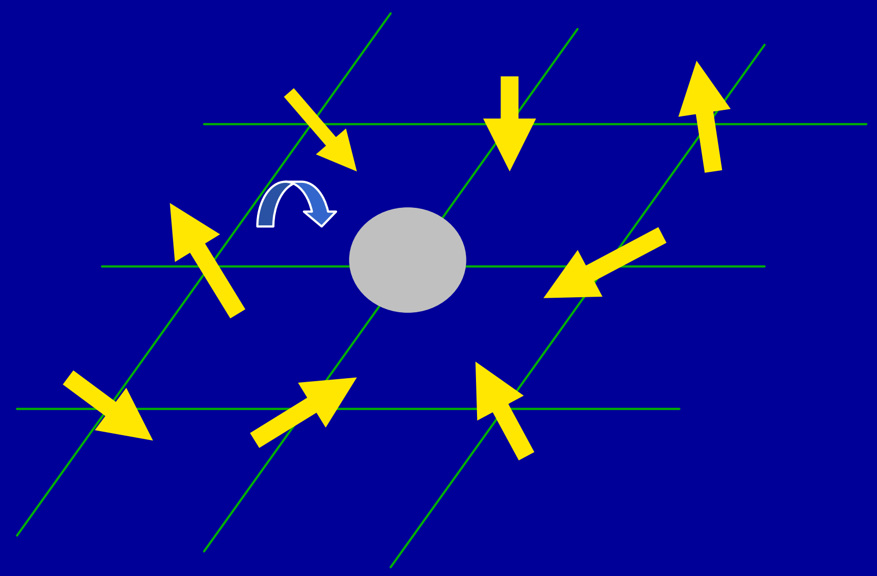
$$\vec{S}_i \rightarrow spin\ {}^1\!/_2,$$

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

t_{ij} = t for nearest neighbor charge hopping,
t' for 2nd neighbors, t'' for 3rd , t' and t'' breaks the particle-hole symmetry

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

Constraint: For hole-doped systems two electrons are not allowed on the same lattice site



Three species: an up spin, a down spin or an empty site or a "hole"

Minimal theoretical models

- 2D Hubbard model – U and t differ by almost an order of magnitude, reliable numerical approaches

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  2D t-J type models –

  - no finite temp. QMC – sign problem and strong constraint
  - ED for 32 sites with 1,2 and 4 holes (Leung, PRB)

Variational Monte Carlo method

Expectation values of an operator O in $|\Phi>$:

$$\langle \hat{O} \rangle = \frac{\langle \Phi | \hat{O} | \Phi \rangle}{\langle \Phi | \Phi \rangle} = \sum_{\alpha,\gamma} \frac{\langle \Phi | \alpha \rangle \langle \alpha | \hat{O} | \gamma \rangle \langle \gamma | \Phi \rangle}{\langle \Phi | \Phi \rangle}$$

$$= \sum_{\alpha} \frac{|\langle \alpha | \Phi \rangle|^2}{\langle \Phi | \Phi \rangle} \sum_{\gamma} \frac{\langle \gamma | \Phi \rangle}{\langle \alpha | \Phi \rangle} \langle \alpha | \hat{O} | \gamma \rangle \equiv \sum_{\alpha} \rho_\alpha f_\alpha$$

$$f_\alpha = \sum_{\gamma} \frac{\langle \gamma | \Phi \rangle}{\langle \alpha | \Phi \rangle} \langle \alpha | \hat{O} | \gamma \rangle$$

Bases: $$|\alpha\rangle = \prod_{i=1}^{N_\uparrow} \prod_{j=1}^{N_\downarrow} c^\dagger_{R_{i\uparrow}} c^\dagger_{R_{j\downarrow}} |0\rangle$$

$$\rho_\alpha = \frac{|\langle \alpha | \Phi \rangle|^2}{\langle \Phi | \Phi \rangle}$$ -- the probability of config. α

$$\langle \alpha | \Phi \rangle = det(\hat{a}_\alpha)$$

Slater determinant

Metropolis algorithm

To improve the trial wave function, we could add a Jastrow factor with more parameters like

$$\hat{J} \bullet |\psi\rangle$$

$$\hat{J} = \prod_{i<j} \left(1 - (1 - r_{ij}^{\alpha}) \cdot n_i^h n_j^h\right)$$

$$r_{ij} = \sqrt{\sin^2\left(\frac{\pi}{L}(x_i - x_j)\right) + \sin^2\left(\frac{\pi}{L}(y_i - y_j)\right)}$$

This term introduces power-law correlation between holes

When we have many variational parameters (p_i) , we could use the Stochastic reconfiguration (SR) method

Casula, *et. al.*, J. Chem. Phys. '04
Sorella, PRB '05
Yunoki and Sorella, PRB '06

Similar to steepest descent (SD) method, we define a "force":

$$F_i \equiv -\frac{\partial}{\partial p_i} E(\Phi_{\mathbf{p}_i})$$

$$\delta p_i = p_i' - p_i = F_i \delta t$$

We can obtain the next parameters p_i' by iterating

The energy improvement is approximately written as

$$\Delta E \equiv E(\Phi_{\mathbf{p}_i'}) - E(\Phi_{\mathbf{p}_i}) \simeq -\sum_{i=1}^{v_p} F_i \delta p_i = -\delta t \sum_{i=1}^{v_p} F_i^2$$

Energy will converge to the minimum when all $F_i=0$.
We can tune $\delta t (>0)$ to control the convergence of iteration.

However, SD method overlooks a possibility that a small δp_i may lead to a large change of the wave function…

Therefore, we also need to minimize a "distance":

$$\Delta_{\mathbf{p}} = 1 - \frac{\langle \Phi_{\mathbf{p}_i} | \Phi_{\mathbf{p}'_i} \rangle}{\sqrt{\langle \Phi_{\mathbf{p}_i} | \Phi_{\mathbf{p}_i} \rangle \langle \Phi_{\mathbf{p}'_i} | \Phi_{\mathbf{p}'_i} \rangle}}$$

A functional is defined as

$$\begin{aligned} f(\delta p_i) &= \Delta E + \lambda \Delta_{\mathbf{p}} \\ &= -\sum_{i=1}^{v_p} F_i \delta p_i + \lambda \sum_{i,j=1}^{v_p} \delta p_i \delta p_j \hat{S}_{ij} \end{aligned}$$

λ is a Lagrange multiplier

Minimization of $f(\delta p_i)$ with respect to δp_i, we have a "new" iterated formula:

$$\delta p_i = \delta t \sum_{j=1}^{v_p} \hat{S}_{ij}^{-1} F_j$$

$\delta t = 1/2\lambda$

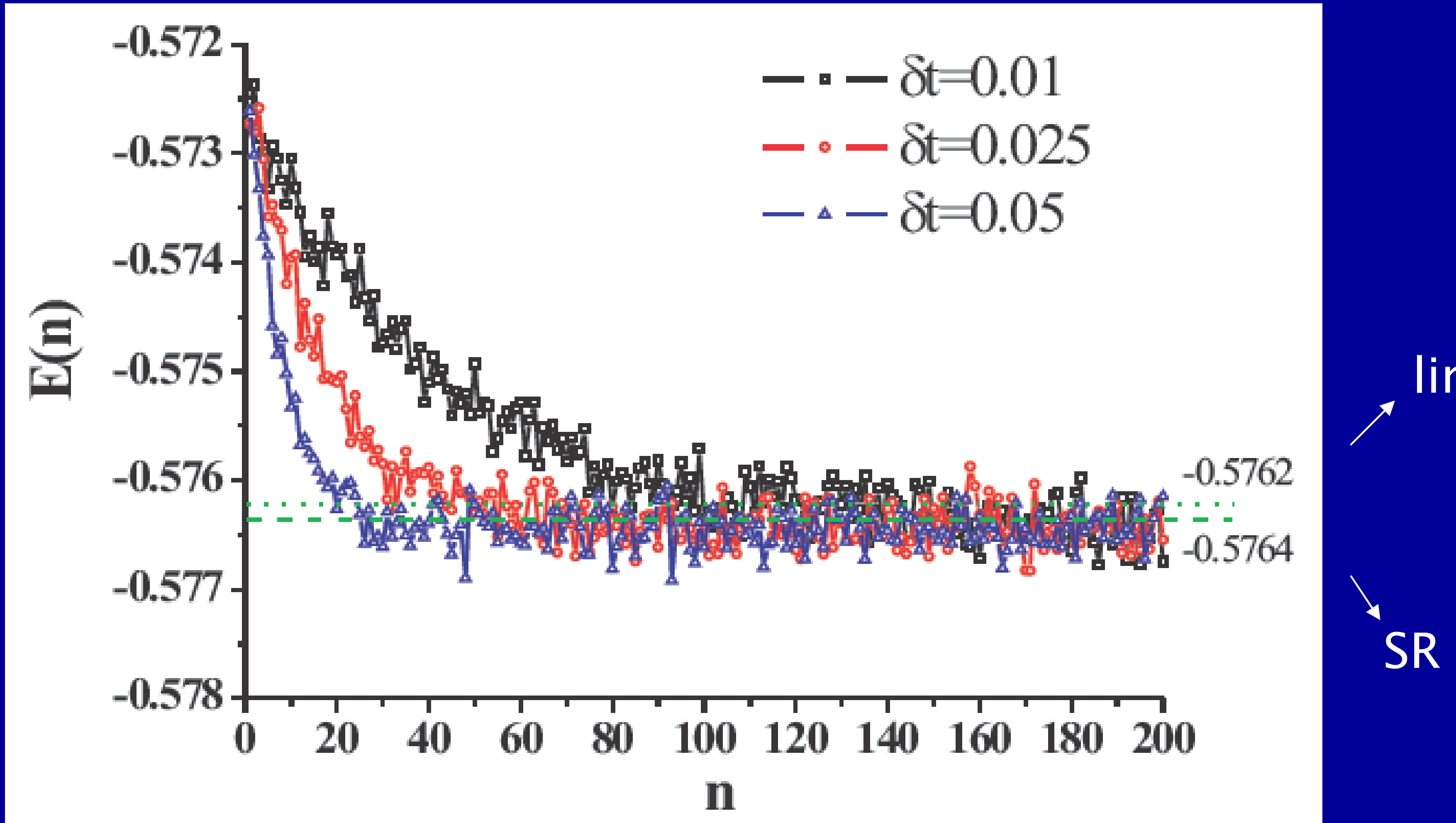
Then, the energy improvement for SR method becomes

$$\Delta E = -\delta t \sum_{i,j=1}^{v_p} \hat{S}_{ij}^{-1} F_i F_j$$

S_{ij} matrix remains positive definite.

Sometimes S_{ij} has no inverse matrix for some unstable iterations. If so, we use the SD method instead.

How do we choose δt in SR method?



2D Lattice size=64

t–t'–t''–J model with (*t'*,*t''*,*J*)=(-0.3,0.2,0.3)

Trial wave function: *d*–wave RVB wave function

n is the number of iterations

Beyond VMC approach – a less biased approach the Power-Lanczos method

For a given trial wave function, $|\Phi>$, we approach the ground state in two steps:

1. Lanczos iteration

$$|\Phi^{(1)}>=|\Phi>+\frac{C_1}{N}\mathbf{H}|\Phi>$$

We denote this state as |PL1>

$$|\Phi^{(2)}>=|\Phi>+\frac{C_1}{N}\mathbf{H}|\Phi>+\frac{C_2}{N^2}\mathbf{H}^2|\Phi>$$

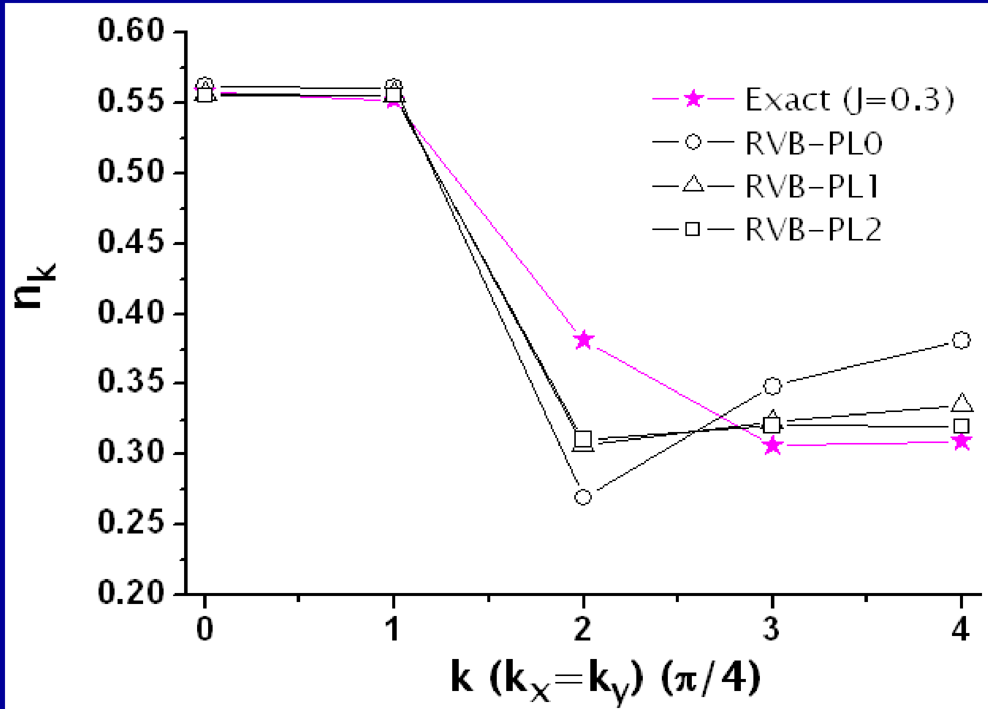
|PL2>

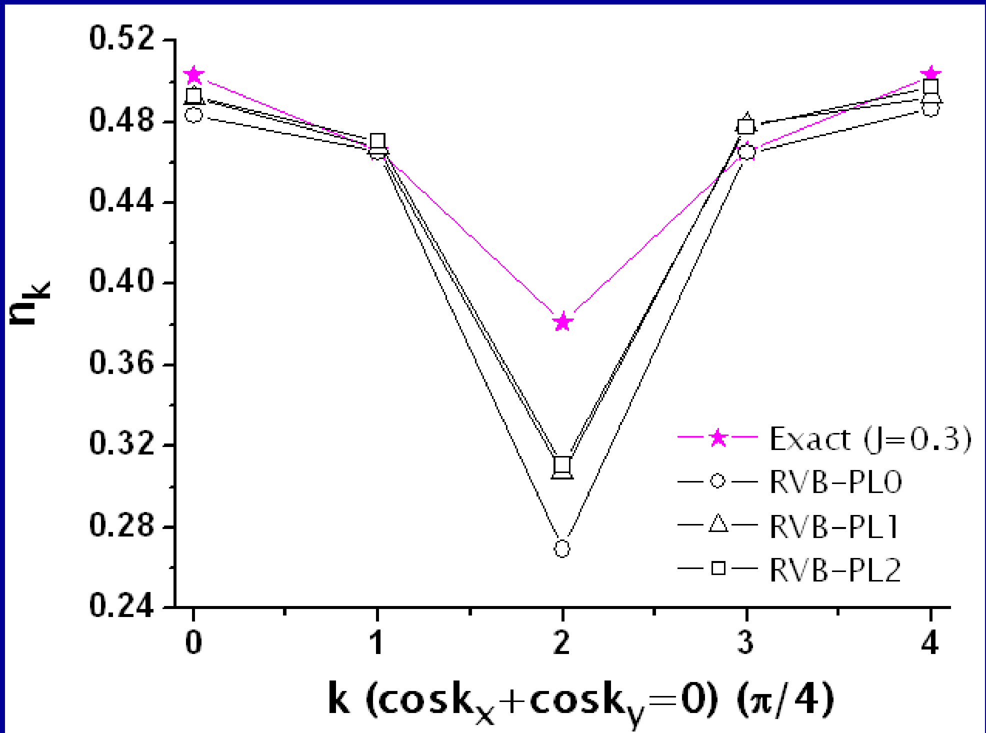
C_1 and C_2 are taken as variational parameters

2. Power Method

$$|\Phi_n^{(l)}>=(W-\mathbf{H})^n|\Phi^{(l)}>$$

$$|GS>=\lim_{n\to\infty}|\Phi_n^{(l)}>=(W-\mathbf{H})^n|\Phi^{(l)}>$$





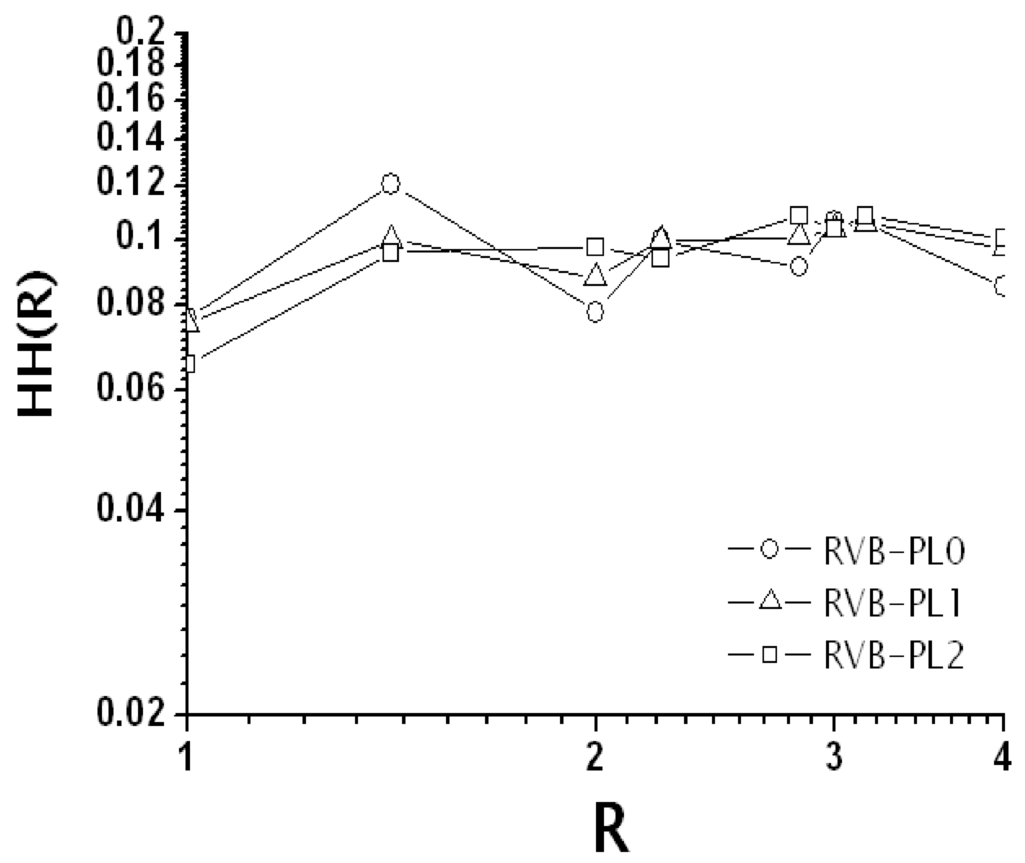
After PL, nk, HH(R), and energy get closer to exact results!

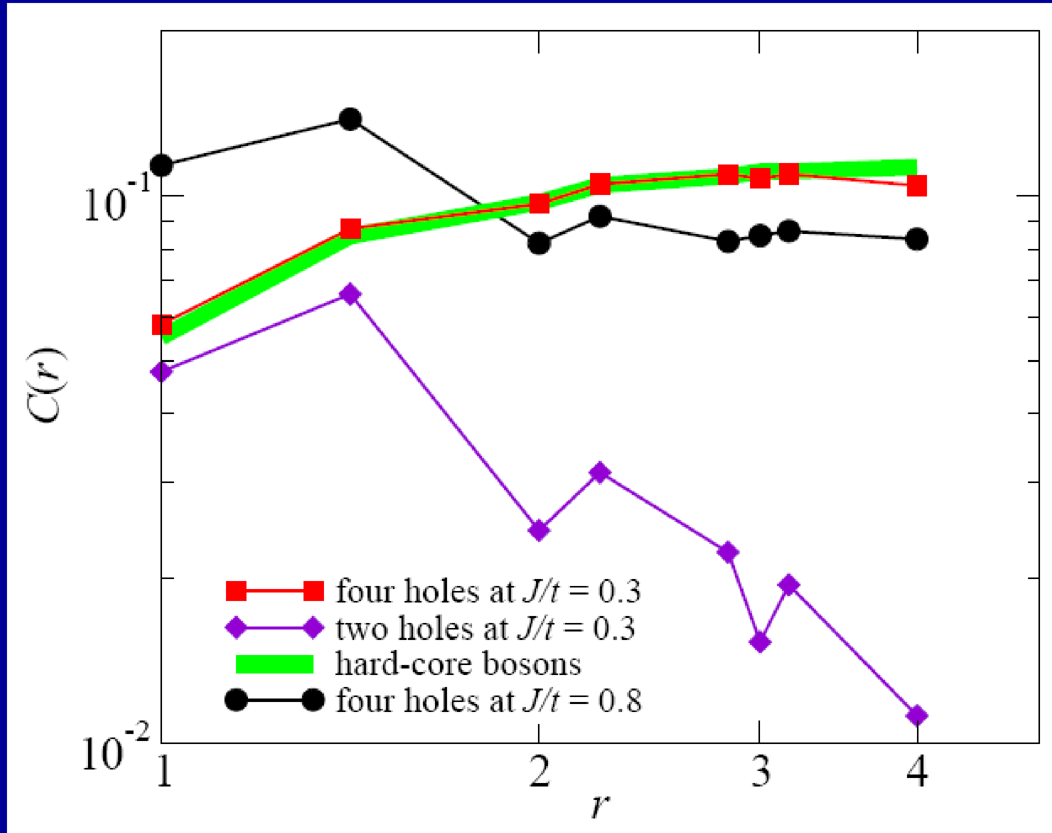
For the t-J model, Leung PRB 2006, 4 holes in 32 sites

PL Energy

J=0.3	E
Exact	−0.583813
RVB(PL0)	−0.5431
RVB(PL1)	−0.5654
RVB(PL2)	−0.5709

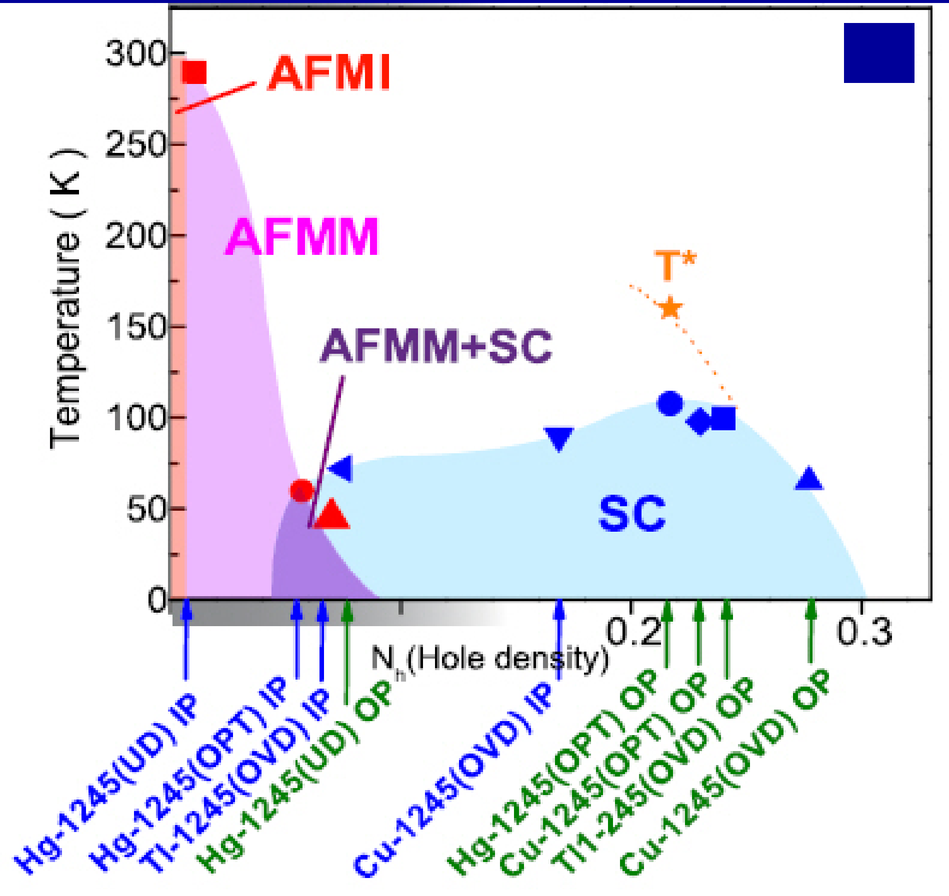
HH(R) - the hole-hole correlation function

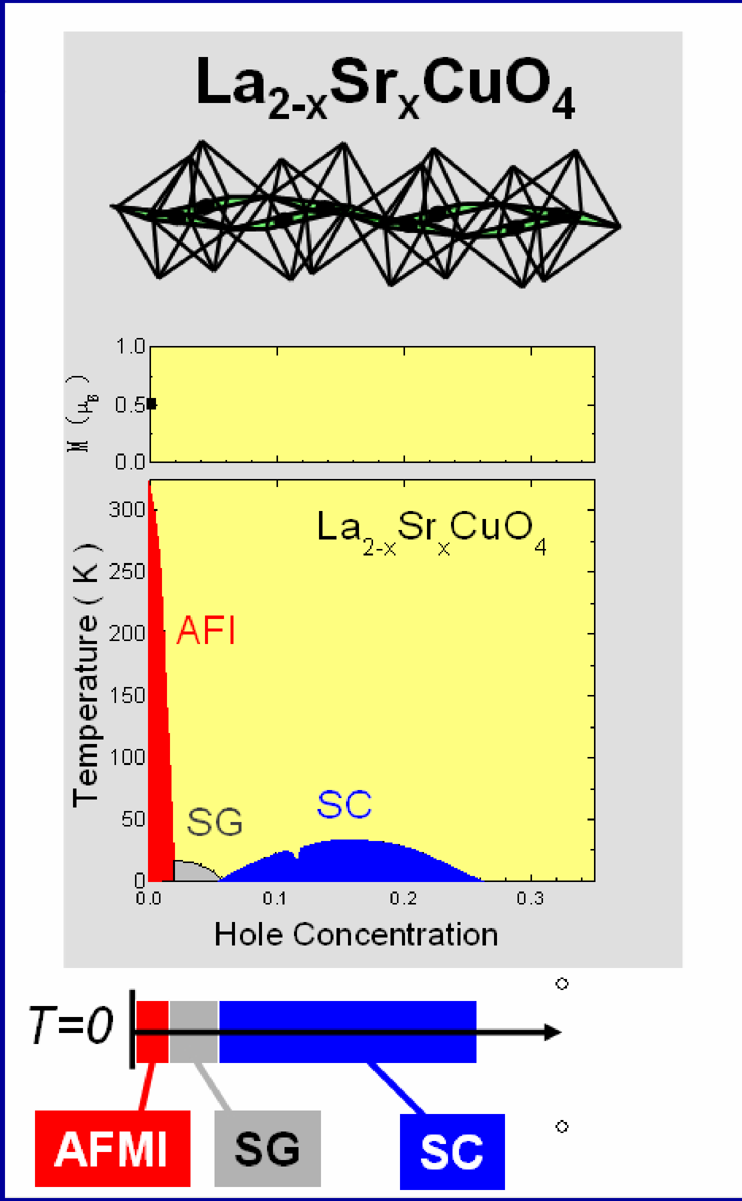




Trial wave functions for hole-doped systems

Must account for : Mott insulator
AFM, SC , AFM+SC?





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

AFM is natural!

D-wave SC?

In 1987, Anderson pointed out the superexchange term

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

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

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

This provides the pairing mechanism!

It can be easily shown that near half-filling this term only favors d-wave pairing for 2D Fermi surface!

Spin or charge pairing?

The resonating-valence-bond (RVB) variational wave function proposed by Anderson (originally for s-wave and no t', t''),

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

The Gutzwiller operator $\mathbf{P_d}$ $\mathrm{P_d} = \prod_i (1 - n_{i\uparrow} n_{i\downarrow})$ **enforces no doubly occupied sites for hole-doped systems**

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

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

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

four variational parameters, t_v' t_v'' Δ_v, and μ_v

d-RVB = A projected d-wave BCS state!

AFM was not considered.

The simplest way to include AFM:

$$|\psi_{tr}\rangle = \exp(h^* \sum_i (-1)^i S_z^i)|\mathrm{RVB}\rangle$$

Lee and Feng, PRB 1988, for t-J

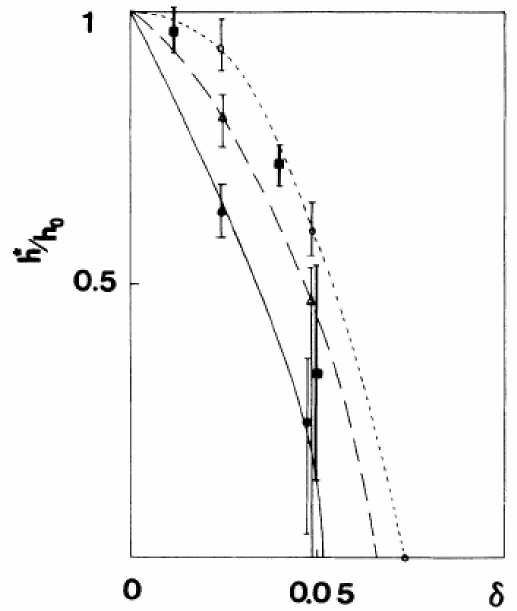


FIG. 3. Data of the ratio h^*/h_0 as a function of the hole concentration δ for $\Delta=0.6$, $t/J=5$ (solid circles), $\Delta=0.6$, $t/J=2.5$ (open circles), $\Delta=0.2$, $t/J=5$ (triangles), and internal field measurement (Ref. 4) of $(La_{1-x}Ba_x)_2CuO_4$ (squares), respectively. Typical error bars are shown.

TABLE I. A comparison of the ground-state energy and sublattice magnetization for the Heisenberg model on a two-dimensional square lattice.

Author(s)	$-\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$	$M_s/2$	Method
Anderson (Ref. 17), Kubo (Ref. 18)	0.329	0.303	Spin wave
Horsch and von der Linden (Ref. 13)	0.3219(9)	0.335	Variational
Oitmaa and Betts (Ref. 12)	0.328(3)	0.24	Finite lattice
Yokoyama and Shiba (Ref. 19)	0.321(1)	0.43	Variational SDW
Gros (Ref. 9)	0.319(1)	0	Variational RVB
Huse and Elser (Ref. 16)	0.3319	0.355	Variational
Liang *et al.* (Ref. 20)	0.3344(2)	0.375	Variational RVB
Present work	0.332(5)	0.37(1)	Variational

Use mean field theory to include AFM,

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

Lee and Feng, PRB38, 1988; Chen, et al., PRB42, 1990; Giamarchi and Lhuillier, PRB43, 1991; Lee and Shih, PRB55, 1997; Himeda and Ogata, PRB60, 1999

Assume AFM 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 + AFM for the half-filled ground state

(no t, t' and t'')

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

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
staggered moment m = 0.367	0.375 ~ 0.3

Liang, Doucot And Anderson

The wave function for adding holes or removing electrons from the half-filled RVB+AFM ground state

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

Creating charge excitations to the Mott Insulator "vacuum".

The state with one hole (two parameters: m_v and Δ_v)

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

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

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.

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

Without the long range hopping terms, t' and t'', the model Hamiltonian, t-J model, has the particle-hole symmetry: $c_{i\sigma}^{+} \rightarrow c_{i\sigma}$

t' and t'' break the symmetry between doping electrons and holes!

From hole-doped to electron-doped, just change

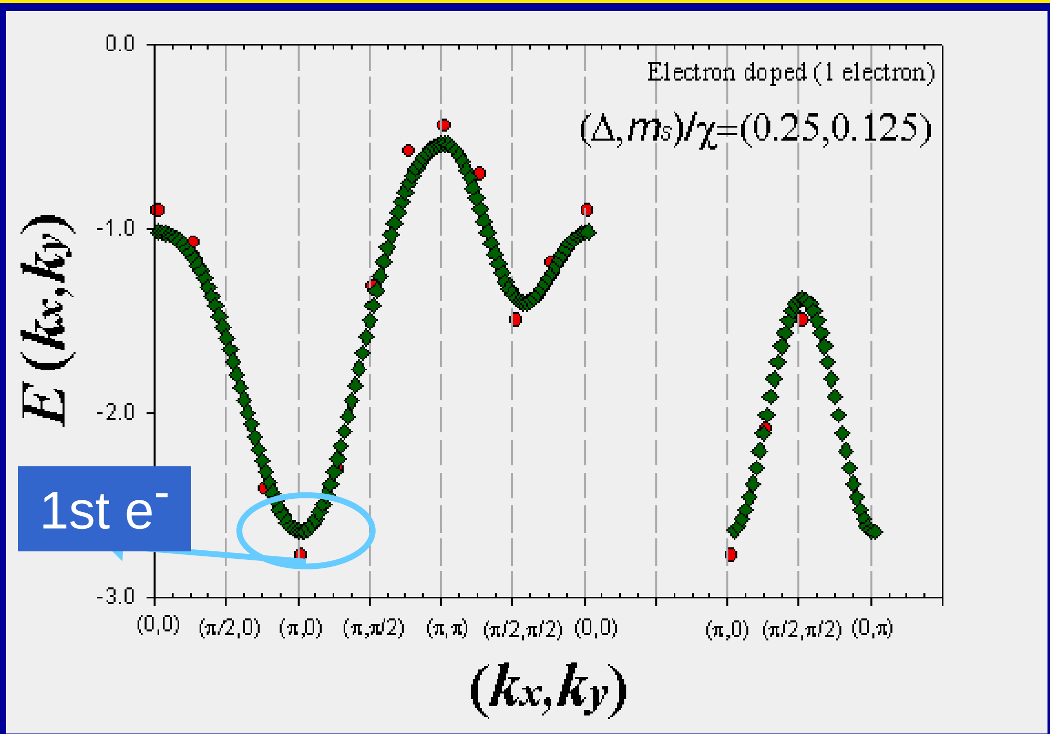
t'/t $\rightarrow$ – t'/t and t"/t $\rightarrow$ – t"/t

Different Hamiltonians – different phase diagram.

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

J/t=0.3

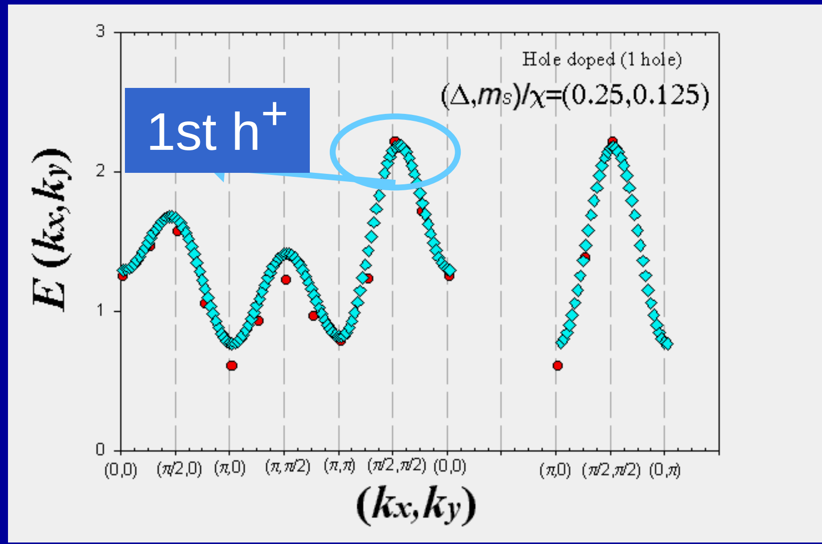
Energy dispersion after one electron is doped. The minimum is at (π , 0).
t'/t= 0.3, t"/t= - 0.2

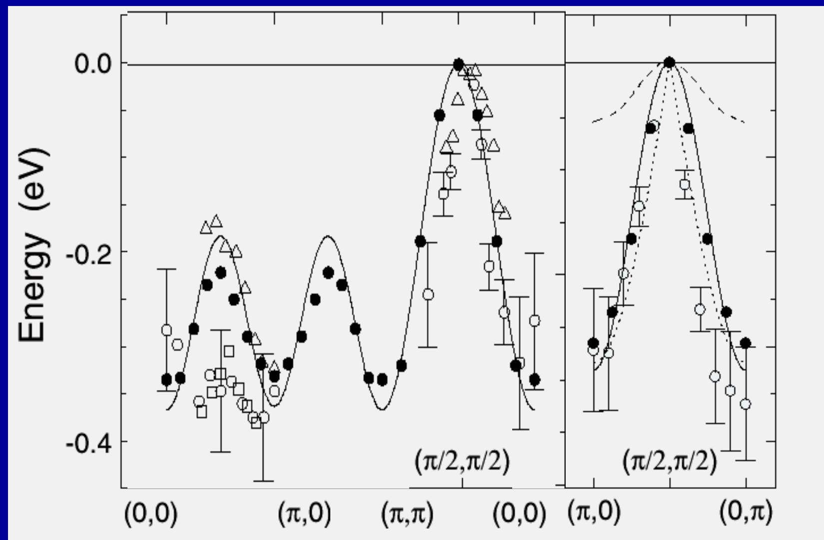


The same wave function is used for both e-doped and hole-doped cases.

There is no information about t' and t" in the wave function used.

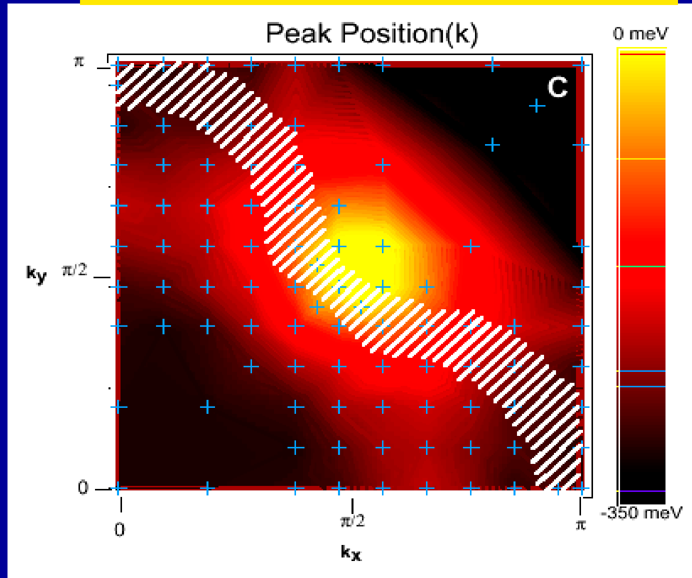
Dispersion for a single hole.
t'/t= - 0.3, t"/t= 0.2





□ 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, Tohyama and Maekawa, SC Sci. Tech. 13, R17 (2000)

ARPES for $Ca_2CuO_2Cl_2$

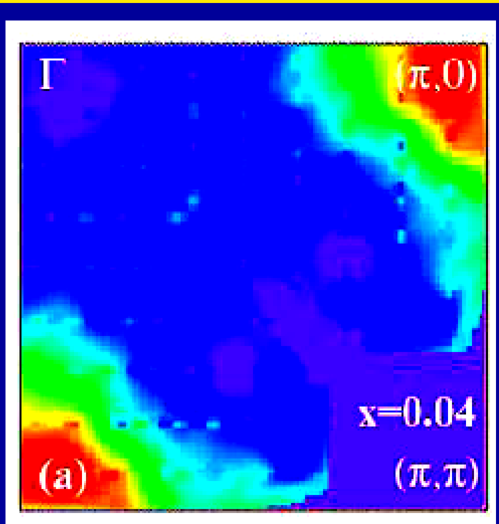


Ronning, Kim and Shen, PRB67 (2003)

The lowest energy at

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

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



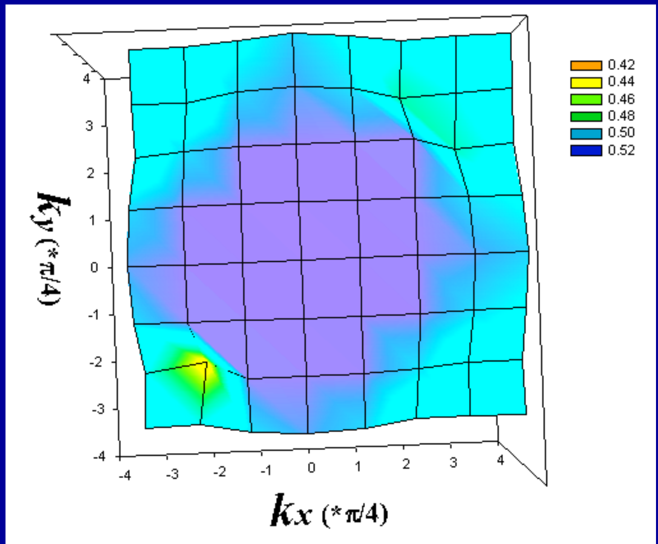
Fermi surface around (π,0) and (0, π)!

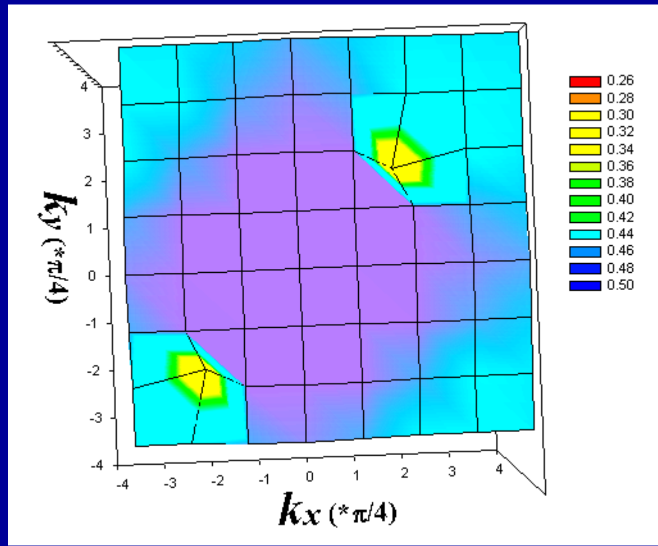
Armitage *et al*., PRL (2002)

Momentum distribution for a single hole calc. by the quasi-particle wave function

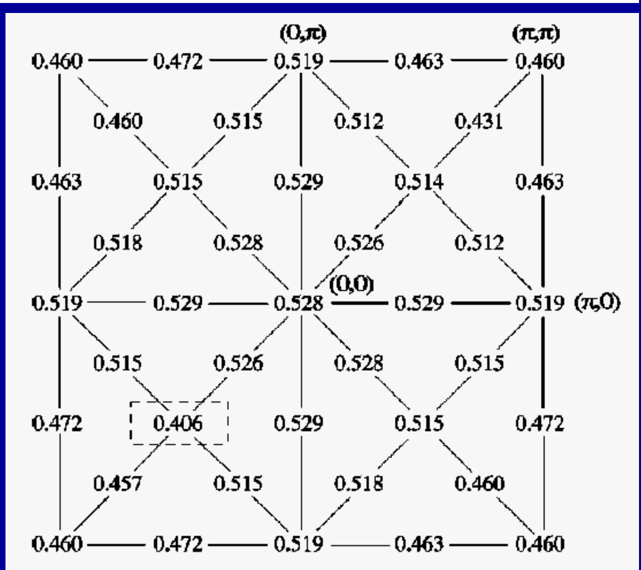
$$\left|\psi_{1h}(k=(\pi/2,\pi/2),S_z=1/2)\right\rangle$$

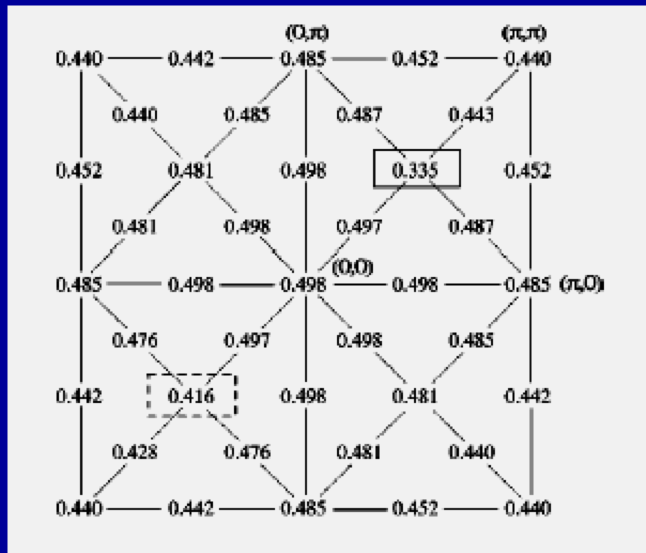
$< n^h_{k\uparrow} >$ $< n^h_{k\downarrow} >$





64 sites





Exact results for the single-hole ground state for 32 sites. Chernyshev et al. PRB58, 13594(98')

Wave Functions for one *hole* system

- Quasi-particle state:

$$P_d C^{+}_{k\downarrow}\Big(\sum_{q\neq -k}{}' A_a a^{+}_{q\uparrow} a^{+}_{-q\downarrow} + B_q b^{+}_{q\uparrow} b^{+}_{-q\downarrow}\Big)^{\frac{N}{2}-1}\left|0\right\rangle$$

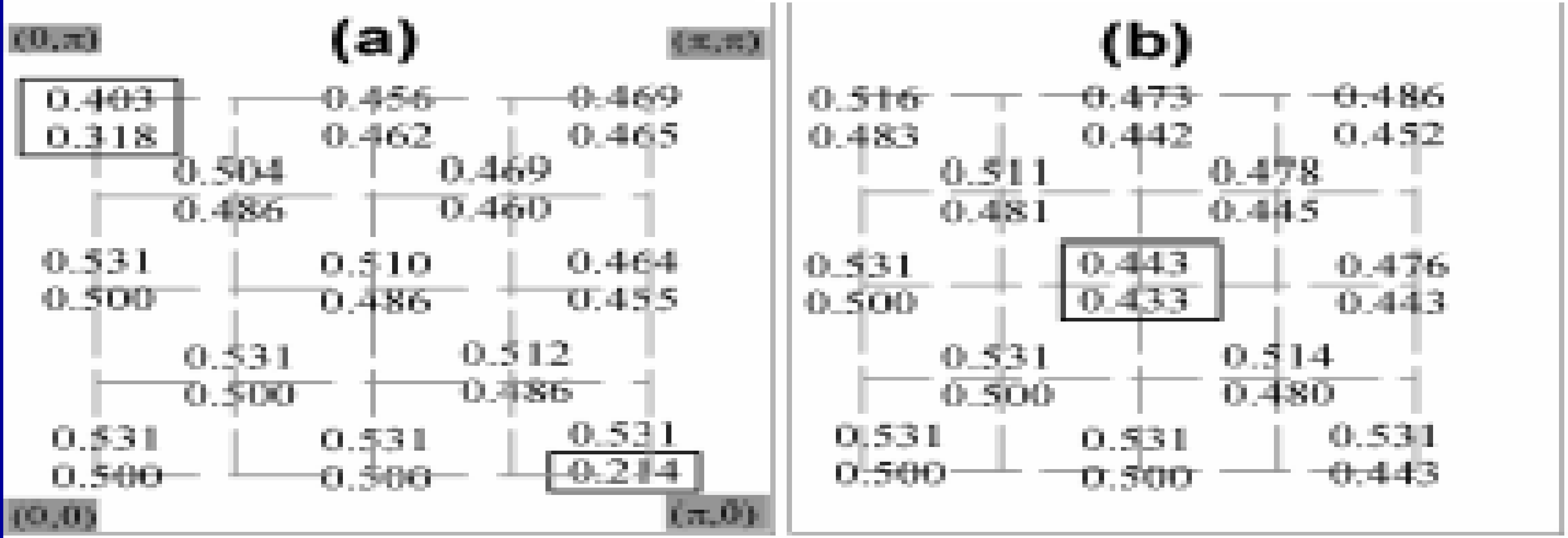
Hole momentum (*k_h*)=unpaired spin momentum (*k_s*) = *k*

- Spin-bag state:

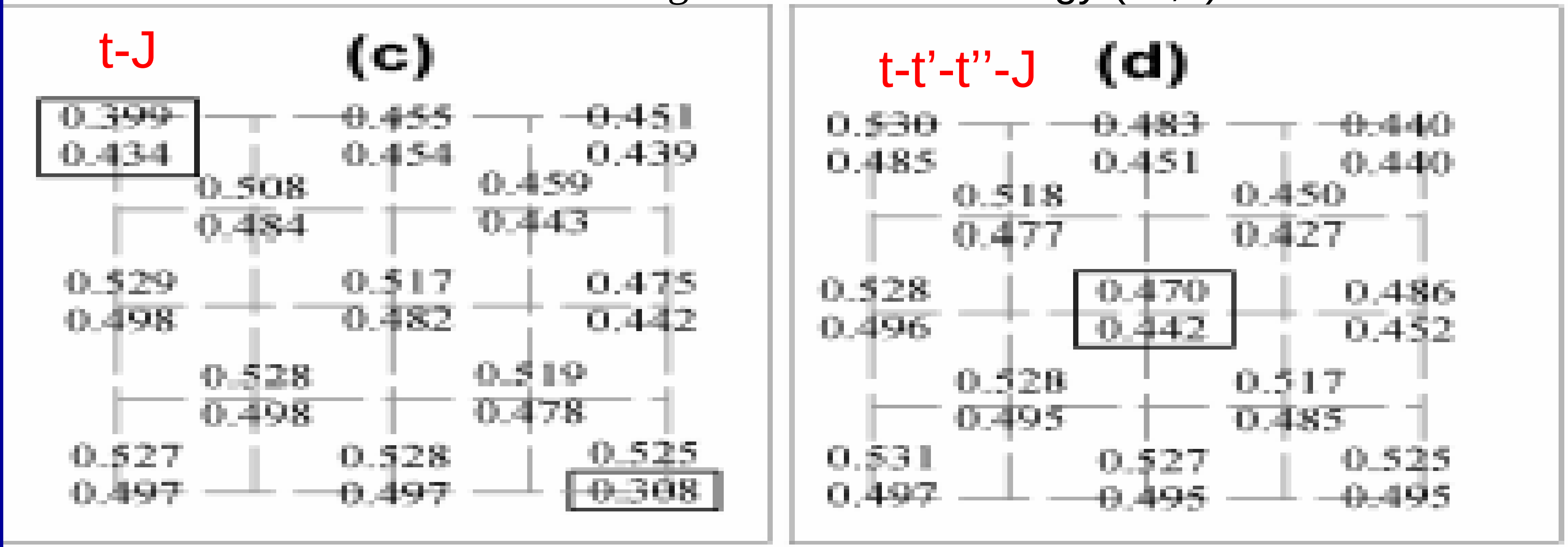
$$P_d C^{+}_{k_s\downarrow}\Big(\sum_{q\neq k_h}{}' A_a a^{+}_{q\uparrow} a^{+}_{-q\downarrow} + B_q b^{+}_{q\uparrow} b^{+}_{-q\downarrow}\Big)^{\frac{N}{2}-1}\left|0\right\rangle$$

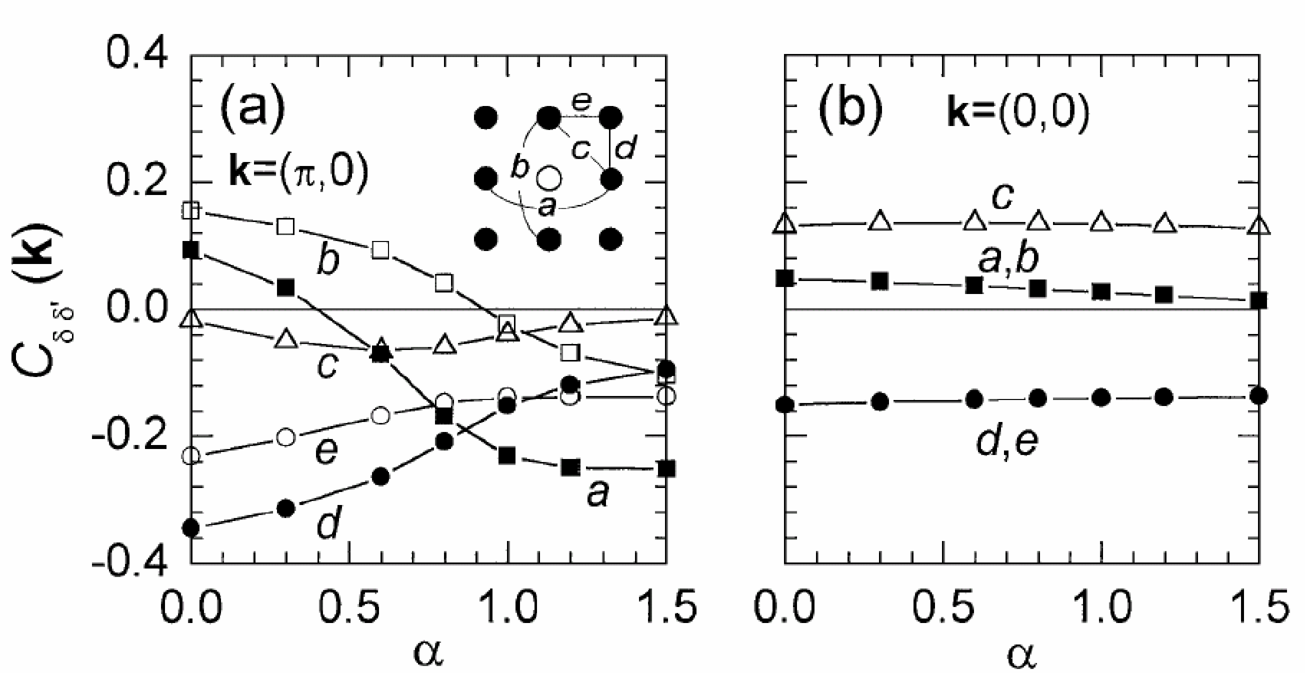
, where $\boldsymbol{k}_s \neq \boldsymbol{k}_h = (\frac{\pi}{2}, \frac{\pi}{2})$

a QP state $\boldsymbol{k_h}=(\pi,0)=\boldsymbol{k_s}$ a SB state $\boldsymbol{k_s}=(\pi,0)$, $\boldsymbol{k_h}=(\pi/2,\pi/2)$



Exact 32 site result from P. W. Leung for the lowest energy $(\pi, 0)$ state





Takami TOHYAMA et al.,

J. Phys. Soc. Jpn. Vol 69, No1, pp. 9-12

J/t=0.4, t'/t≈- α /3
and t"/t'=2/3

	(0,0) QP	(0,0) SB	(π/2,π/2) QP	(π,0) QP	(π,0) SB
a	0.188	-0.0288	-0.0044	0.123	-0.0313
b	0.188	-0.0254	-0.0052	0.159	-0.0085
c	0.202	-0.0302	-0.0005	0.071	-0.002
d	-0.273	-0.203	-0.2241	-0.353	-0.1921
e	-0.264	-0.195	-0.2154	-0.279	-0.2115

Our Result: (π , 0) is QP at t-J model, but SB for t-t'-t"-J.

(0, 0) is QP for both

QP:Quasi-Particle state

SB: Spin-Bag state

The state with two holes

$$\left|\psi_{2h}(k_{total}=0, S_Z=0)\right\rangle \propto c_{k_h\uparrow} c_{-k_h\downarrow}\left|\psi_0\right\rangle$$

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

Ground state is $k_h=(\pi/2, \pi/2)$ for two 0e holes; $k_h=(\pi, 0)$ for two 2e holes.

Similar construction for more holes and more electrons.

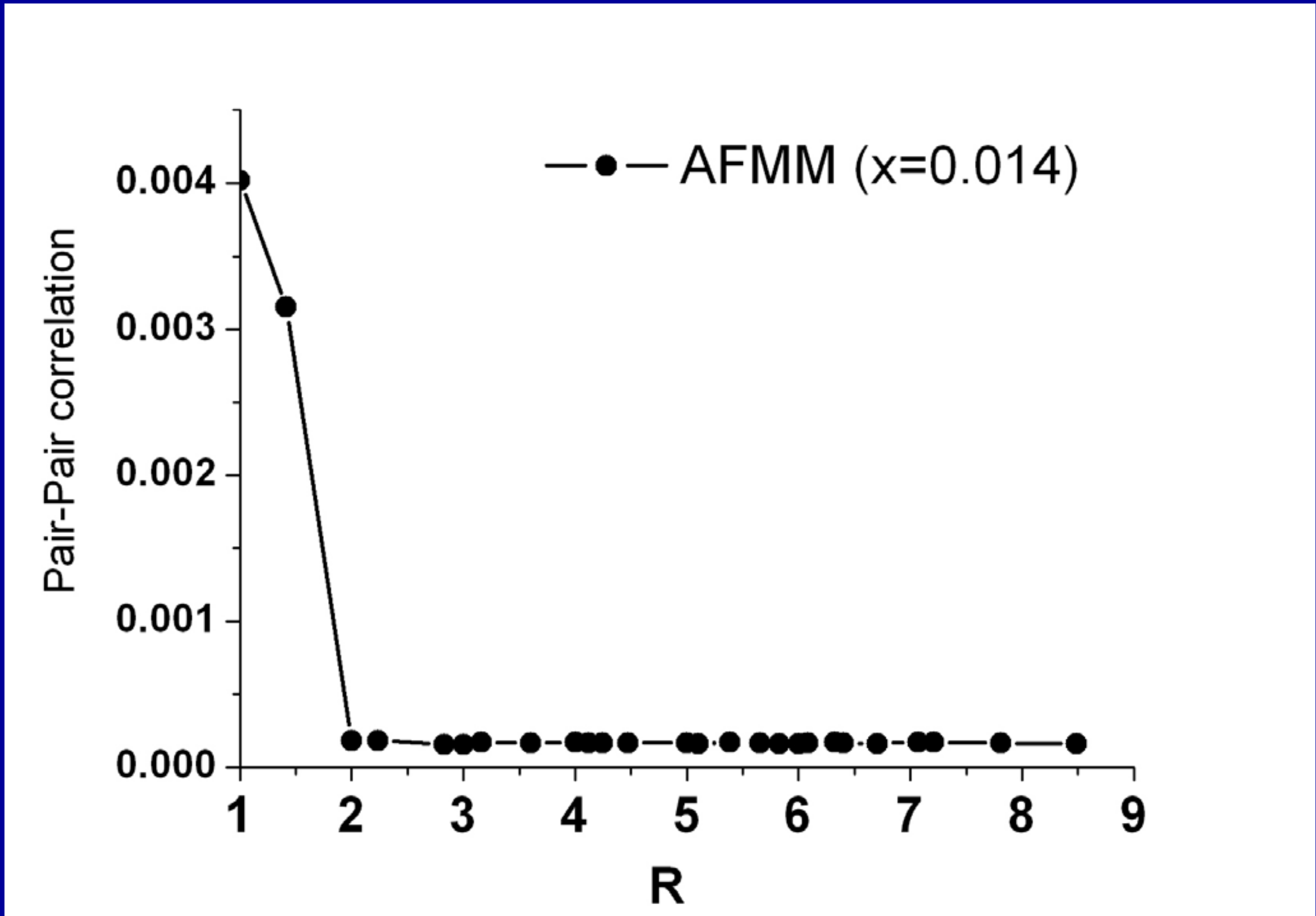
The Mott insulator at half-filling is considered as the vacuum state. Thus hole- and electron-doped states are considered as the negative and positive charge excitations .

Fermi surface becomes pockets in the k-space!

Lee *et al*., PRL 90 (2003); Lee *et al*. PRL 91 (2003).

d-wave pairing correlation function

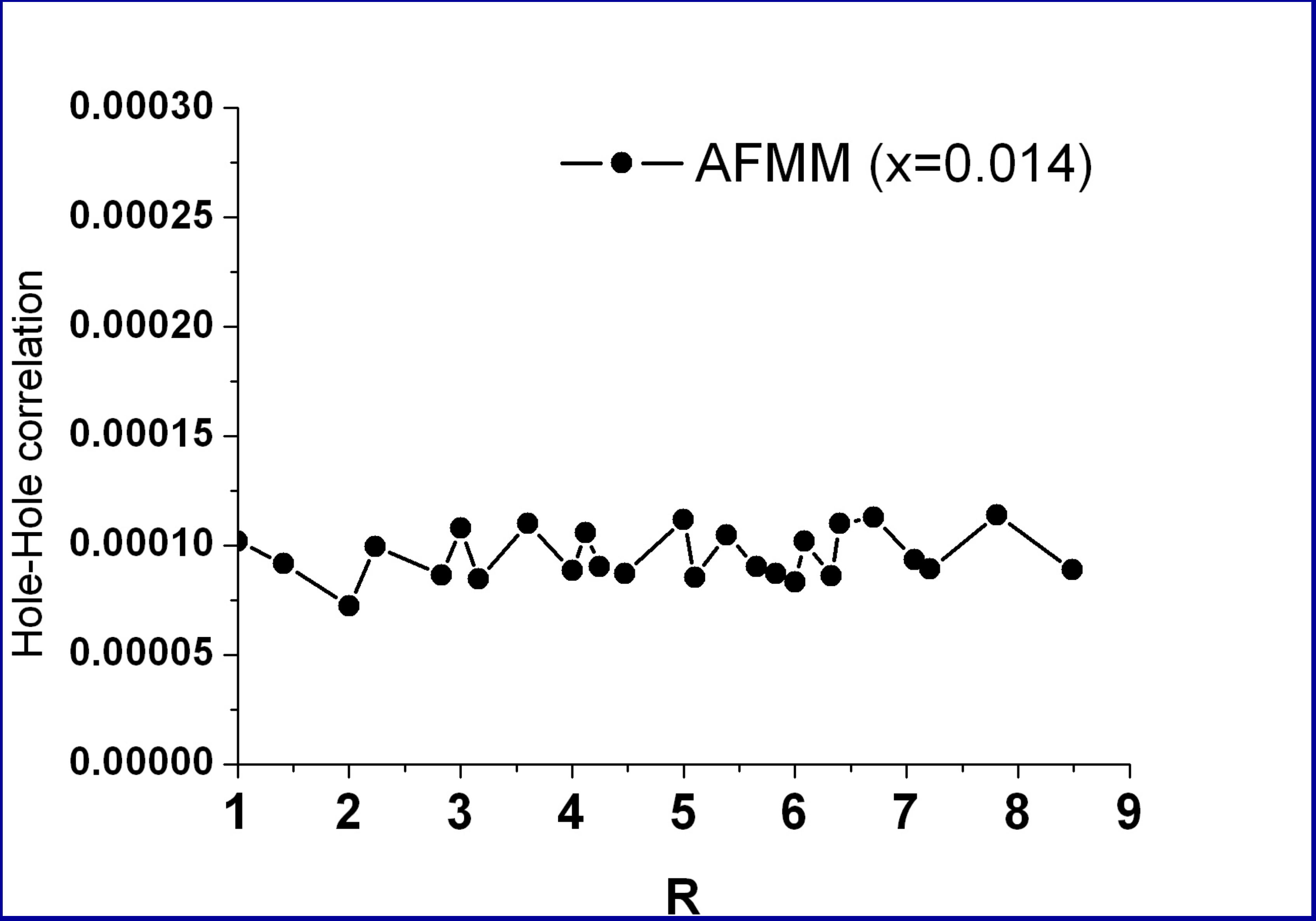
$$P_{s \text{ or } d}(R) = \frac{1}{N_s} \sum_i \langle \Delta_i^\dagger \Delta_{i+R} \rangle \quad \Delta_i = c_{i\uparrow}(c_{i+\hat{x}\downarrow} + c_{i-\hat{x}\downarrow} \pm c_{i+\hat{y}\downarrow} \pm c_{i-\hat{y}\downarrow})$$



2 holes
in 144 sites

The new wave function has AFM but negligible pairing.
It could be used to represent an AFM metallic (AFMM) phase.

2 holes
in 144 sites



Increase doping, pockets are connected to form a Fermi surface:

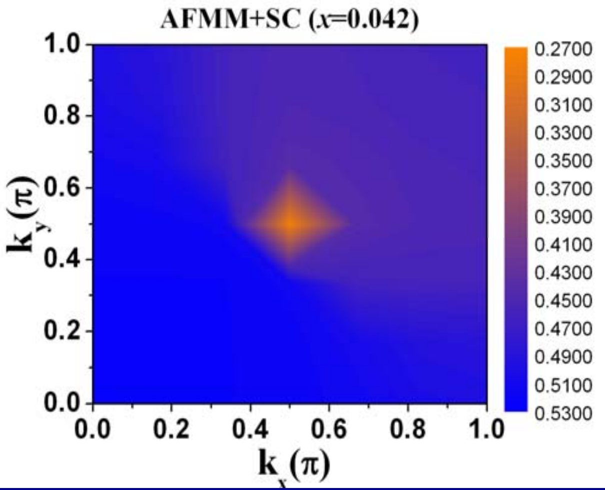
Cooper pairs formed by SDW quasiparticles

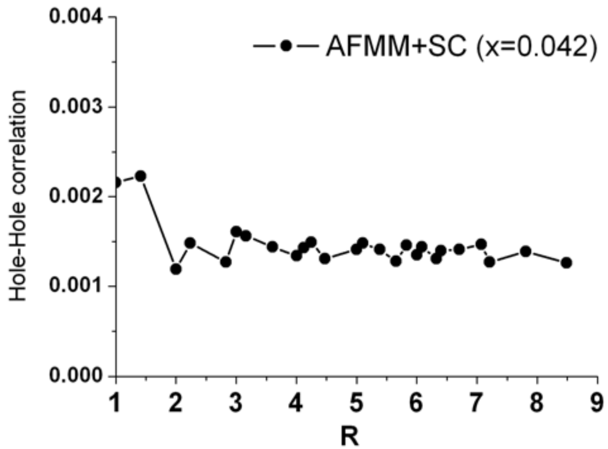
$$| N_e\rangle_{AFMM+SC} = P_d \left(\sum_{\mathbf{k}\in MBZ} A_{\mathbf{k}} a^{\dagger}_{\mathbf{k}\uparrow} a^{\dagger}_{-\mathbf{k}\downarrow} + B_{\mathbf{k}} b^{\dagger}_{\mathbf{k}\uparrow} b^{\dagger}_{-\mathbf{k}\downarrow} \right)^{N_e/2} | 0\rangle$$

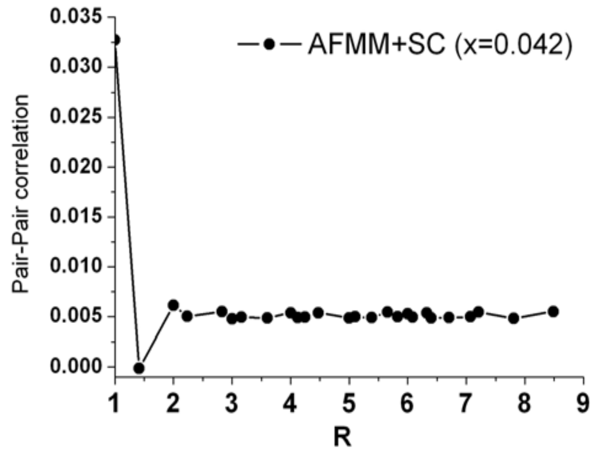
$$\xi^{\pm}_{\mathbf{k}} = \pm\sqrt{\epsilon^2_{\mathbf{k}} + m^2_v} - \mu_v - t'_v cosk_x cosk_y - t''_v(cos2k_x + cos2k_y)$$

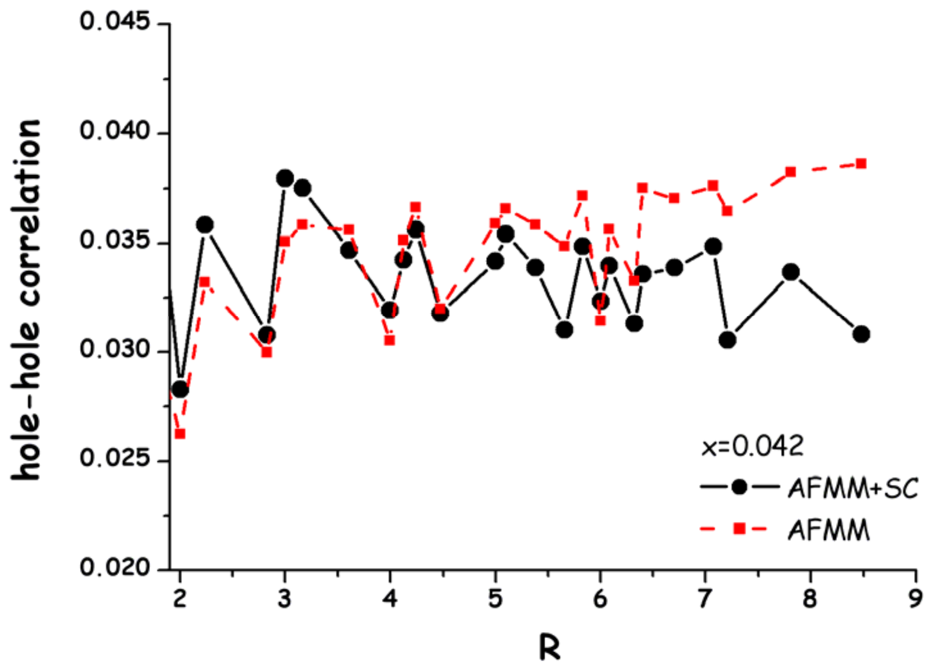
$$\epsilon_{\mathbf{k}} = -(cosk_x + cosk_y)$$

three new variational parameters: μ_v, t'_v and t''_v

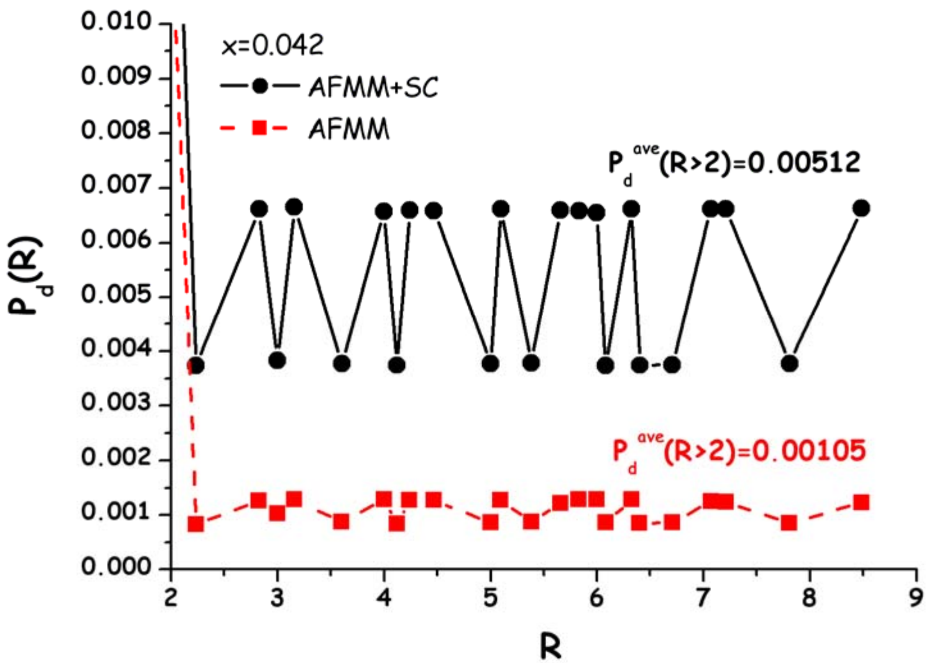




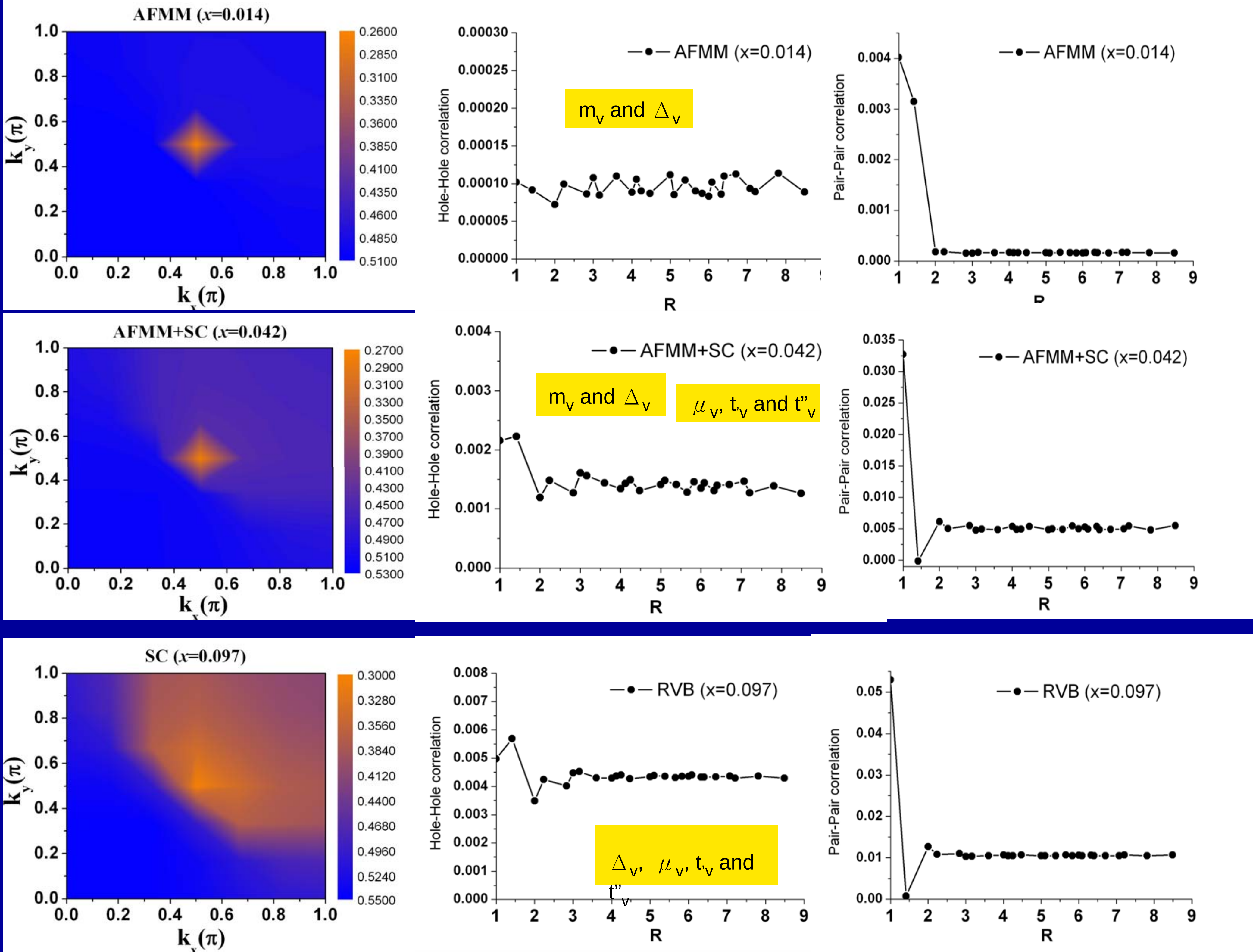




AFMM shows stronger hole-hole repulsive correlation than AFMM+SC.



The pair-pair correlation of AFMM is much smaller than AFMM+SC.

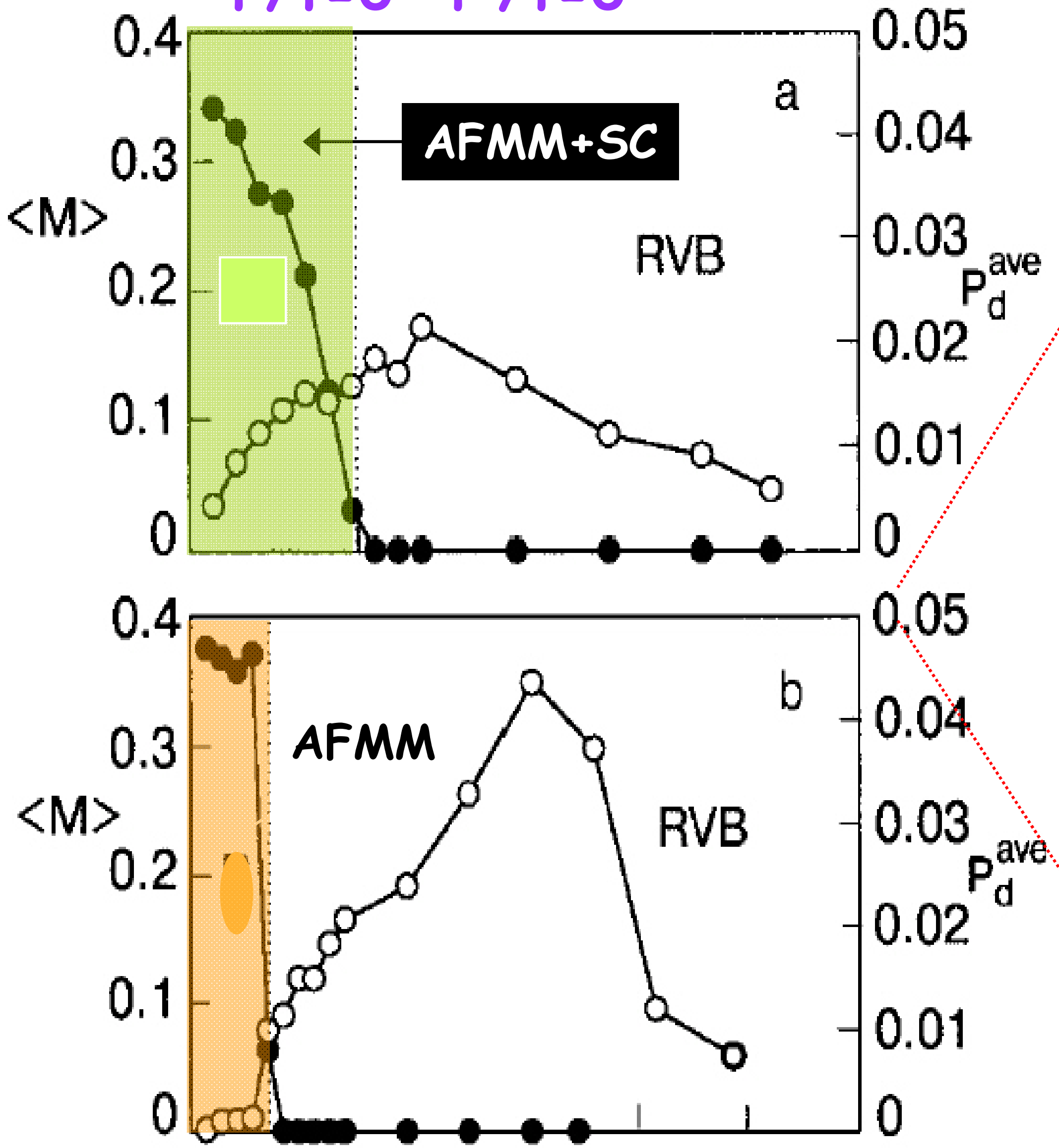


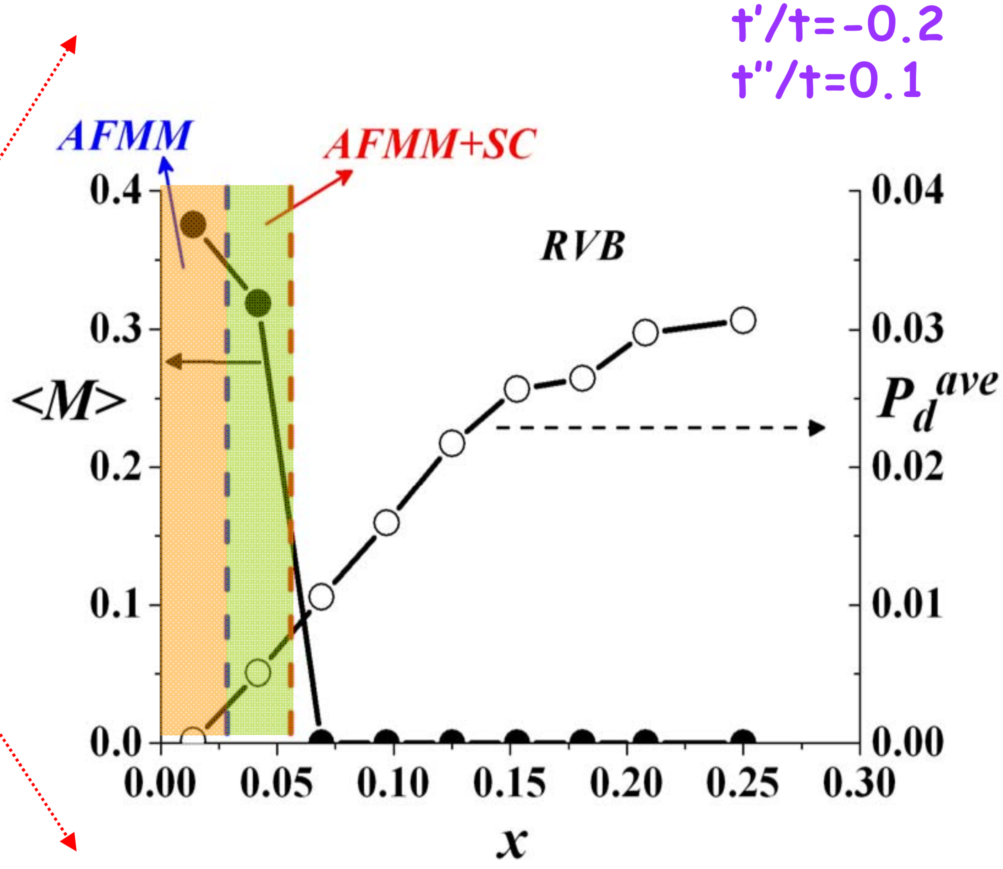
AFMM (x=0.014)
AFMM+SC (x=0.042)
SC (x=0.097)
$k_y (\pi)$
$k_x (\pi)$
Hole-Hole correlation
Pair-Pair correlation
R
—●— AFMM (x=0.014)
—●— AFMM+SC (x=0.042)
—●— RVB (x=0.097)
m_v and Δ_v
m_v and Δ_v
μ_v, t_v and t''_v
Δ_v, μ_v, t_v and t''_v

Possible Phase Diagrams for the t-J model

CT Shih et al., LTP ('05) and PRB ('04)

t'/t=0 t"/t=0

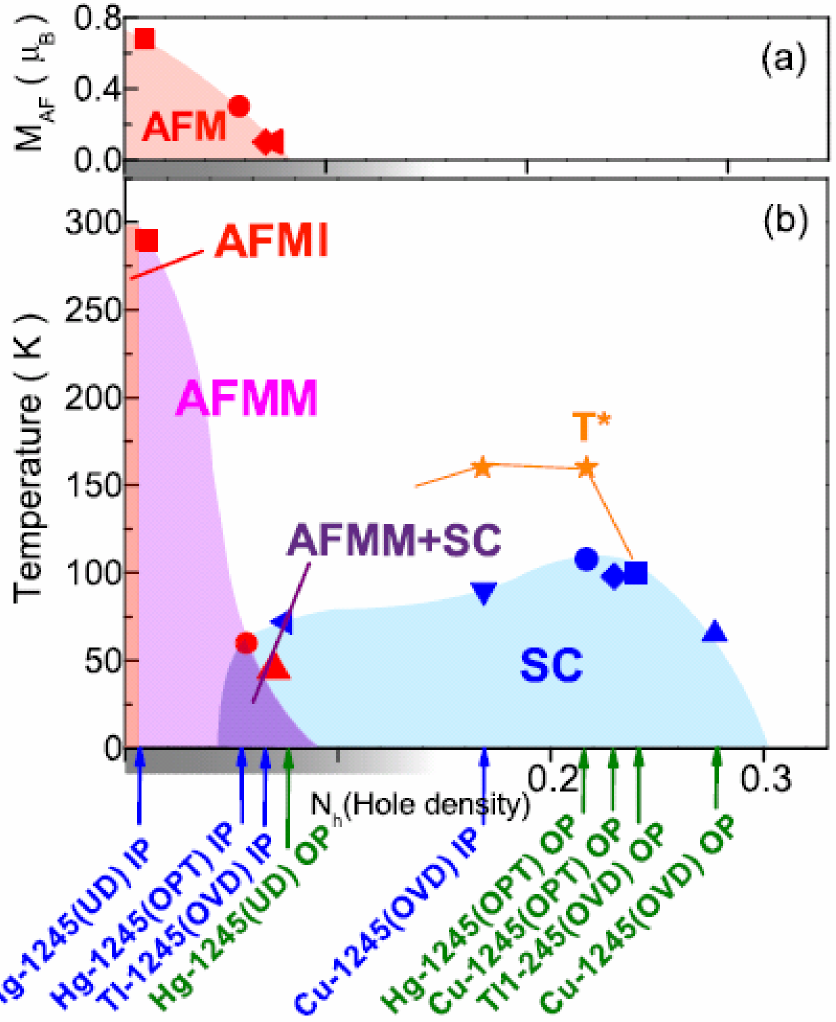




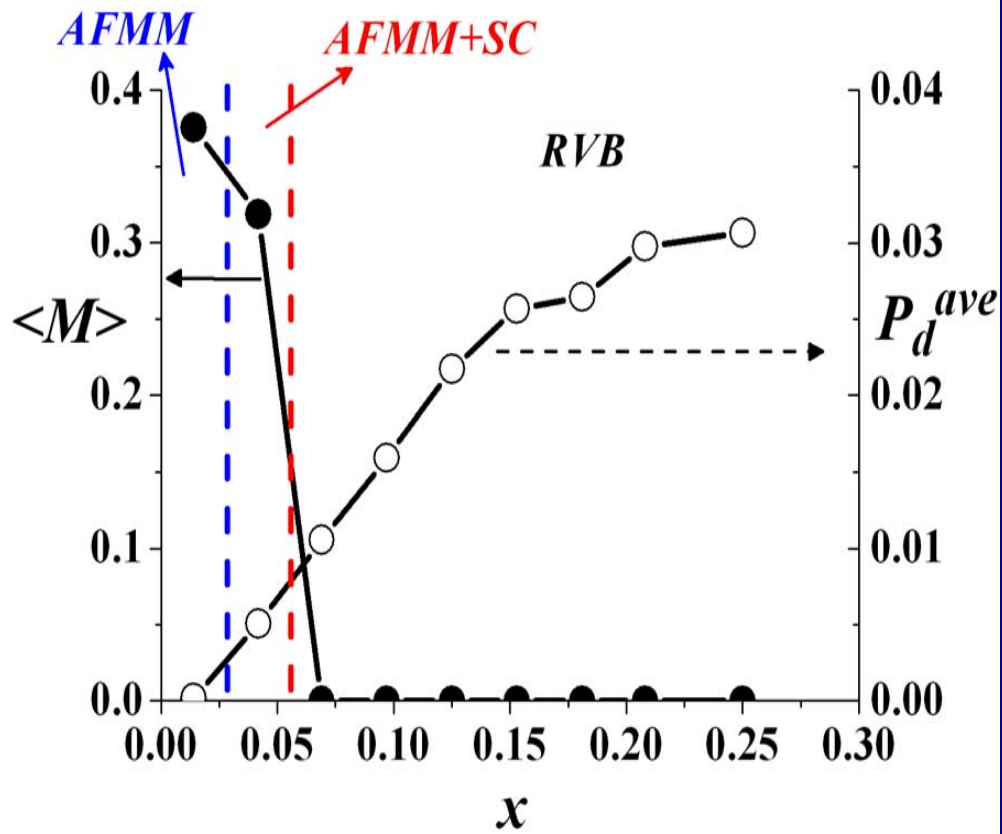
t'/t=-0.3, t"/t=0.2

Phase diagram for hole-doped systems

The "ideal" Cu-O plane

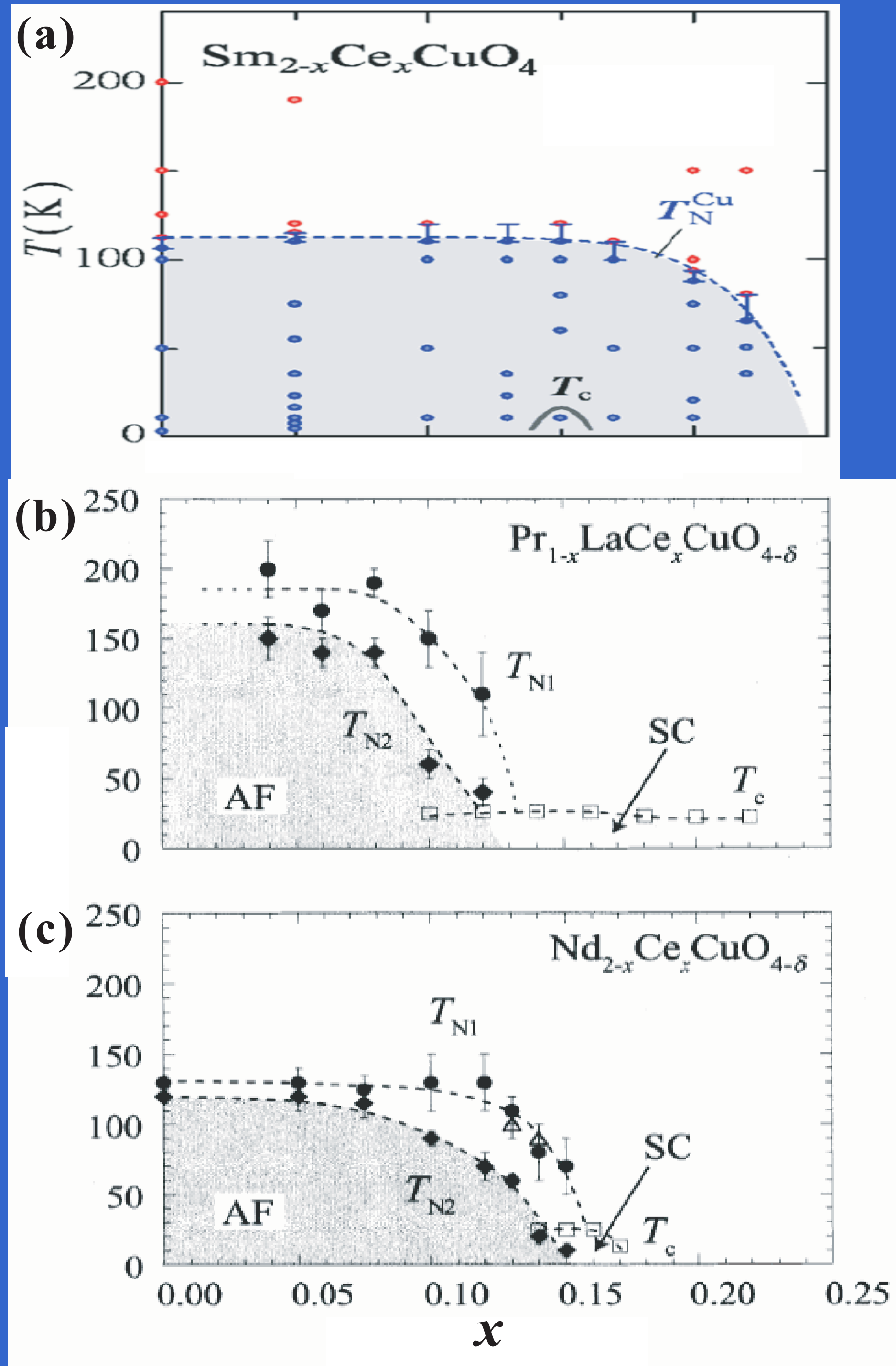


Extended t-J model, t'/t=-0.2, t''/t=0.1



H Mukuda et al., PRL ('06)

Experiments for electron-doped cuprates



M. Ikeda, thesis '06

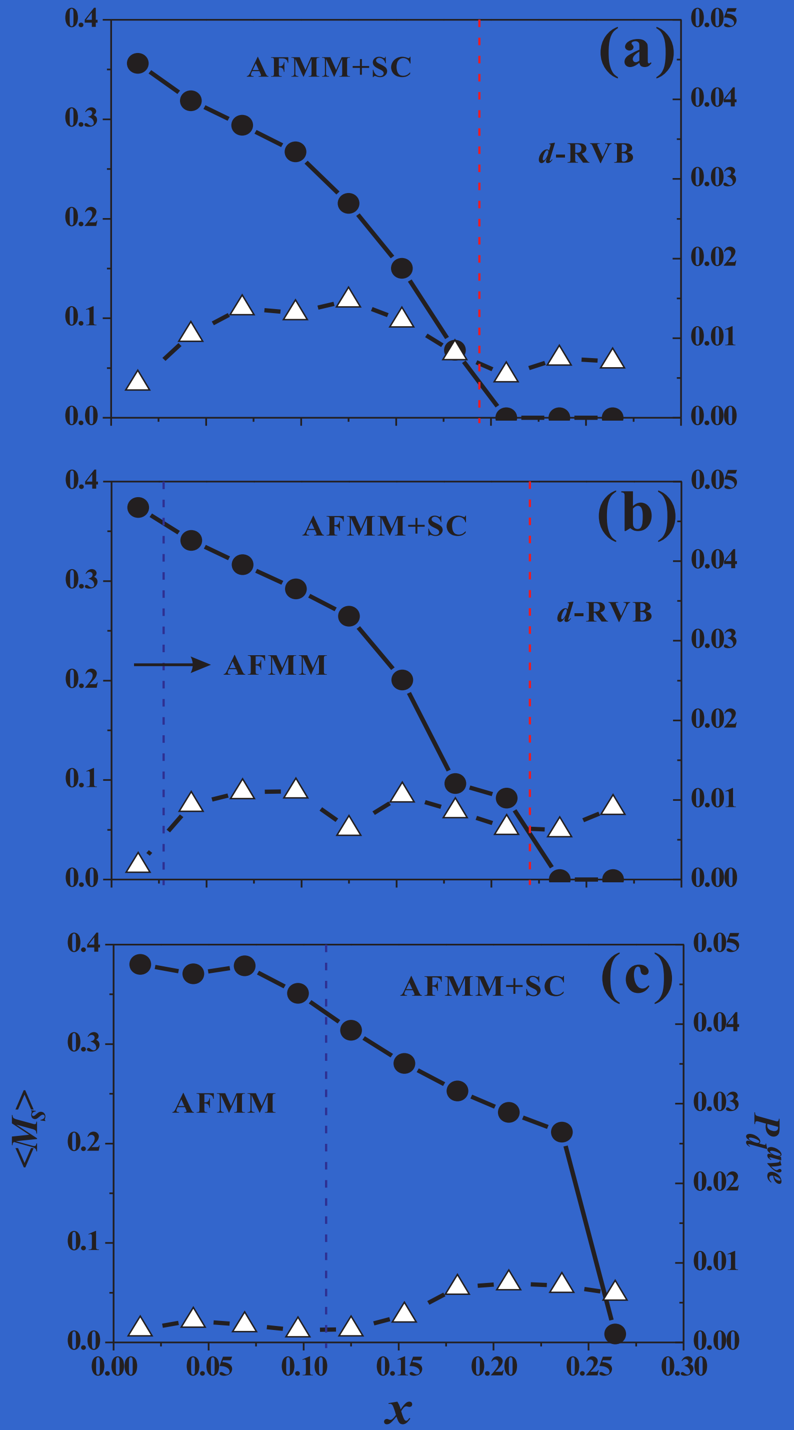
T. Kubo, Physica C '02

VMC (t',t'')

(0.1,−0.05)

(0.15,−0.1)

(0.3,−0.2)



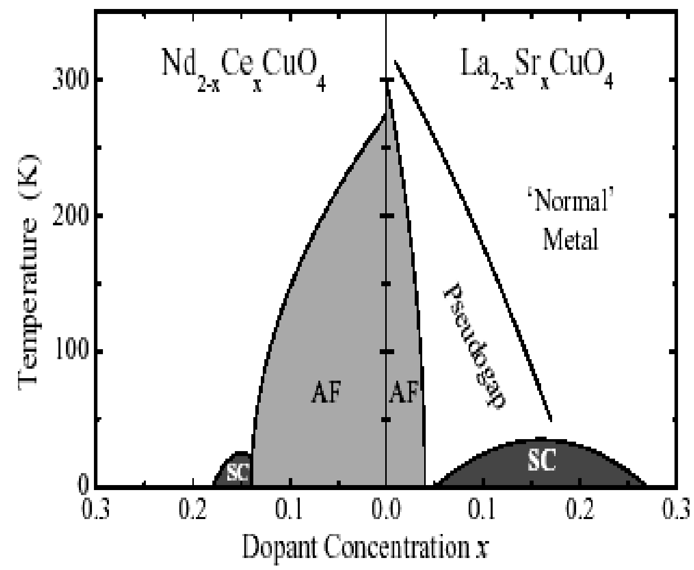


FIG. 1. Phase diagram of n and p-type superconductors.

Excitations in the SC state

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

With a fixed-number of holes, the d-RVB state becomes

$$| N_e\rangle = P_d \left(\sum_{\mathbf{q}} a_{\mathbf{q}} c^\dagger_{\mathbf{q}\uparrow} c^\dagger_{-\mathbf{q}\downarrow} \right)^{N_e/2} | 0\rangle$$

$$a_q = v_q / u_q = \frac{E_q - \xi_q}{\Delta_q}, \Delta_q = \Delta(\cos q_x - \cos q_y)$$

Quasi-particle excitation $\left|N_e + 1, k\right\rangle = \mathrm{P_d} C^+_{k,\uparrow} (\sum_q a_q C^+_{q,\uparrow} C^+_{-q,\downarrow})^{N_e/2} \left|0\right\rangle$

Excitation energies are fitted with $E_k = \sqrt{(\varepsilon_k^2 + \Delta_k^2)}$

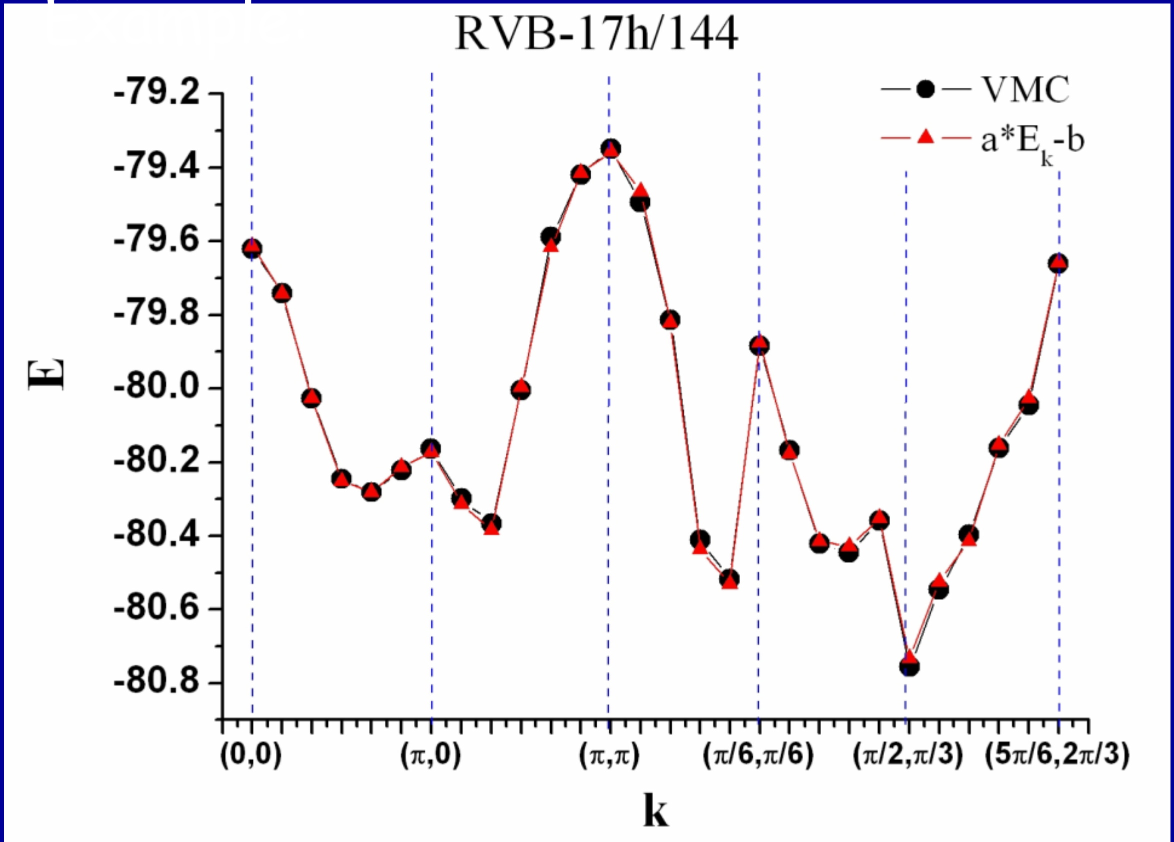
QP excitation

$$|N_e+1\rangle \equiv P_d c^\dagger_{\mathbf{k}\sigma} |\overline{N_e}\rangle$$

$$|N_e-1\rangle \equiv P_d c^\dagger_{-\mathbf{k}-\sigma} |\overline{N_e-2}\rangle \propto P_d c_{\mathbf{k}\sigma} |\overline{N_e}\rangle$$

$$\left|N_e+1,k\right\rangle = \mathrm{P_d} C^+_{k,\uparrow}\left(\sum_q a_q C^+_{q,\uparrow} C^+_{-q,\downarrow}\right)^{N_e/2} \left|0\right\rangle$$

Excitation energies are fitted with $E_k = \sqrt{(\varepsilon_k^2 + \Delta_k^2)}$

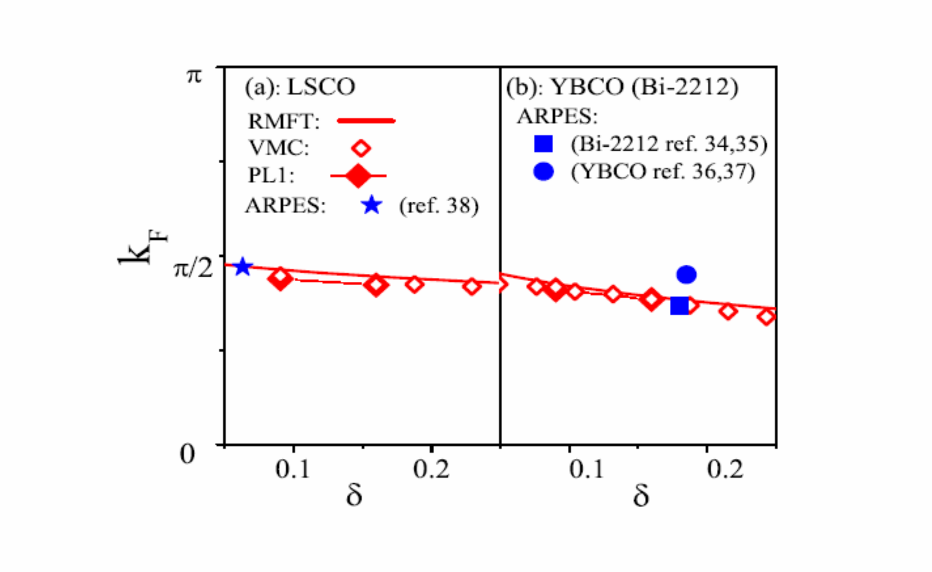


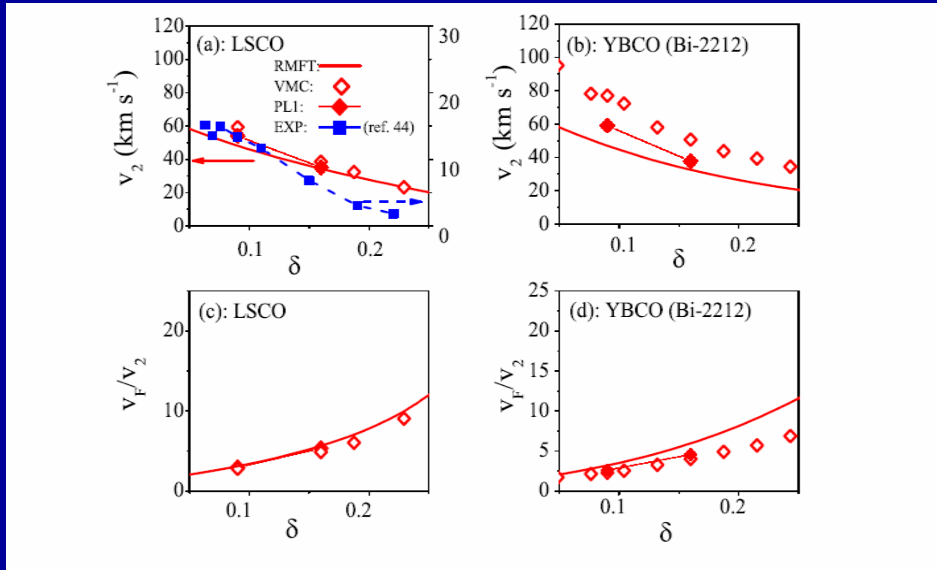
t'/t, t"/t, and μ/t are renormalized and "Fermi surface" is determined by Setting Δ=0 in the excitation energy.

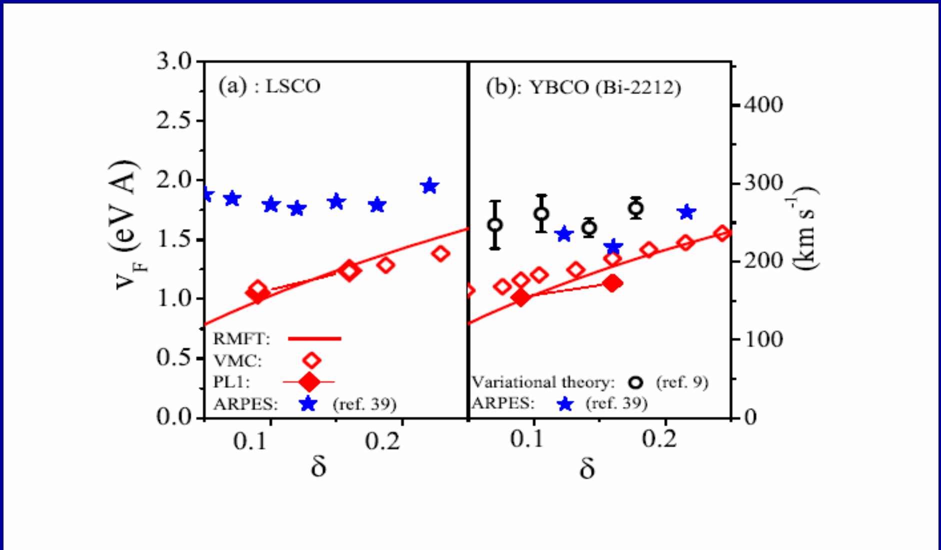
J/t=0.3, t=0.3eV

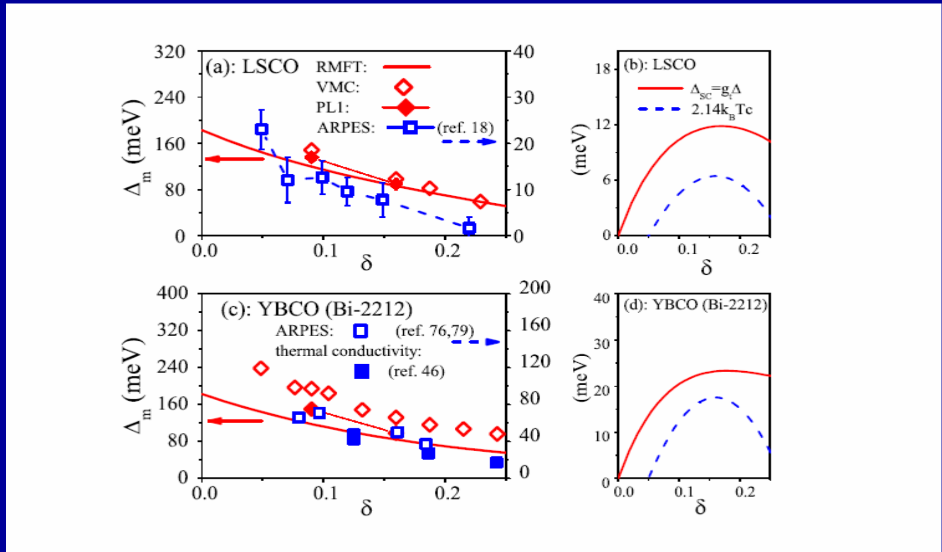
t'/t=-0.3 & t''/t=0.2 for YBCO and BSCO

but t'/t=-0.1 & t''/t=0.05 for LSCO









Our VMC overestimates the gap by a factor of 2, PRB 2006

Anomalies in the spectral weight for the low-lying excitations.

$$A(k,\omega) = \sum_m \left|\langle m | C_{k,\sigma} | 0 \rangle\right|^2 \delta(\omega + E_m - E_0) + \sum_m \left|\langle m | C^+_{k,\sigma} | 0 \rangle\right|^2 \delta(\omega - E_m + E_0)$$

$$Z^+_{\mathbf{k}\sigma} = \frac{|\langle N_e + 1 | c^\dagger_{\mathbf{k}\sigma} | N_e \rangle|^2}{\langle N_e | N_e \rangle \langle N_e + 1 | N_e + 1 \rangle}$$

$$Z^-_{\mathbf{k}\sigma} = \frac{|\langle N_e - 1 | c_{\mathbf{k}\sigma} | N_e \rangle|^2}{\langle N_e | N_e \rangle \langle N_e - 1 | N_e - 1 \rangle}$$

$$| N_e + 1 \rangle \equiv P_d c^\dagger_{\mathbf{k}\sigma} | \overline{N_e} \rangle$$

$$| N_e - 1 \rangle \equiv P_d c^\dagger_{-\mathbf{k}-\sigma} | \overline{N_e - 2} \rangle \propto P_d c_{\mathbf{k}\sigma} | \overline{N_e} \rangle$$

For ideal Fermi gas :

$Z^+_k = 1 - n^0_{k\sigma}$ $Z^-_k = n^0_{k\sigma}$

For BCS theory :

$Z^+_k = u^2_k$ $Z^-_k = v^2_k$

For Gutzwiller-projected wave functions??

Using the identities,

$$[c_{\mathbf{k}\sigma}, P_d]P_d = 0;$$
$$P_d c_{\mathbf{k}\sigma}[c^{\dagger}_{\mathbf{k}'\sigma}, P_d] = P_d[\frac{1}{N}\sum_i e^{i(\mathbf{k}'-\mathbf{k})\cdot\vec{R}_{i\sigma}} n_{i,-\sigma}]P_d$$

Exact Identity :

S. Yunoki, cond-mat/0508015,
C.P. Nave *et al.*, cond-mat/0510001

$$Z^+_{\mathbf{k}\sigma} = \frac{1+x}{2} - n_{\mathbf{k}\sigma}$$

$$Z^+_{ave} \equiv \frac{1}{N}\sum_{\mathbf{k}} Z^+_{\mathbf{k}\sigma} = x$$

No exact relation is known about

$$Z^-_{\mathbf{k}\sigma}$$

So what is $Z^{-}_{\mathbf{k}\sigma}$?

BCS theory predicts

$$Z^{-}_{\mathbf{k}\sigma} Z^{+}_{-\mathbf{k}-\sigma} = u^2_{\mathbf{k}} \; v^2_{\mathbf{k}} \propto \Delta^2_{\mathbf{k}}$$

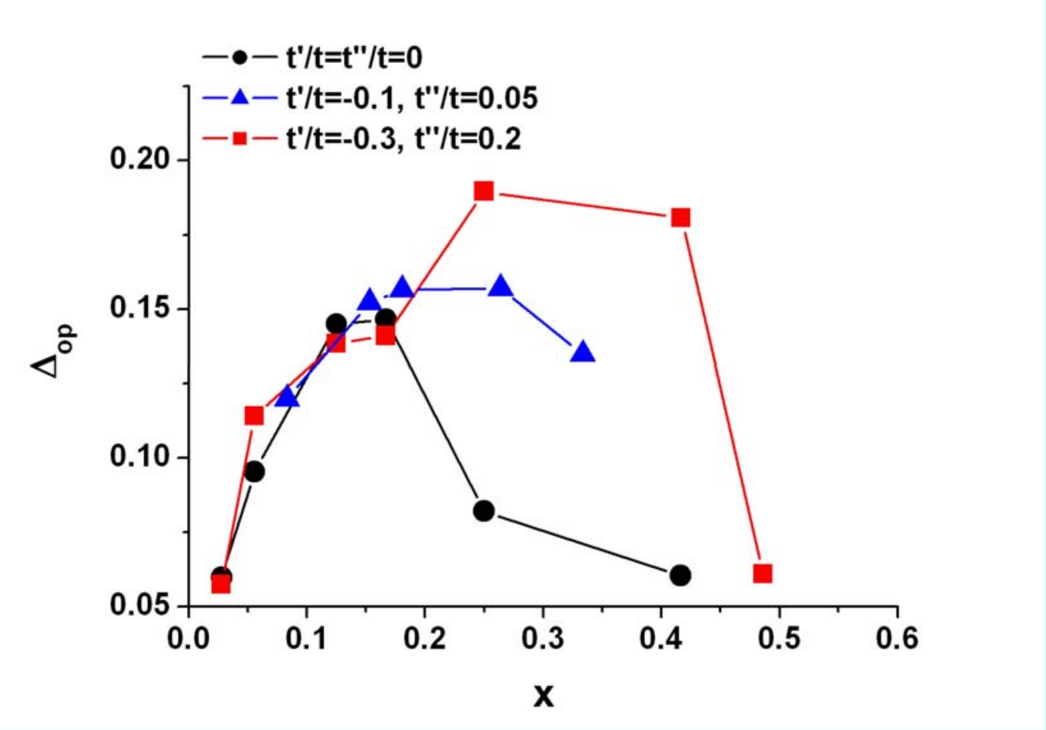
Is this relation between pairing amplitude and spectral weight also true for projected wave functions?

$$P_{\mathbf{k}} \equiv \frac{|\langle N_e \mid c^{\dagger}_{\mathbf{k}\sigma} c^{\dagger}_{-\mathbf{k}-\sigma} \mid N_e - 2\rangle|^2}{\langle N_e \mid N_e\rangle\langle N_e - 2 \mid N_e - 2\rangle} = Z^{-}_{\mathbf{k}\sigma} \cdot Z^{+}_{-\mathbf{k}-\sigma}$$

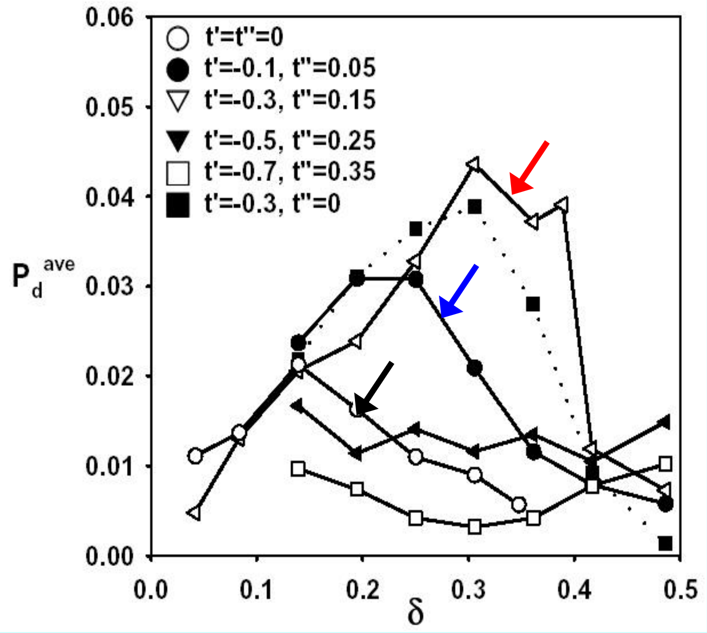
YES!!

Pairing amplitude by VMC (II):

$$\Delta_{op} = \frac{2}{N}\sum_{\mathbf{k}} |\cos(\mathbf{k}_x) - \cos(\mathbf{k}_y)| \sqrt{P_{\mathbf{k}}}$$



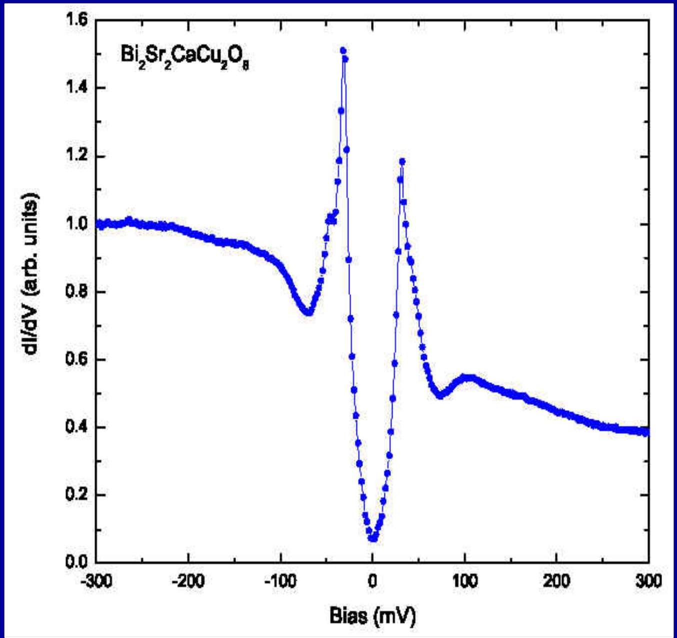
Long-range pair-pair correlation



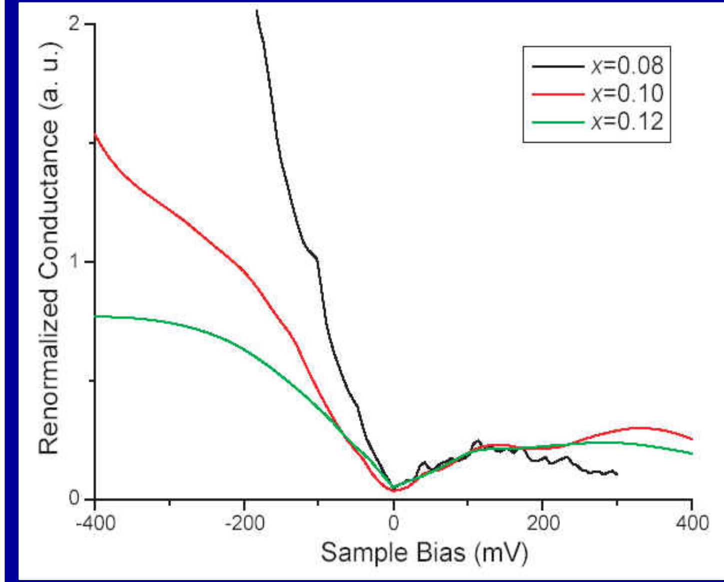
C.T. Shih *et al.*, PRL

Anomalies in STS conductance

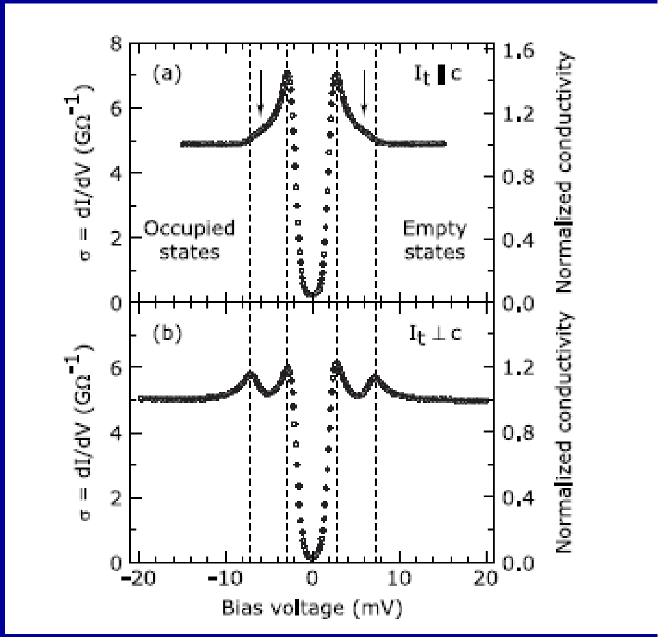
MgB$_2$



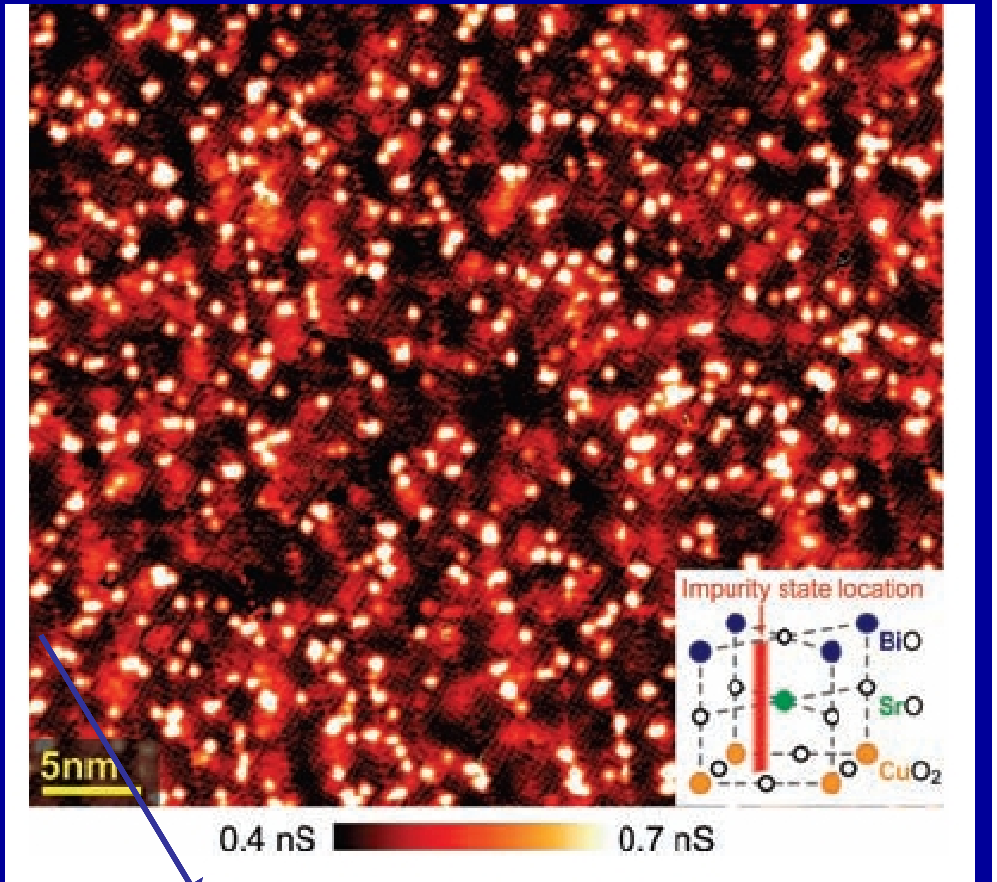
S.H. Pan *et al.*, unpublished data

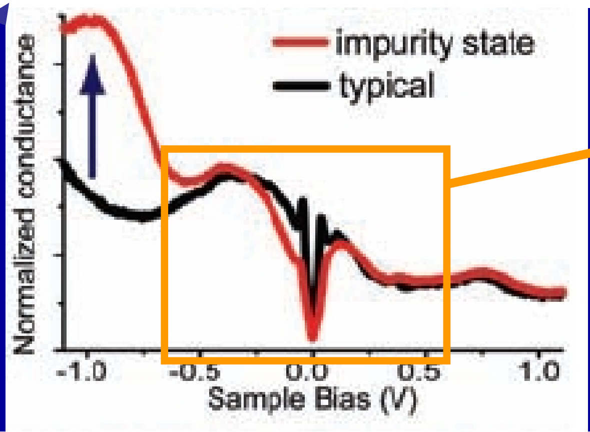


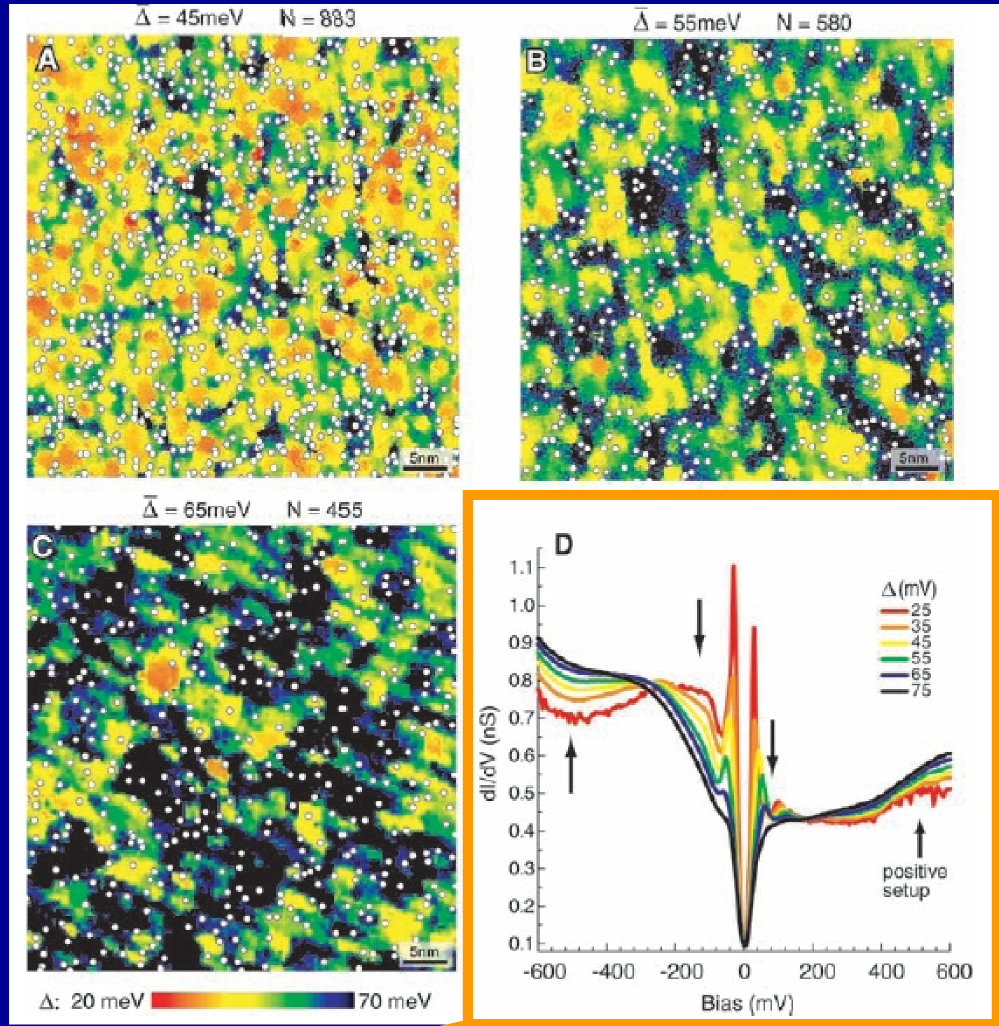
T. Hanaguri *et al.*, Nature

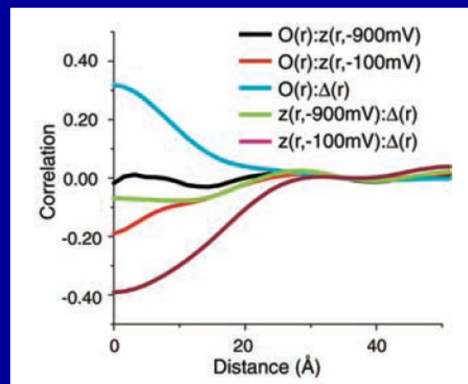


McElroy et al. Science (05)

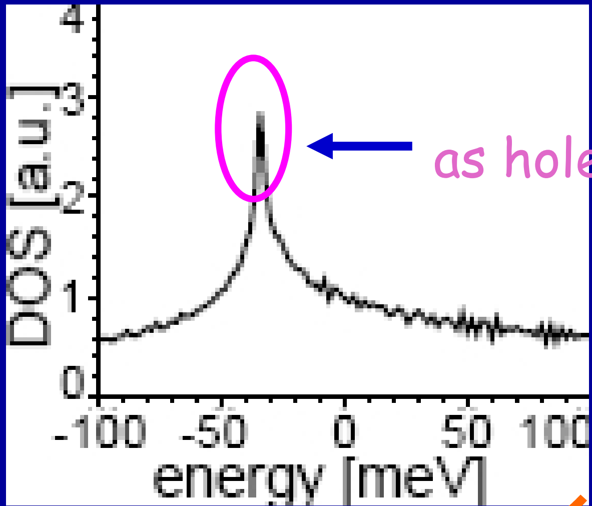






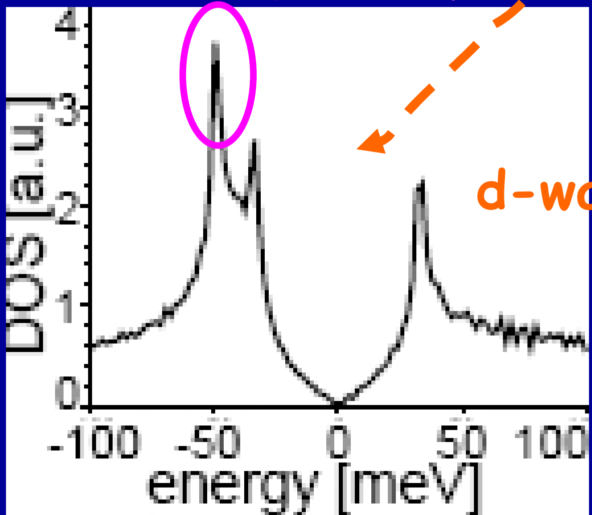


Could the asymmetry be DOS effects ?



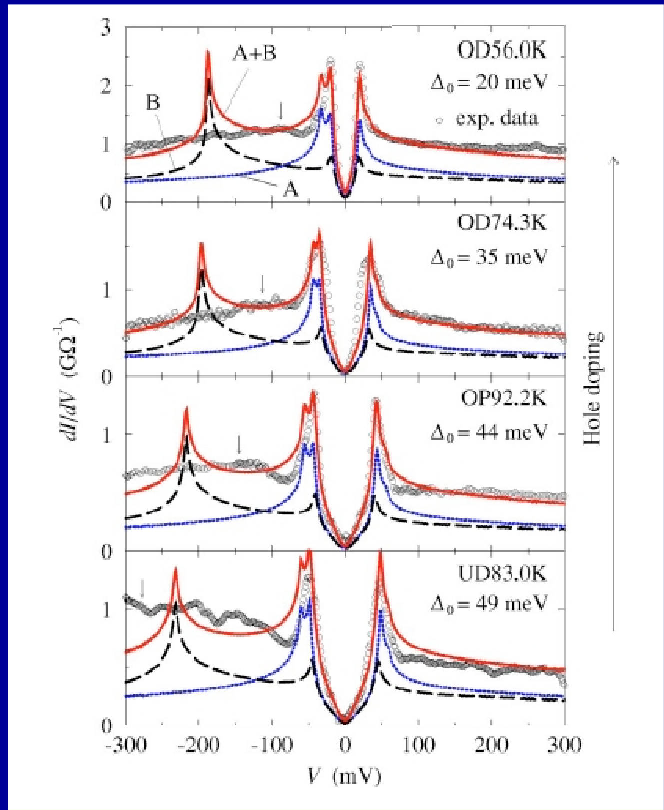
as hole doped

DOS singularity



Hoffman

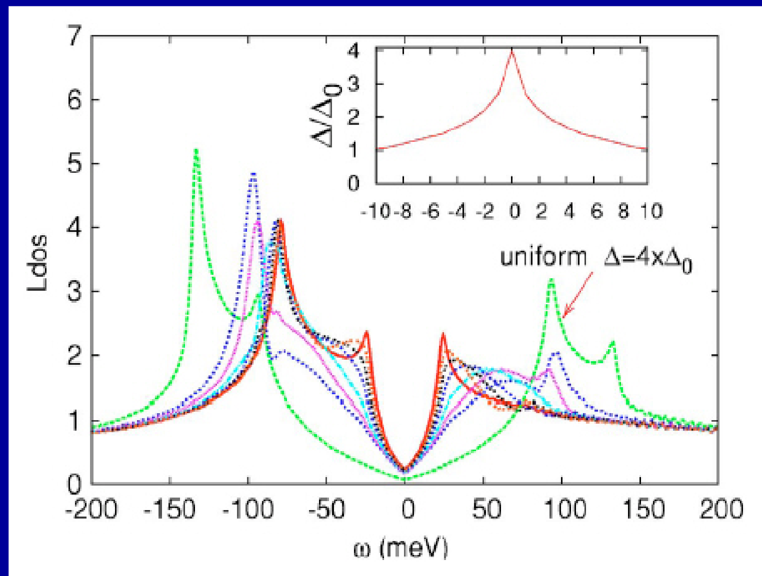
d-wave gap opened !



d-BCS with 2 bands

B. W. Hoogenboom et al. PRB ('03)

M. Cheng et al. PRB ('05)



Particle-hole asymmetry for STS conductance

Conductance is related to the spectral weight

$$A(k,\omega) = \sum_m \left| \langle m | C_{k,\sigma} | 0 \rangle \right|^2 \delta(\omega + E_m - E_0) + \sum_m \left| \langle m | C_{k,\sigma}^{+} | 0 \rangle \right|^2 \delta(\omega - E_m + E_0)$$

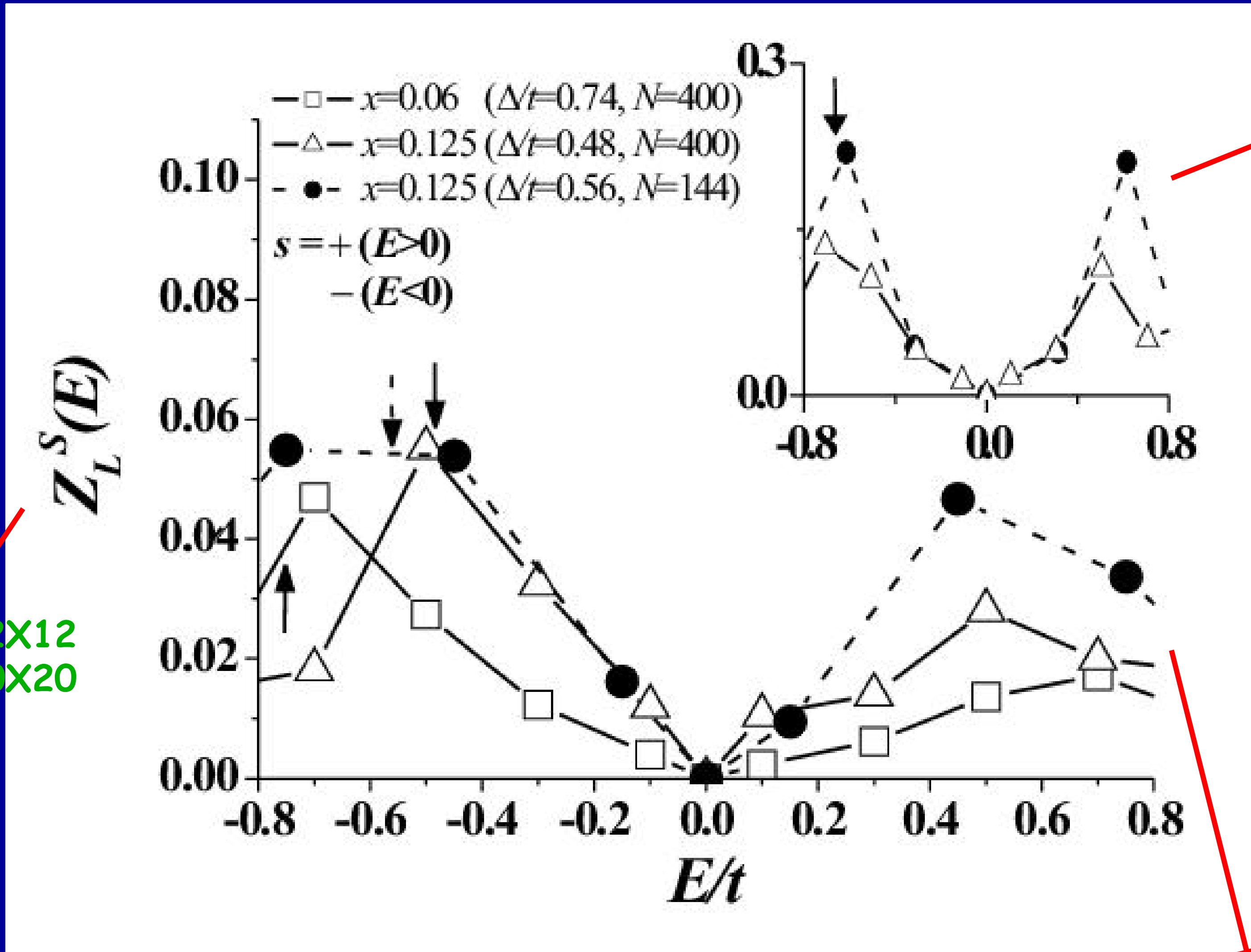
the tunneling conductance at negative bias:

$$\sum_m \left| \langle m | C_{k,\sigma} | 0 \rangle \right|^2 \delta(\omega + E_m - E_0) = \sum_k Z_k^{-} \delta(\omega - E_k + E_0)$$

For positive bias:

$$\sum_k Z_k^{+} \delta(\omega - E_k + E_0)$$

Quasi-particle contribution to the conductance ratio



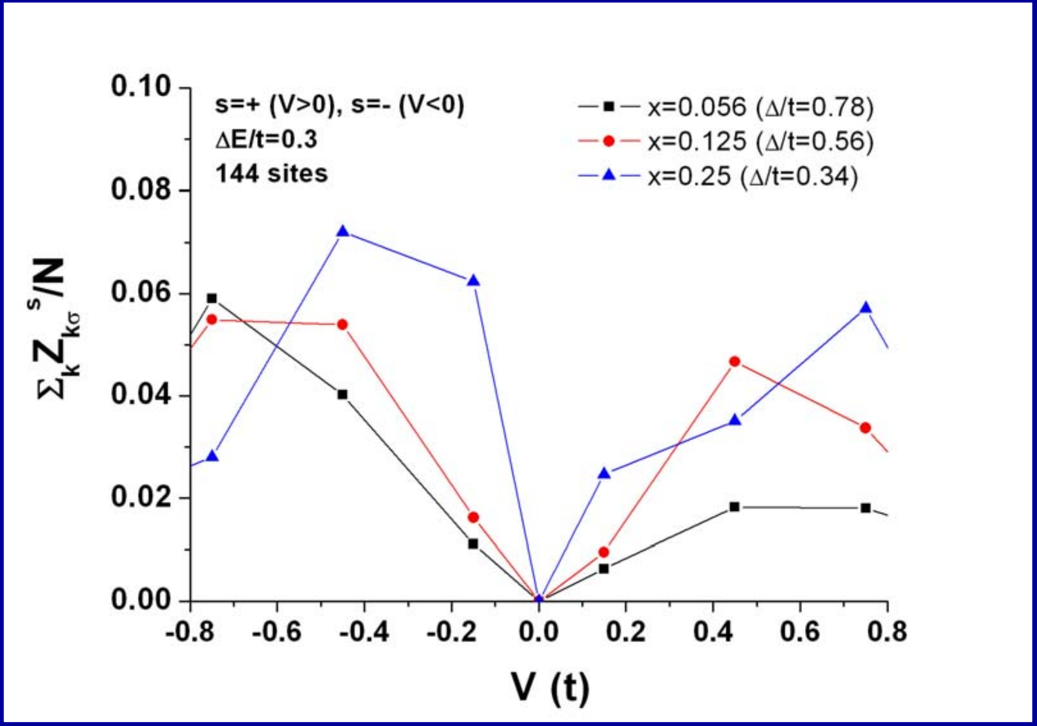
d-BCS

ΔE=0.3t for 12X12
ΔE=0.2t for 20X20

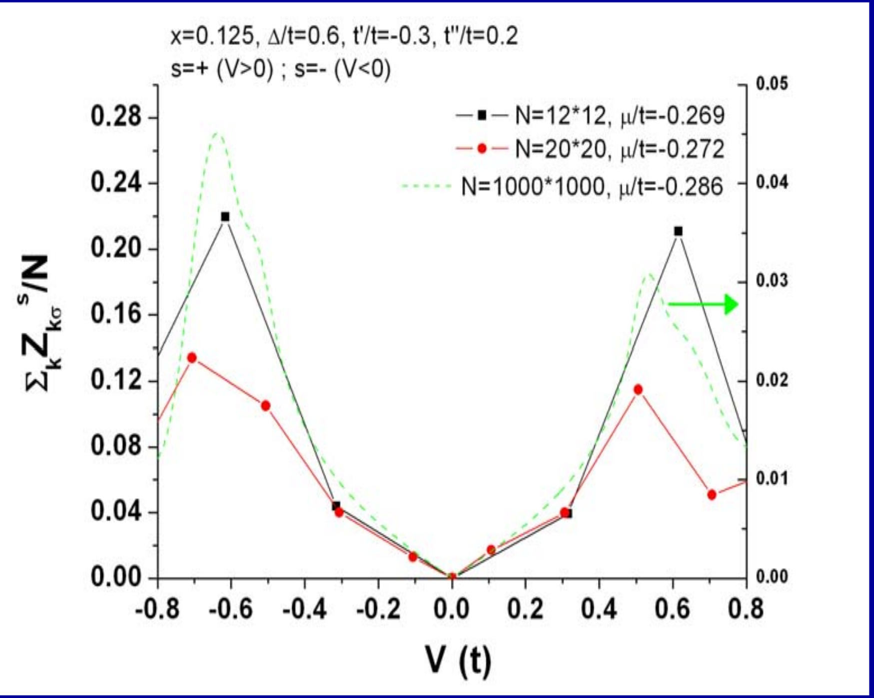
d-RVB (t'=-0.3, t''=0.2)

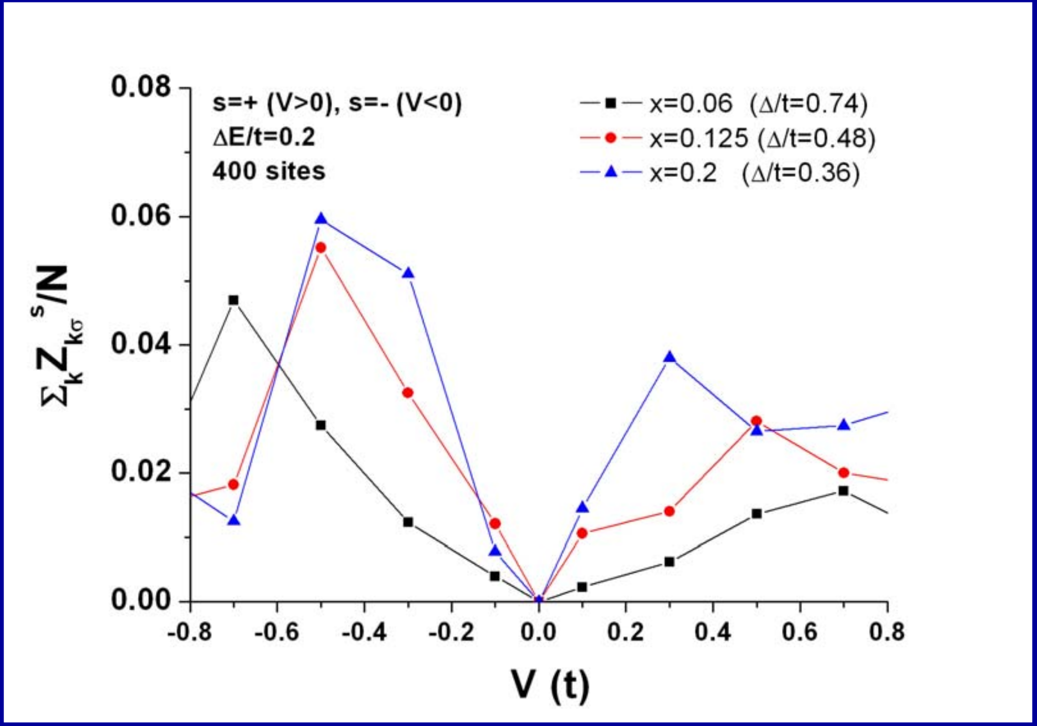
Quasi-particle contribution to the conductance ratio :

d-RVB (t'=-0.3, t''=0.2)

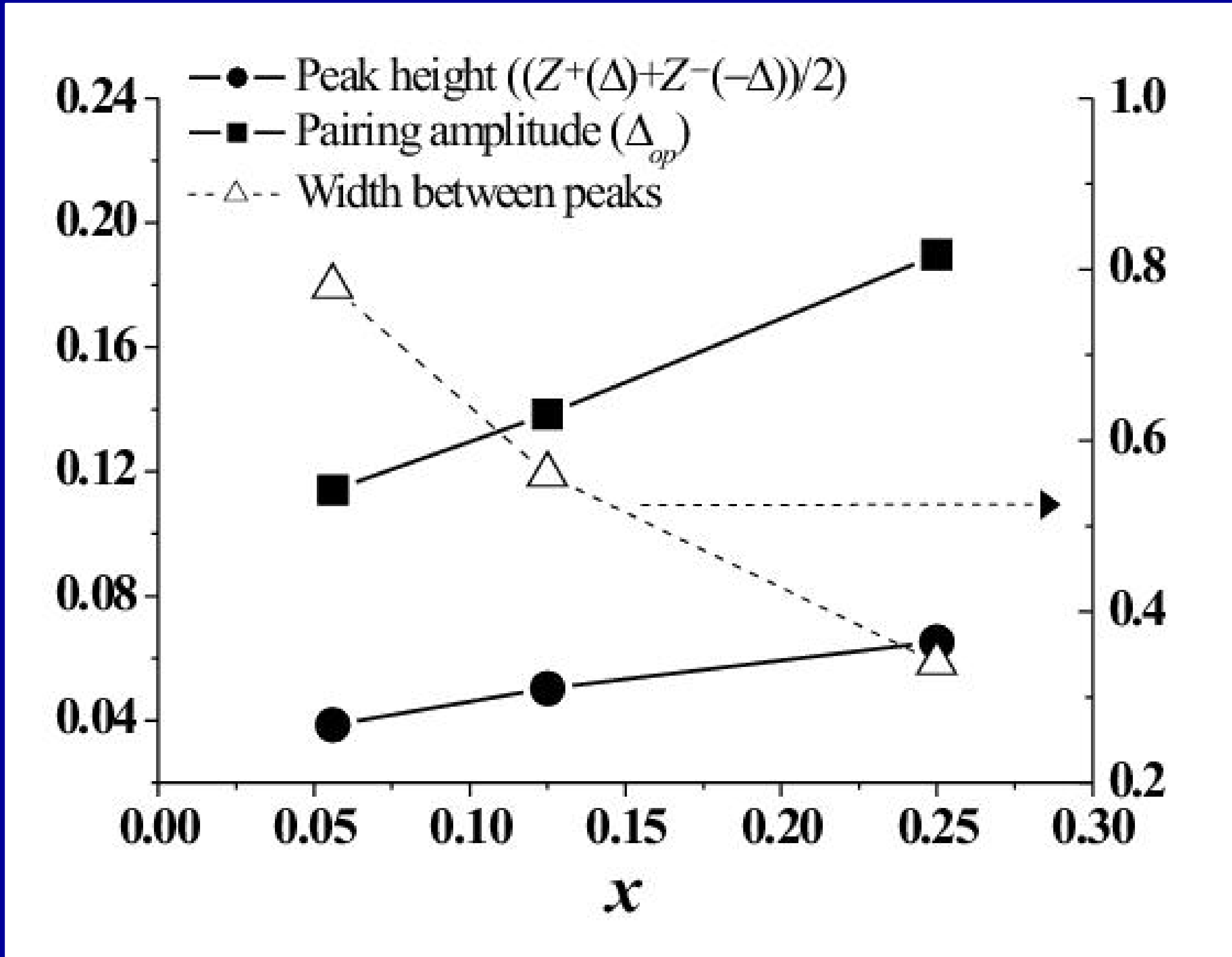


d-BCS

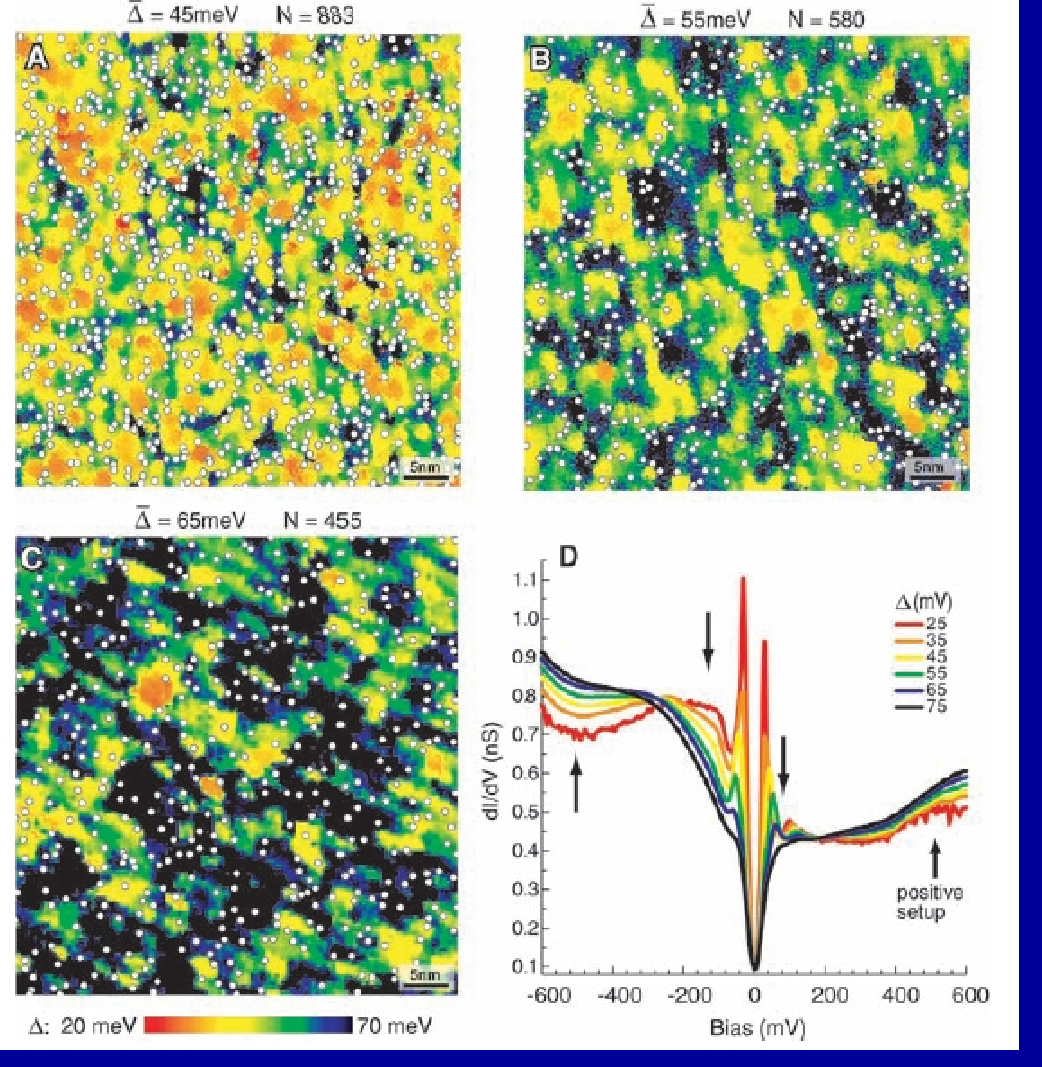




Spectral weight PEAK HEIGHTS and GAP SIZES



Why is d-wave SC so robust?



McElroy et al. Science (05)

Consider the impurity elastic scattering matrix element

$$V_{k,k'} : \langle k | C^{+}_{k,\sigma} C_{k',\sigma} \; | k' \rangle$$

For BCS theory, this is just $u_k \, u_{k'} - v_k \, v_{k'}$

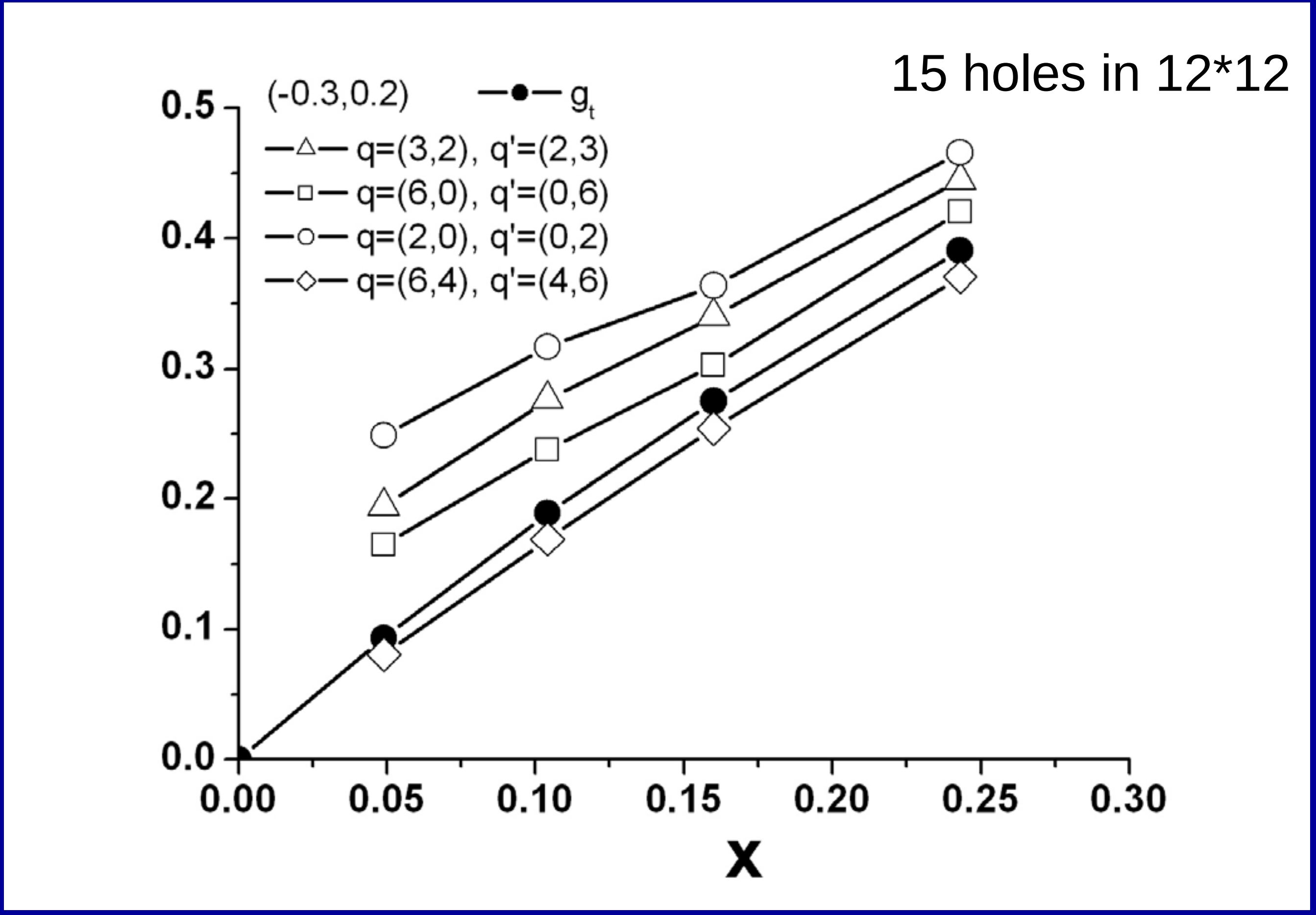
But for projected states, there is a strong renormalization

$$|N_e + 1, k\rangle \; = \mathrm{P_d} C^{+}_{k,\uparrow} \Big(\sum_q a_q C^{+}_{q,\uparrow} C^{+}_{-q,\downarrow} \Big)^{N_e/2} |0\rangle$$

$$V_{k,k'} : \langle N_e + 1, k | C^{+}_{k,\sigma} C_{k',\sigma} \; | N_e + 1, k' \rangle$$

$$V_{k,k'} : \langle N_e + 1, k | C^+_{k,\sigma} C_{k',\sigma} | N_e + 1, k' \rangle$$

$$| N_e + 1, k \rangle = P_d C^+_{k,\uparrow} \left(\sum_q a_q C^+_{q,\uparrow} C^+_{-q,\downarrow} \right)^{N_e/2} | 0 \rangle$$



$g_t = 2x/(1+x)$
Renormalized Mean-field theory ,
Garg et al,
Cond-mat/0609666

Summary

- Variational approach provides a semi-quantitative way to understand the t-J or extended t-J model by taking into account the projection rigorously.

- Based on the RVB concept, trial wave functions for the doped system have been constructed to represent the AFMM, AFMM+SC and SC phases, these phase were observed in multilayer cuprates.

- With the values of t, t’ and J in the range of experiments, the phase diagram obtained agree with cuprates below optimal doping.
- Same theory shows that the AFM is much more robust in electron-doped system.

Summary

- In addition to studying ground states, variational approach could also study excitation spectra, STM conductance asymmetry, effects of disorder (why d-wave is so robust) etc..
- Questions unanswered: stripes, competing states, ..

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