The multielectron approach to the electronic structure, normal and superconducting states of high-Tc cuprates.

Sergey G.Ovchinnikov

L.V.Kirensky Institute of Physics, Siberian Branch of Russian Academy of Science, Krasnoyarsk, Russia

In collaboration with

- V.Gavrichkov, E.Shneyder, (Krasnoyarsk)
- M.Korshunov (Krasnoyarsk-> Florida)
- Ekaterinburg team: I.Nekrasov, Z.Pchelkina (from Anisimov group)

Outline

- Generalized tight binding (GTB) and LDA+GTB approach to electrons in strongly correlated systems
- Energy dependent effective Hamiltonian. Microscopically derived t-t’-t”-J* model from ab initio multiband p-d model
- Strongly correlated electrons and spin-liquid with short AFM order
- Doping evolution of the Fermi surface and Lifshitz quantum phase transitions
- Magnetic and phonon contributions to d-pairing
- Isotope effect
- conclusions

LEHMANN REPRESENTATION: electron in strong correlated system as a superposition of Hubbard-type quasiparticles

Single electron GF $G_\sigma = \langle\langle a_{k\sigma} | a^{+}_{k\sigma} \rangle\rangle_\omega$ **can be written as**

$$G_\sigma(k,\omega) = \sum_m \left(\frac{A_m(k,\omega)}{\omega - \Omega_m^{+}} + \frac{B_m(k,\omega)}{\omega - \Omega_m^{-}} \right) \qquad (1)$$

where the QP energies are given by

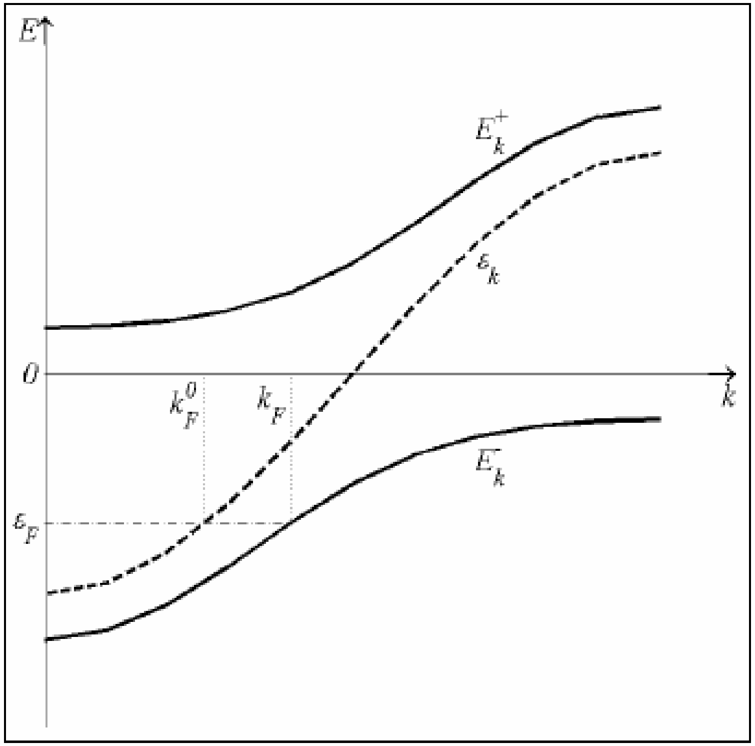
$$\Omega_m^{+} = E_m(N+1) - E_0(N) - \mu, \qquad \Omega_m^{-} = E_0(N) - E_m(N-1) - \mu,$$

and the QP spectral weight is equal to

$$A_m(k,\omega) = \left| \langle 0,N | a_{k\sigma} | m,N+1 \rangle \right|^2, \qquad B_m(k,\omega) = \left| \langle m,N-1 | a_{k\sigma} | 0,N \rangle \right|^2.$$

Strong electron correlations within the Hubbard model

$$H=\sum_{f,\sigma}\left((\varepsilon-\mu)n_{f,\sigma}+\frac{U}{2}n_{f,\sigma}n_{f,\bar{\sigma}}\right)+\sum_{f,g,\sigma}t_{fg}a^{+}_{f,\sigma}a_{g,\sigma}. \qquad n_{f,\sigma}=a^{+}_{f,\sigma}a_{f,\sigma},\ \bar{\sigma}\equiv-\sigma.$$



Hubbard-I decoupling [***J.C. Hubbard****, Proc. Roy. Soc. A 276, 328 (1963)*]:

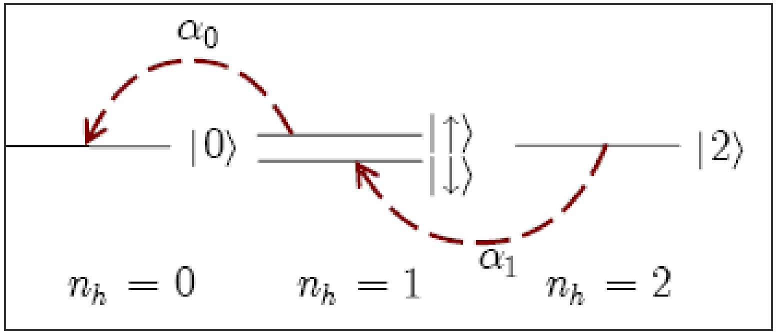
$$\langle\langle a_{f+h,\sigma}n_{f,\bar{\sigma}}\,|\,a^{+}_{g,\sigma}\rangle\rangle\rightarrow\langle n_{f,\bar{\sigma}}\rangle\langle\langle a_{f+h,\sigma}\,|\,a^{+}_{g,\sigma}\rangle\rangle$$

Basis intracell states for the Hubbard model:

$|0\rangle$ - zero-particle vacuum,

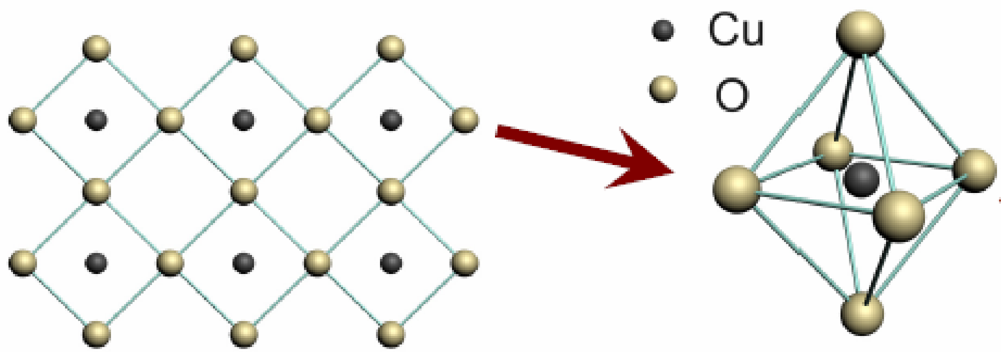
$|\sigma\rangle=a^{+}_{f\sigma}|0\rangle$ - one-particle state with spin σ,

$|2\rangle=a^{+}_{f\sigma}a^{+}_{f\bar{\sigma}}|0\rangle$ - two-particle state.

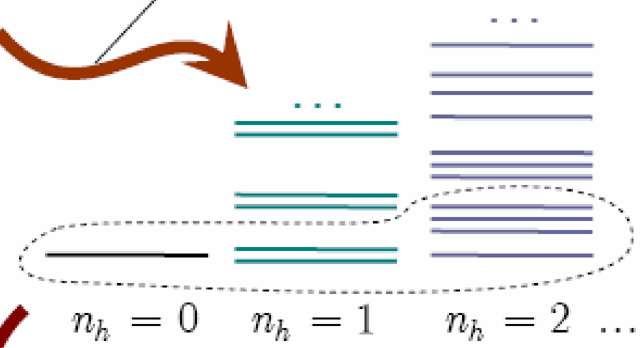


Hubbard X-operators: $X^{pq}_{f\sigma}=|p\rangle\langle q|$, $[X^{pq}_{f},X^{mn}_{g}]_{\pm}=\delta_{fg}\left(\delta_{qm}X^{pn}_{f}\pm\delta_{pn}X^{mq}_{f}\right)$

The GTB method consists of 3 steps:



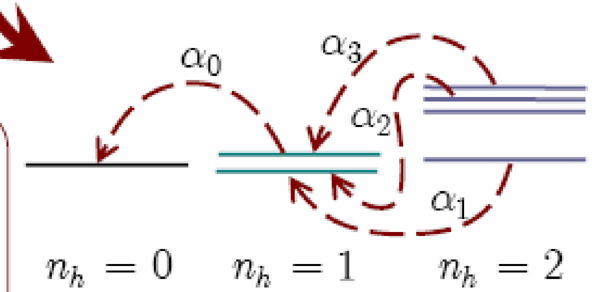
I. Exact diagonalization of $H_c(i) \rightarrow |p\rangle = |m, n_h\rangle,\ \varepsilon_p$

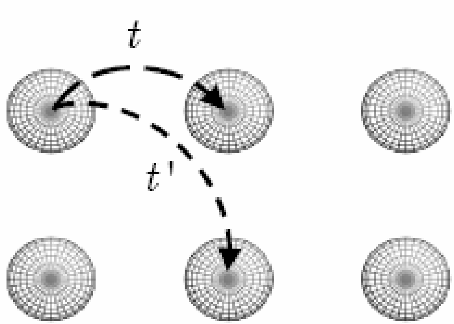


II. The intracell X-operators are constructed:

$$X_f^n \leftrightarrow X_f^{p,q} \equiv |p\rangle\langle q| = |m, n_h\rangle\langle m', n_h'|$$

$$a_{f\lambda\sigma} = \sum_n \gamma_{\lambda\sigma}(n) X_f^n$$





III. Hamiltonian in the X-representation:

$$H = \sum_{f,p} (\varepsilon_p - N\mu) X_f^{pp} + \sum_{f \neq g} \sum_{n,n'} t_{fg}^{nn'} X_f^{n\dagger} X_g^{n'}$$

Dyson equation in the X-method

Val'kov, Ovchinnikov 2001

$$a_{k\lambda} = \sum_m \gamma_\lambda(m) X_k^m \qquad X_k^m \equiv X_k^{p,q}$$

Single-electron GF: $$G_{\lambda\lambda'}(k,\omega_n) = \sum_{m,m'} \gamma_\lambda(m)\gamma_{\lambda'}(m')D^{mm'}(k,\omega_n)$$

$$D^{mm'}(k,\omega_n) = \left\langle\left\langle X_k^m \middle| X_k^{m'} \right\rangle\right\rangle_{\omega_n}$$

Dyson equation:

$$\hat{D}(k,\omega_n) = \left[\hat{G}_0^{-1}(\omega_n) - \hat{P}(k,\omega_n)t_k + \hat{\Sigma}(k,\omega_n)\right]^{-1}\hat{P}(k,\omega_n)$$

local propagator

hopping

self-energy

strength operator

Strength operator $\hat{P}(k,\omega_n)$ results from X-operators algebra
(similar to spin algebra → Baryakhtar, Yablonsky, Krivoruchko, 1983)
Renormalization of the spectral weight (oscillator strength) due to $\hat{P}(k,\omega_n)$

"Hubbard I" approximation:

$$\hat{\Sigma} = 0, \quad P^{mm'} \to F(m)\delta_{mm'}, \quad G_0^{mm'}(\omega_n) = \delta_{mm'} / \left\{i\omega_n - \left(\varepsilon_p - \varepsilon_q\right)\right\},$$

$$F(m) = \langle X^{pp}\rangle + \langle X^{qq}\rangle, \quad m = m(p,q)$$

Multiband p-d model

[***Yu.B. Gaididei and V.M. Loktev***, *Phys.Stat.Sol.B147, 307 (1988)*]

$$H_{pd} = \sum_{f,\lambda,\sigma} (\varepsilon_\lambda - \mu) n_{f\lambda\sigma} + \sum_{f\neq g} \sum_{\lambda,\lambda',\sigma} T_{fg}^{\lambda\lambda'} c_{f\lambda\sigma}^{+} c_{f\lambda'\sigma} + \frac{1}{2} \sum_{f,g,\lambda,\lambda'} \sum_{\sigma_1,\sigma_2,\sigma_3,\sigma_4} V_{fg}^{\lambda\lambda'} c_{f\lambda\sigma_1}^{+} c_{f\lambda\sigma_3} c_{g\lambda'\sigma_2}^{+} c_{g\lambda'\sigma_4}$$

where $\lambda = \left\{ d_{x^2-y^2}, d_{z^2} \equiv d_{3z^2-r^2}, p_x, p_y, p_z \right\}$,

$$T_{fg}^{\lambda\lambda'} = \left\{ t_{pd}, d_x \leftrightarrow p_{x,y}; t_{pd}/\sqrt{3}, d_z \leftrightarrow p_{x,y}; t'_{pd}, d_z \leftrightarrow p_z, t_{pp}, p_x \leftrightarrow p_y; t'_{pp}, p_{x,y} \leftrightarrow p_z \right\}$$

$$V_{fg}^{\lambda\lambda'} = \left\{ U_d, U_p, V_p, V_p, V_{pd}, J_p, J_d \right\}.$$

3-band p-d model:

[***V.J. Emery***, *PRL 58, 2794 (1987)*, ***C.M. Varma et al.***, *Solid State Commun. 62, 681 (1987)*]

$Cu(d_{x^2-y^2})$,

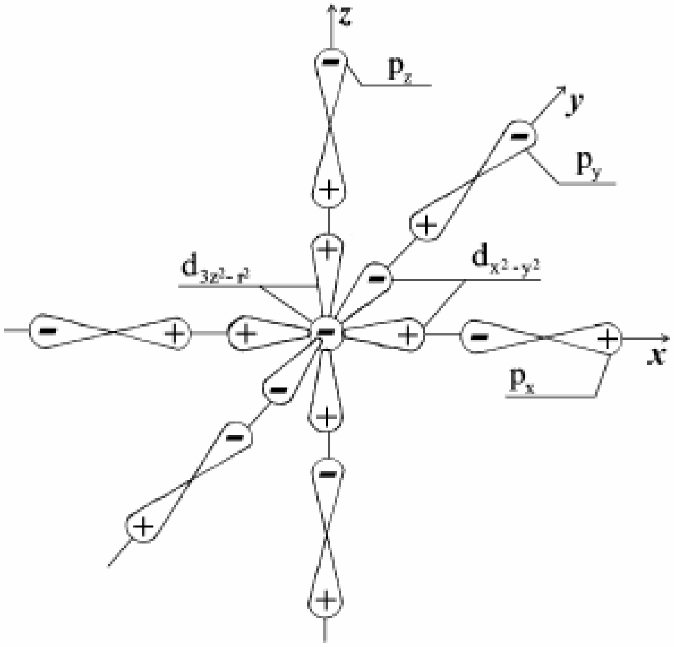
planar $O(p_x, p_y)$.

Multiband p-d model:

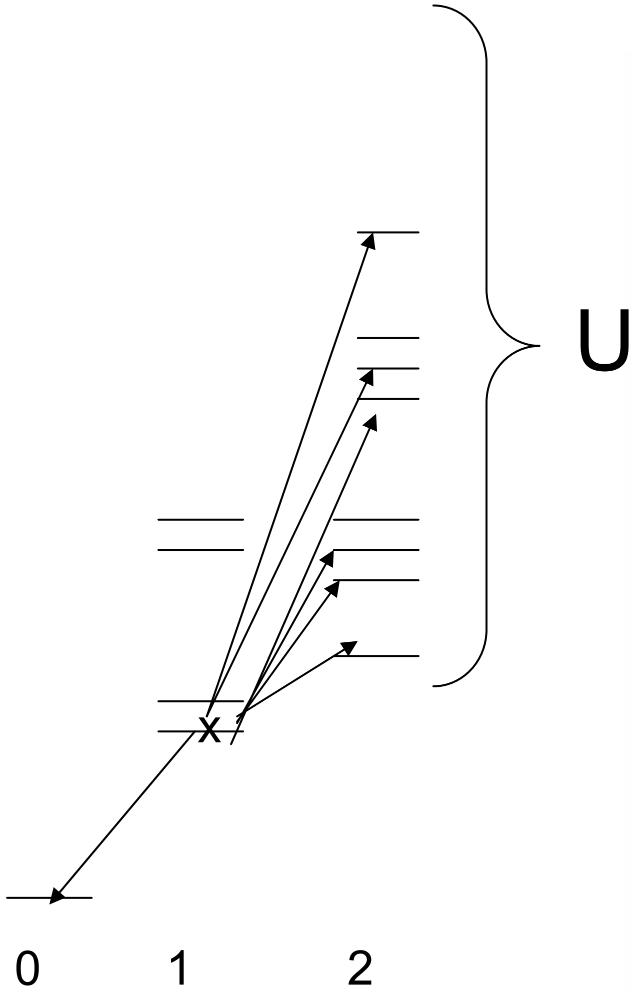
$Cu(d_{x^2-y^2}, d_{3z^2-r^2})$,

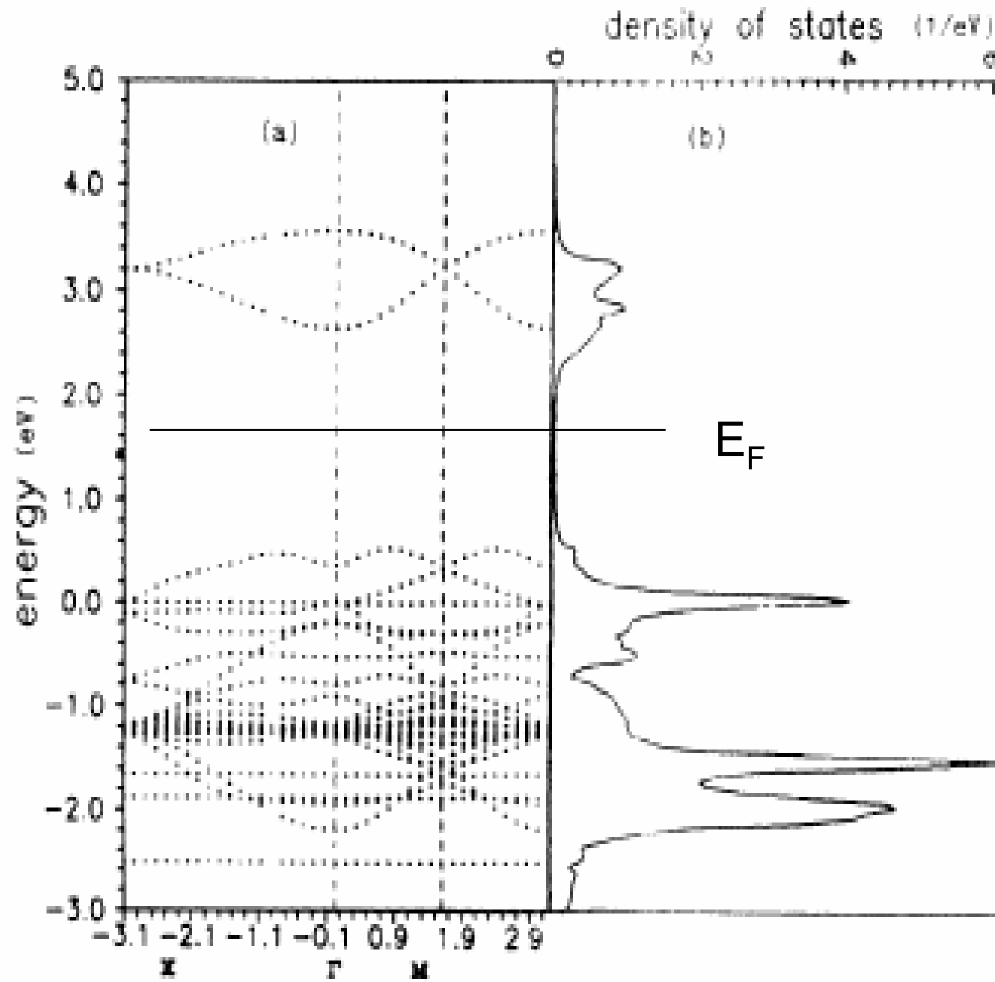
planar $O(p_x, p_y)$,

apical $O(p_z)$.



Band structure and density of states of undoped antiferromagnetic La2CuO4 at the energy scale E~U (Ovchinnikov, PRB49, 9891,1994)





Band structure of undoped cuprates

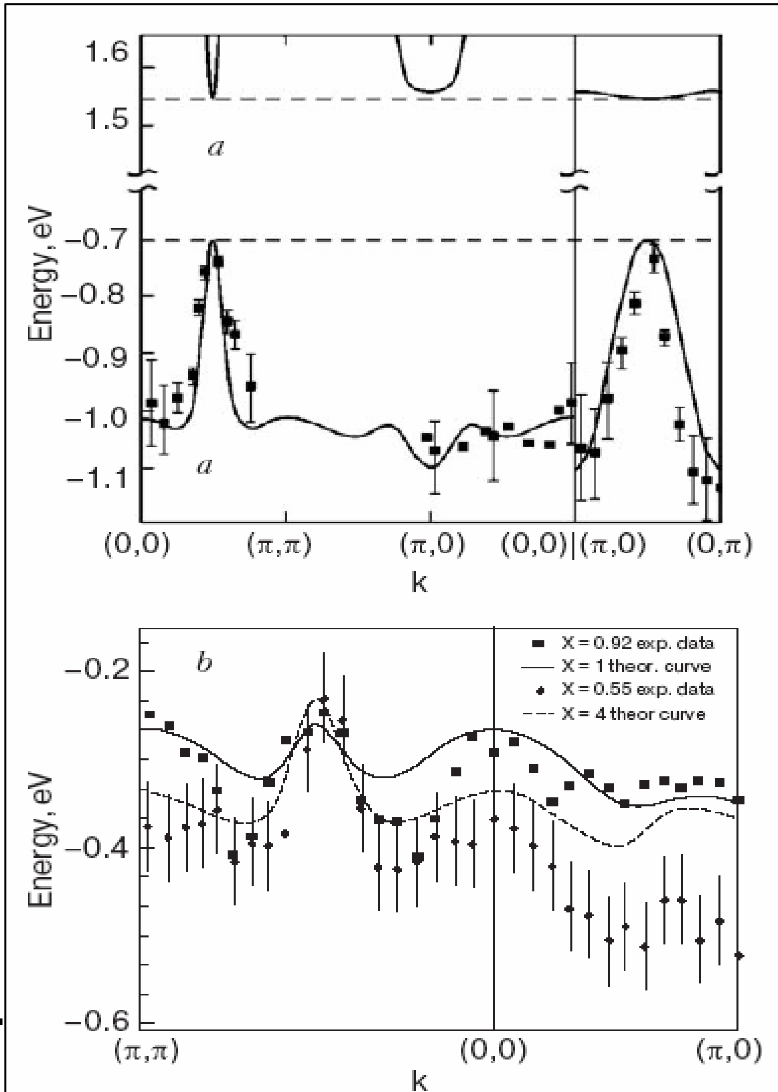
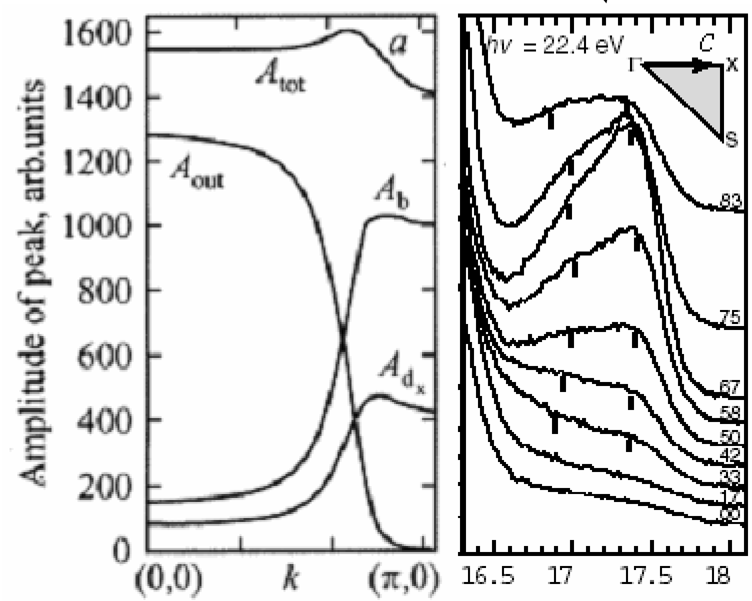


Fig. 2. The quasiparticle dispersion for the top of the valence band in $Sr_2CuO_2Cl_2$ [8] (*a*) and in $Bi_2Sr_2Ca_{1-x}Y_xCu_2O_{8+y}$ [23] (*b*) and its comparison to the ARPES data.

Experimental data from ARPES measurements

B.O. Wells et al. Phys. Rev. Lett. 74, 964 (1995) – left, C. Kim et al., Phys. Rev. Lett. 80, 4245 (1998) - right



V. … 0)

V.A. Gavrichkov et al., Phys. Rev. B 64, 235124 (2001)

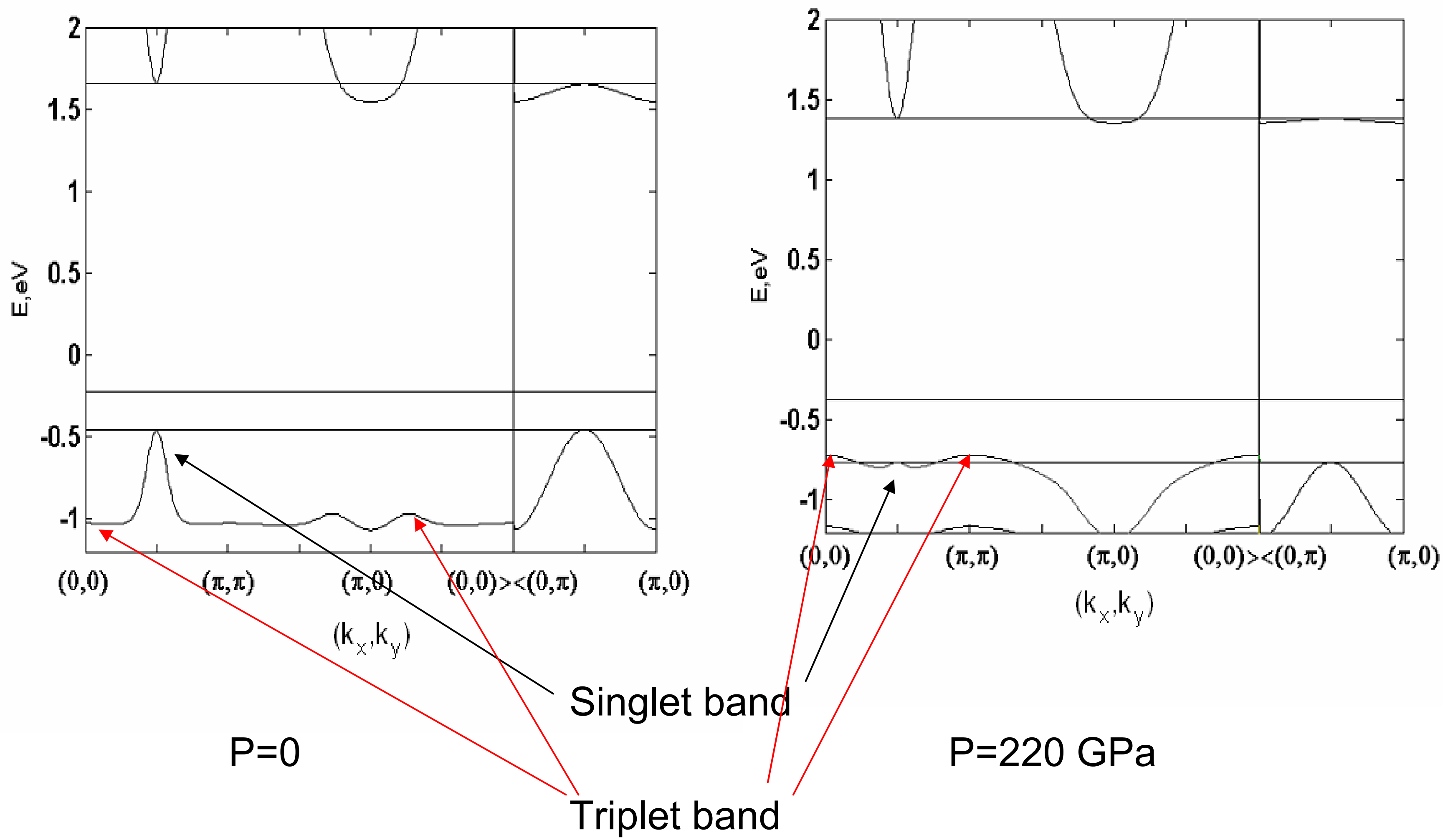
C.Janowitz, V.A.Gavrichkov etal, JETP Lett.80,692 (2004)

Hybrid LDA+GTB scheme without fitting parameters (in collaboration with prof.V.I.Anisimov group, Ekaterinburg, (Korshunov etal, PRB2005))

- Projection of LDA band structure and construction the Wannier functions for p-d –model
- *Ab initio* calculation of p-d –model parameters
- Quasiparticle band structure GTB calculations in the strongly correlated regime with *ab initio parameters*
- Comparison of La_2CuO_4 and Nd_2CuO_4 band structure with fitting and LDA+GTB parameters

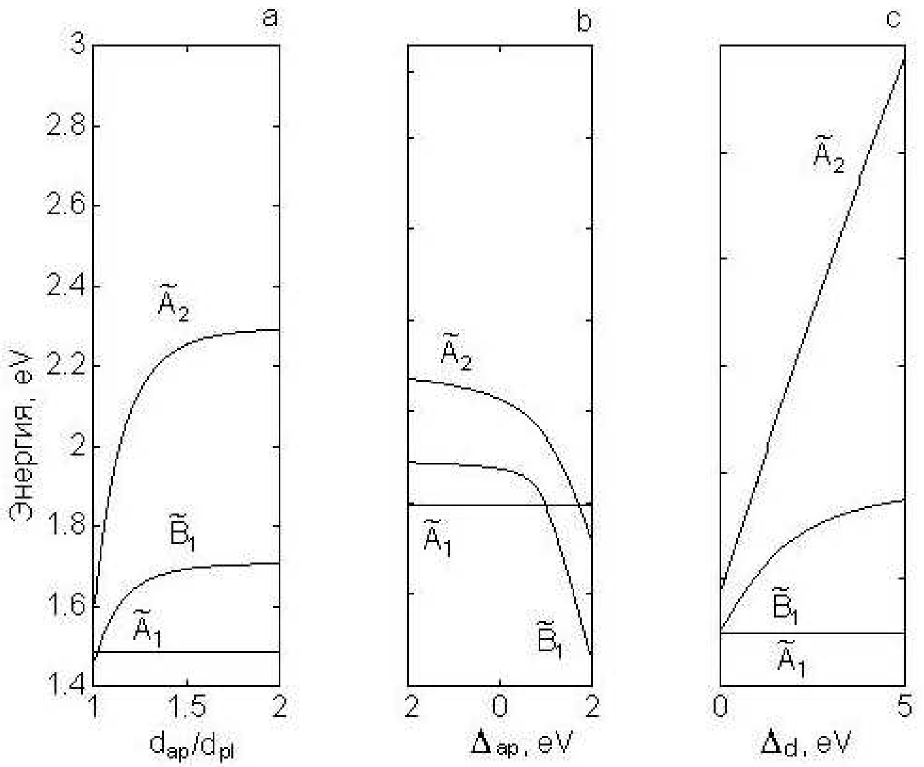
Effect of uniaxial pressure on the bands in La_2CuO_4

(*Gavrichkov, Ovchinnikov, Ul'm, Sol.st.phys.2007*)



Exact diagonalization of CuO6 cluster, two hole states

Gavrichkov etal, JETP 2000



The dependence of the lowest in energy singlet 1*A*1, 1*A*2 and triplet 3*B*1 terms of the *CuO*6 cluster on the following parameters: a) the ratio of the (*Cu*-apical O)/(*Cu*-plane O) distances with =2 eV, =0.5 eV; b) the oxygen crystal field splitting, Δ*ap* with *dap*/*dpl*=1.2, Δ*d*=2 eV; c) the copper crystal field splitting Δ*d* with *dap*/*dpl*=1.2, Δ*ap*=0.5 eV.

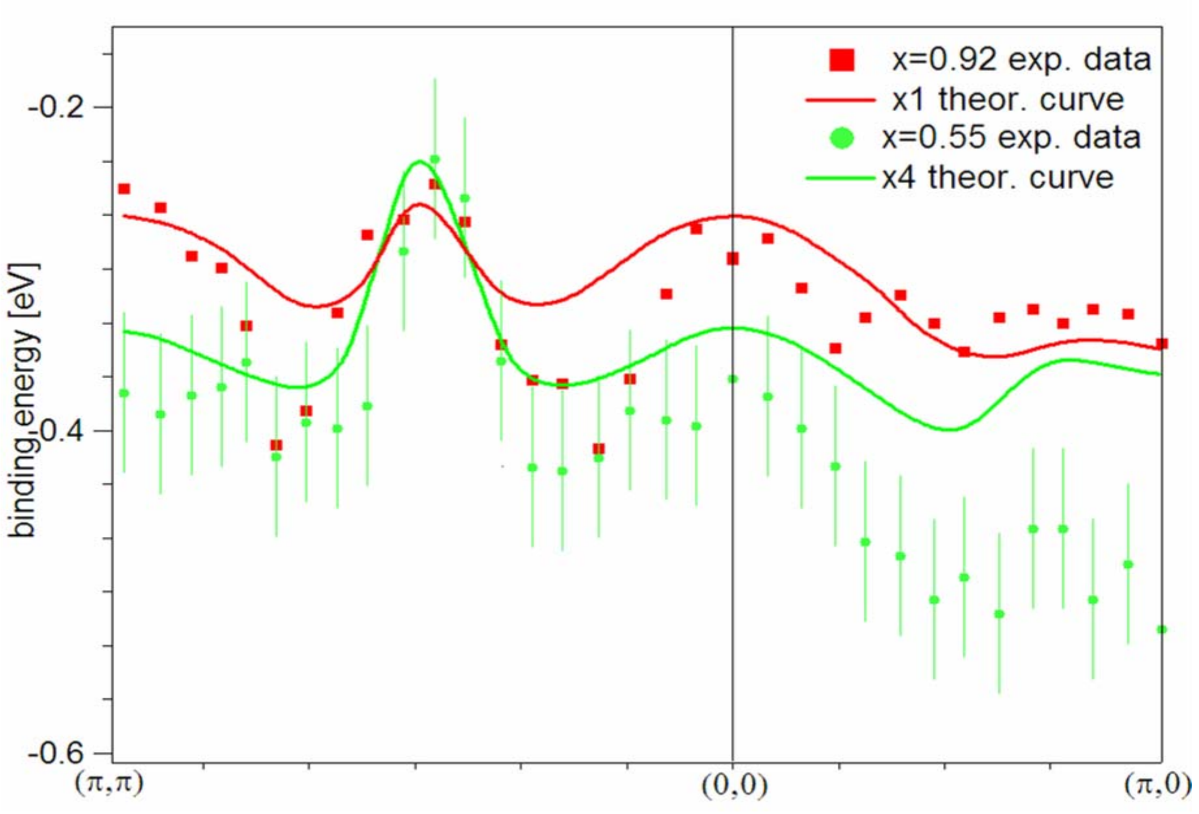
Effect of chemical pressure on electronic structure of $Bi_2Sr_2Ca_{1-x}Y_xCu_2O_8$

by ARPES measurements

C.Janowitz, V.A.Gavrichkov ,R.Manzke, SGO, JETP Lett.80,692 (2004)

strong lattice parameter dependence on the *Y* – content:
parameter c decreases and in-plane parameters *a,b* increase

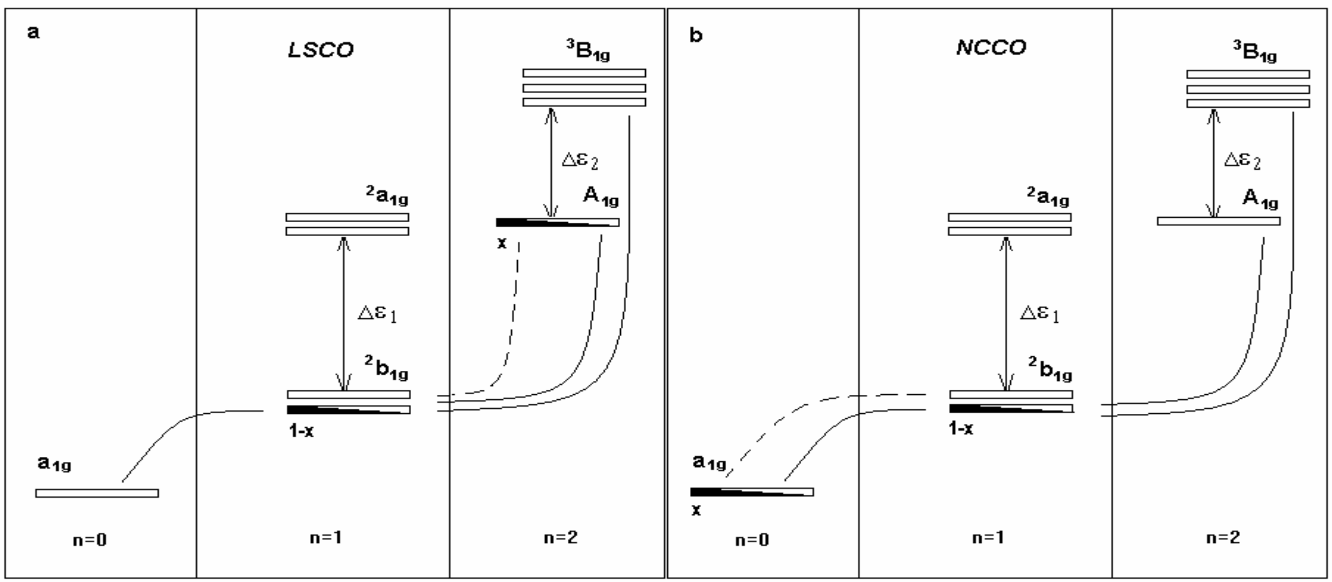
with the Y- concentration x



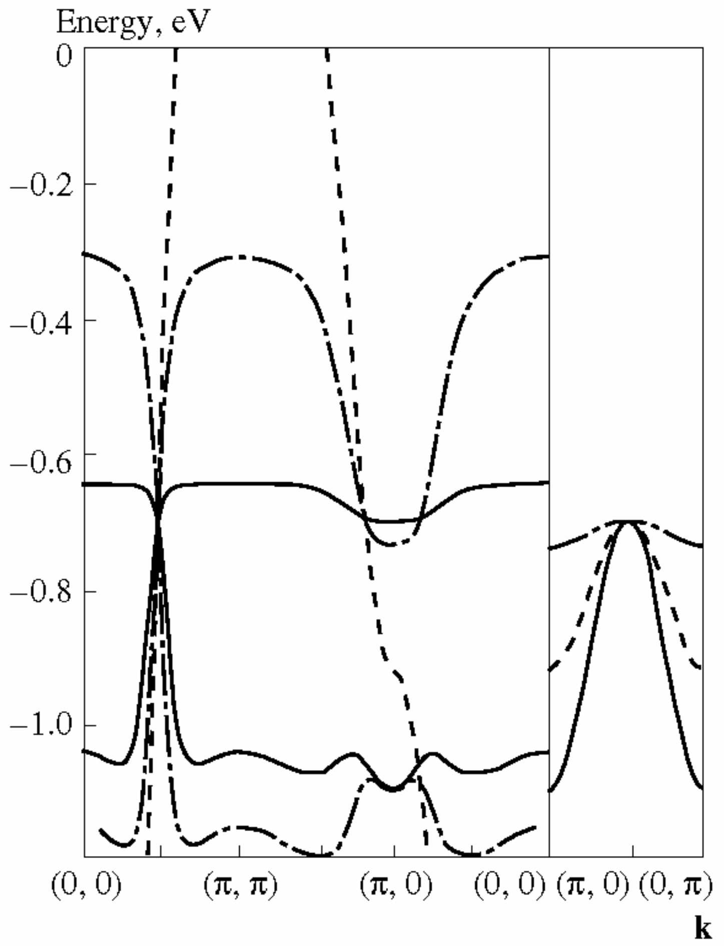
The in-gap states induced by doping

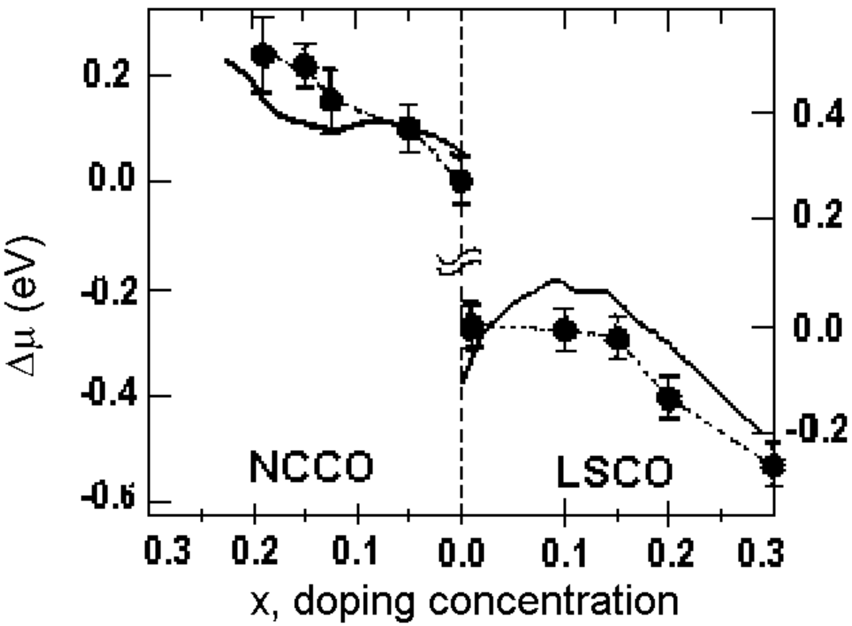
The configuration spaces for *LSCO* and *NCCO*. Solid lines correspond to the quasiparticle transitions resulting in the rigid band, dotted lines - the “impurity” bands.

LSCO: N0=0, N1=1-x, N2=x   NCCO: N0=x, N1=1-x, N2=0



In-gap states and doping dependent band structure



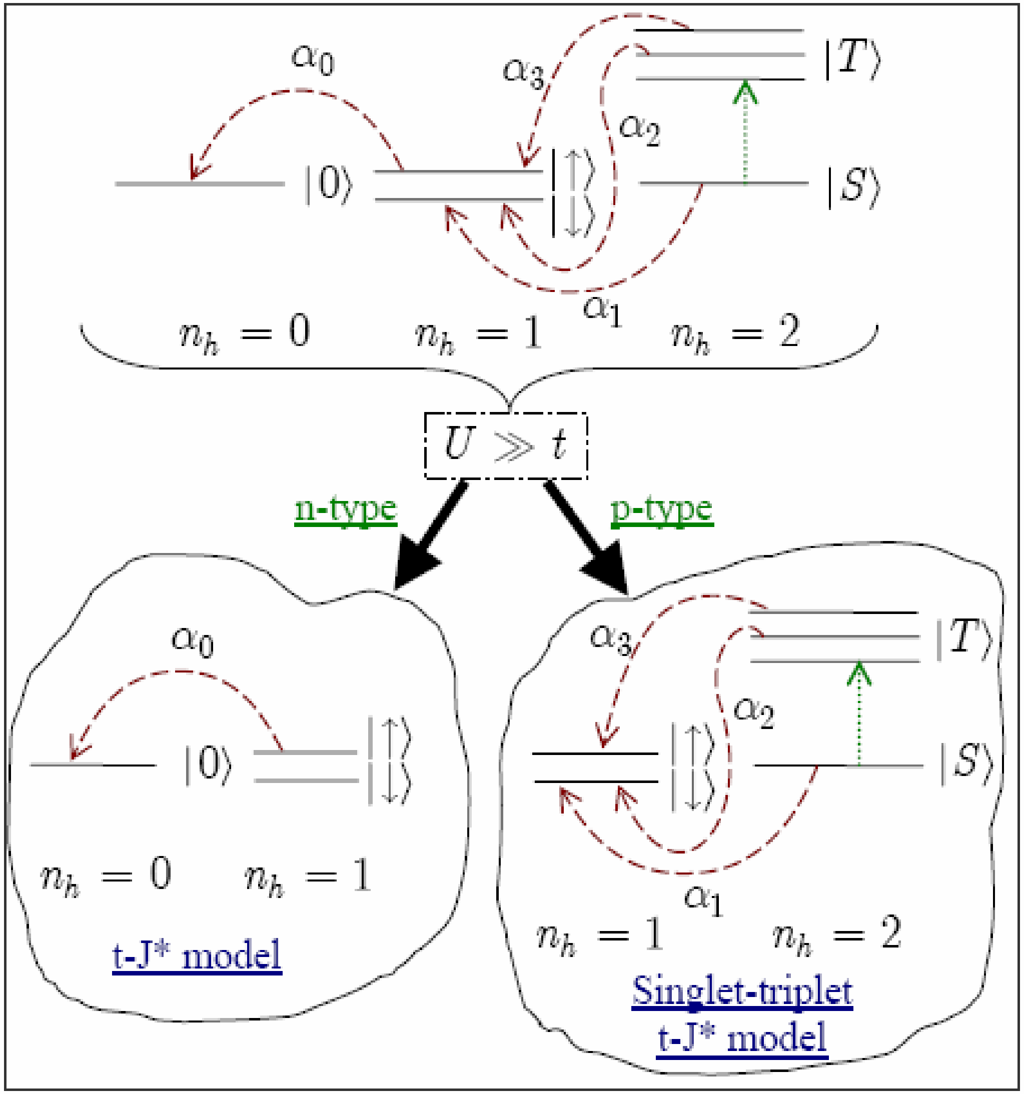


V.A. Gavrichkov et al., JETP 91, 369 (2000)

Doping x=0.01, 0.1, and 0.2

V.A. Gavrichkov and S.G. Ovchinnikov, JETP 98, 556 (2004), experimental data from N.Harima etal, PRB 64, 220507 (2001)

Effective low-energy Hamiltonian



Multiband Hubbard Hamiltonian

↓ ↓ ↓ ↓

Unitary transformation to exclude intersubband (between LHB and UHB) hoppings is applied

↓ ↓ ↓ ↓

Effective singlet-triplet model

[*M.M. Korshunov and S.G. Ovchinnikov, Phys.Sol.State 43, 416 (2001)*]

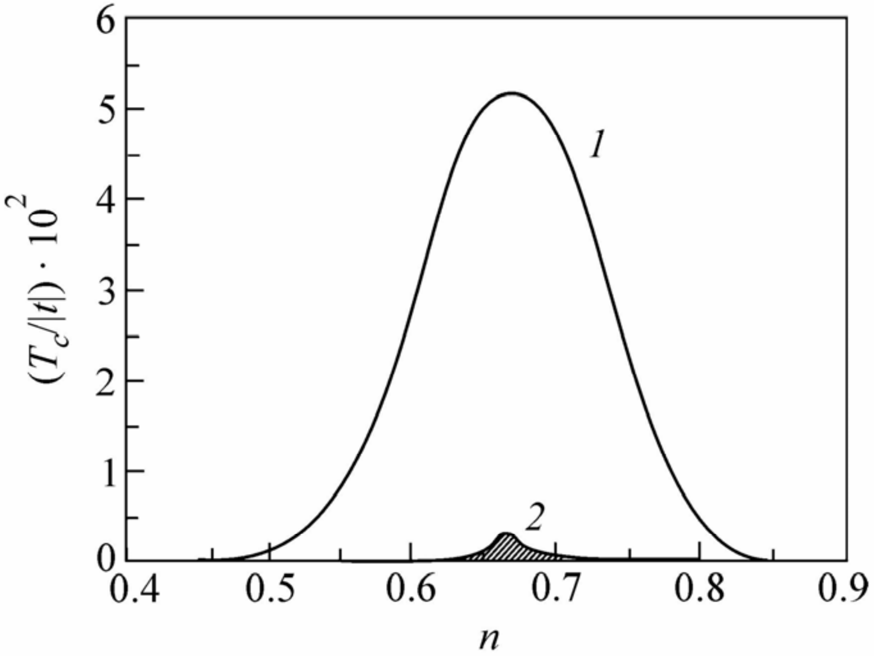
* state that the 3-center interaction terms are included in the model

Effective Hamiltonian for n-type cuprates – t-J model:*

$$H_{t-J^*} = H_{t-J} + H_3$$

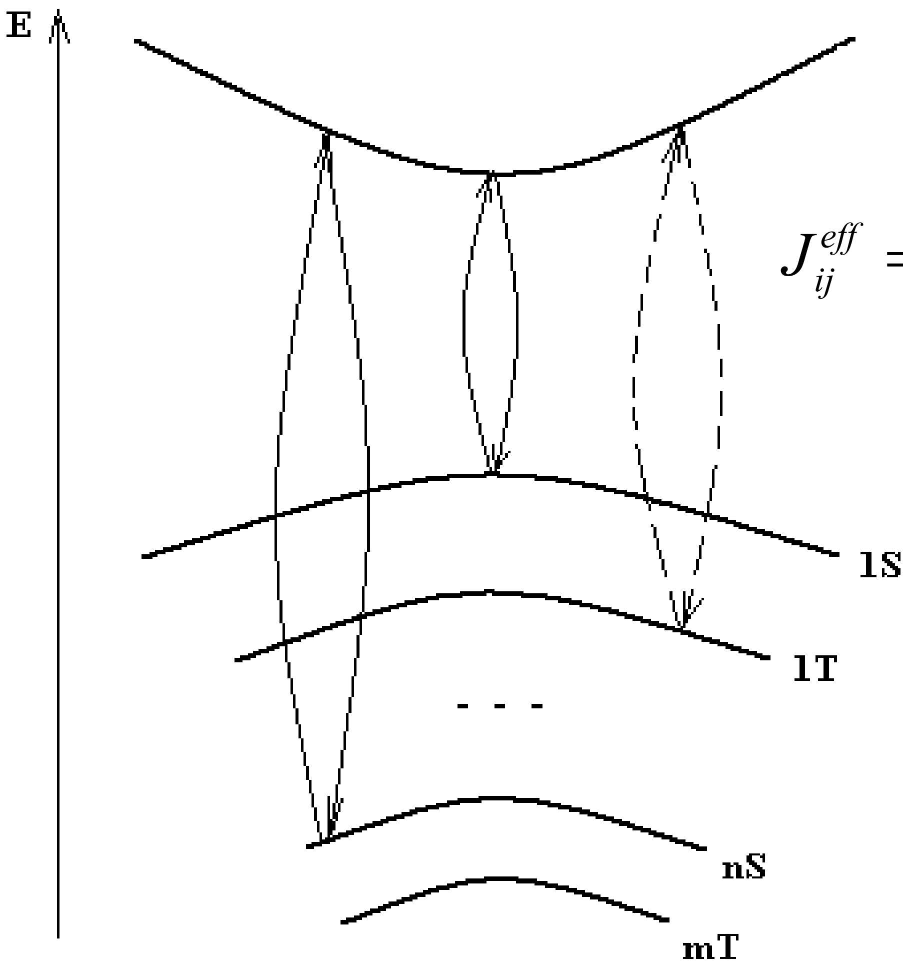
$$H_{t-J} = \sum_{f,\sigma} \varepsilon_1 X_f^{\sigma\sigma} + \sum_{<f,g>,\sigma} t_{fg}^{00} X_f^{\sigma 0} X_g^{0\sigma} + \sum_{<f,g>} J_{fg} \left(\mathbf{S}_f \mathbf{S}_g - \frac{1}{4} \tilde{n}_f \tilde{n}_g \right),$$

$$H_3 = - \sum_{<f,g,m>,\sigma} \frac{t_{fm}^{0S} t_{mg}^{0S}}{E_{ct}} \left(X_f^{\sigma 0} X_m^{\bar{\sigma}\bar{\sigma}} X_g^{0\sigma} - X_f^{\sigma 0} X_m^{\bar{\sigma}\sigma} X_g^{0\bar{\sigma}} \right).$$



V.V. Val'kov, T.A. Val'kova, D.M. Dzebisashvili, S.G. Ovchinnikov, JETP Letters 75, 378 (2002)

Exchange interaction from ab initio LDA+GTB



$$J_{ij}^{eff} = \sum_{n=1}^{N_S} \left| t_{ij}^{0,nS} \right|^2 \Big/ \Delta_{nS} - \sum_{m=1}^{N_T} \left| t_{ij}^{0,mT} \right|^2 \Big/ 2\Delta_{mT}$$

$\Delta_{nS} = E_{nS} - 2\varepsilon_1$, $\Delta_{mT} = E_{mT} - 2\varepsilon_1$,

With ab initio parameters for La_2CuO_4 from Korshunov, Gavrichkov etal (PRB2005)

J=0.146eV

Hole dynamics in SCES at the short range order antiferromagnetic background. SCBA for Self-energy. At low T correlations are static (Barabanov et al, JETP 2001, Valkov and Dzebisashvili, JETP 2005, Plakida and Oudovenko JETP 2007, Korshunov and Ovchinnikov Eur.Phys.J.B, 2007)

$$G_\sigma(\mathbf{k},E)=\frac{(1+x)/2}{E-\varepsilon_0+\mu-\frac{1+x}{2}t(\mathbf{k})-\frac{1-x^2}{4}\cdot t_{01}^2(\mathbf{k})/U+\sum(\mathbf{k})}$$

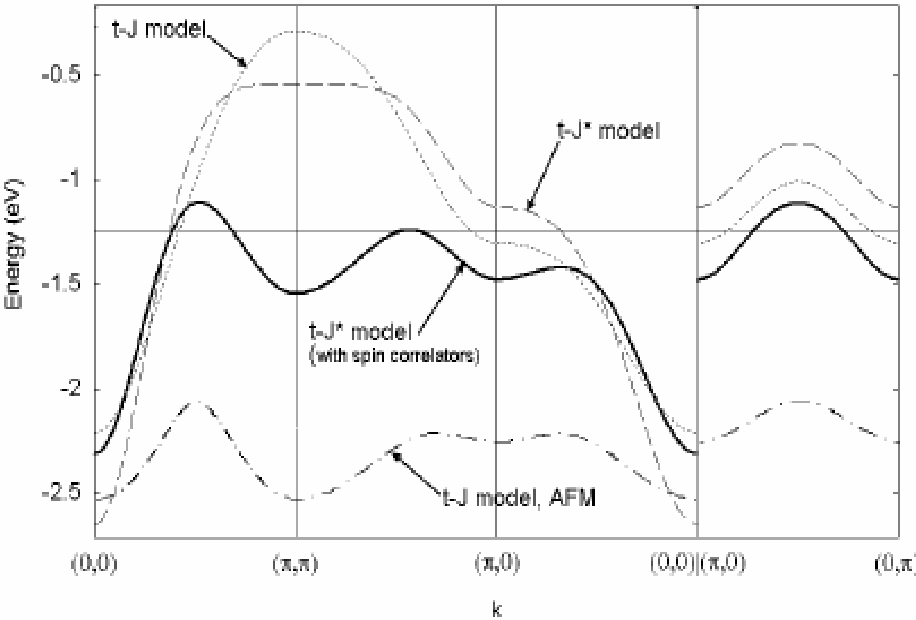
$$\sum(\mathbf{k})=\frac{2}{1+x}\frac{1}{N}\sum_{\mathbf{q}}\left\{\left[t(\mathbf{q})-\frac{1-x}{2}J(\mathbf{k}-\mathbf{q})-x\frac{t_{01}^2(\mathbf{q})}{U}-(1+x)\frac{t_{01}^2(\mathbf{k})t_{01}^2(\mathbf{q})}{U}\right]K(\mathbf{q})+\right.$$

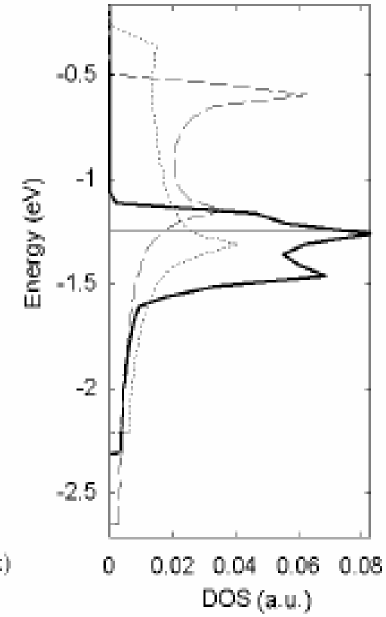
$$\left.\left[t(\mathbf{k}-\mathbf{q})-\frac{1-x}{2}\left(J(\mathbf{q})-\frac{t_{01}^2(\mathbf{k}-\mathbf{q})}{U}\right)-\frac{(1+x)t_{01}(\mathbf{k})t_{01}^2(\mathbf{k}-\mathbf{q})}{U}\right]\cdot\frac{3}{2}C(\mathbf{q})\right\}$$

$$K(\mathbf{q})=\sum_{\mathbf{f}-\mathbf{g}}e^{-i(\mathbf{f}-\mathbf{g})\mathbf{q}}\left\langle X_{\mathbf{f}}^{2\bar{\sigma}}X_{\mathbf{g}}^{2\bar{\sigma}}\right\rangle \quad C(\mathbf{q})=\sum_{\mathbf{f}-\mathbf{g}}e^{-i(\mathbf{f}-\mathbf{g})\mathbf{q}}\left\langle X_{\mathbf{f}}^{\sigma\bar{\sigma}}X_{\mathbf{g}}^{\bar{\sigma}\bar{\sigma}}\right\rangle=2\sum_{\mathbf{f}-\mathbf{g}}e^{-i(\mathbf{f}-\mathbf{g})\mathbf{q}}\left\langle S_{\mathbf{f}}^z S_{\mathbf{g}}^z\right\rangle$$

Correlation functions are calculated follow Valkov and Dzebisashvili, JETP 2005

Quasiparticle dispersion in the t-J and t-J* models

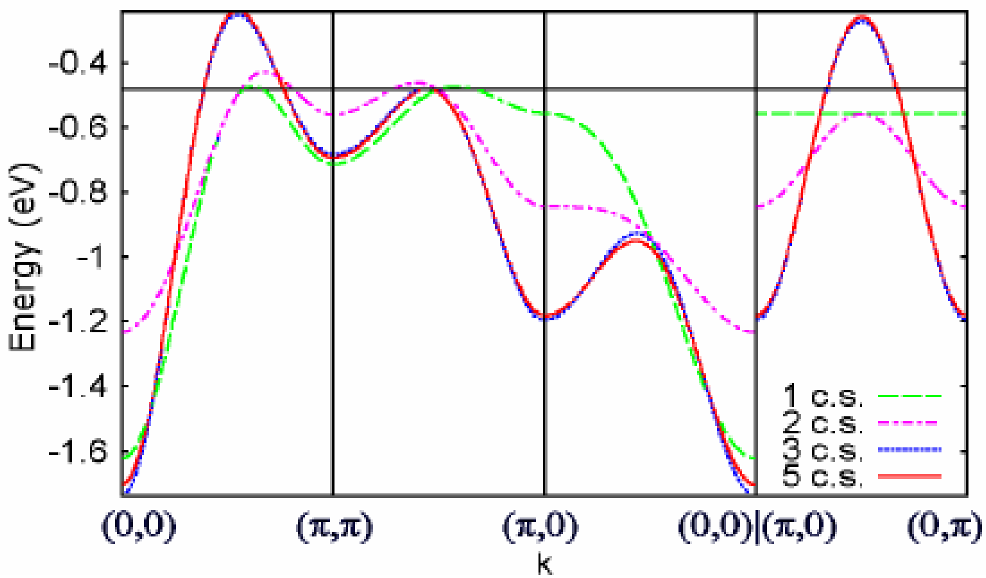


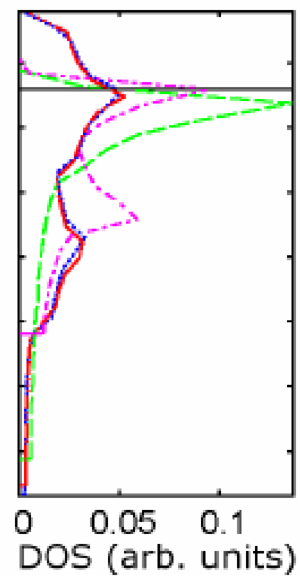


In the BCS-type theory:

$$T_c \propto \exp(-1/N(\varepsilon_F)V)$$

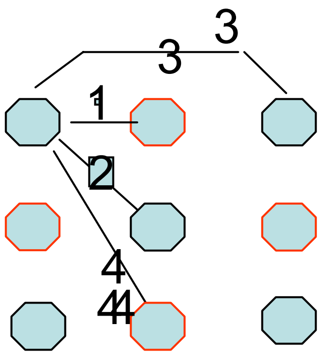
Appearance of the new Van-Hove singularity and corresponding maximum in $T_c(x)$ at low x: [***V.V. Val'kov and D.M. Dzebisashvili,*** *JETP 100, 608 (2005)*]





vF in nodal direction:
1.6-2.0 eV A - theory
1.8+-0.4 eV A – ARPES for 0<x<0.2,
Zhou etal, Nature, 2003

Beyond the Hubbard 1: short range magnetic order in spin liquid state up to 9-th neighbor

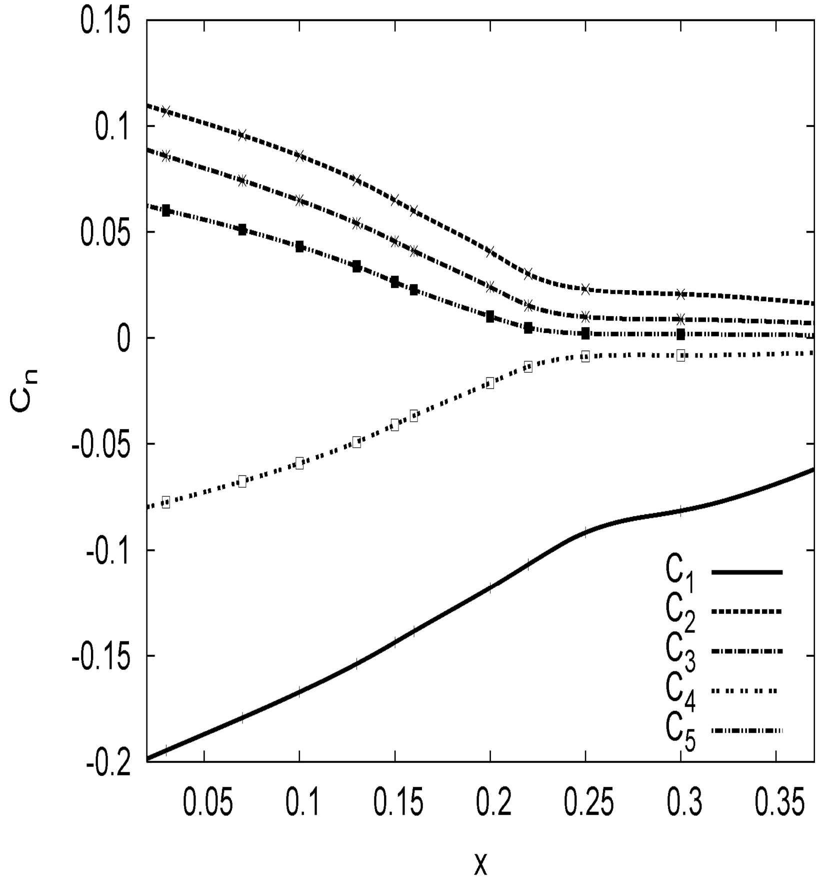


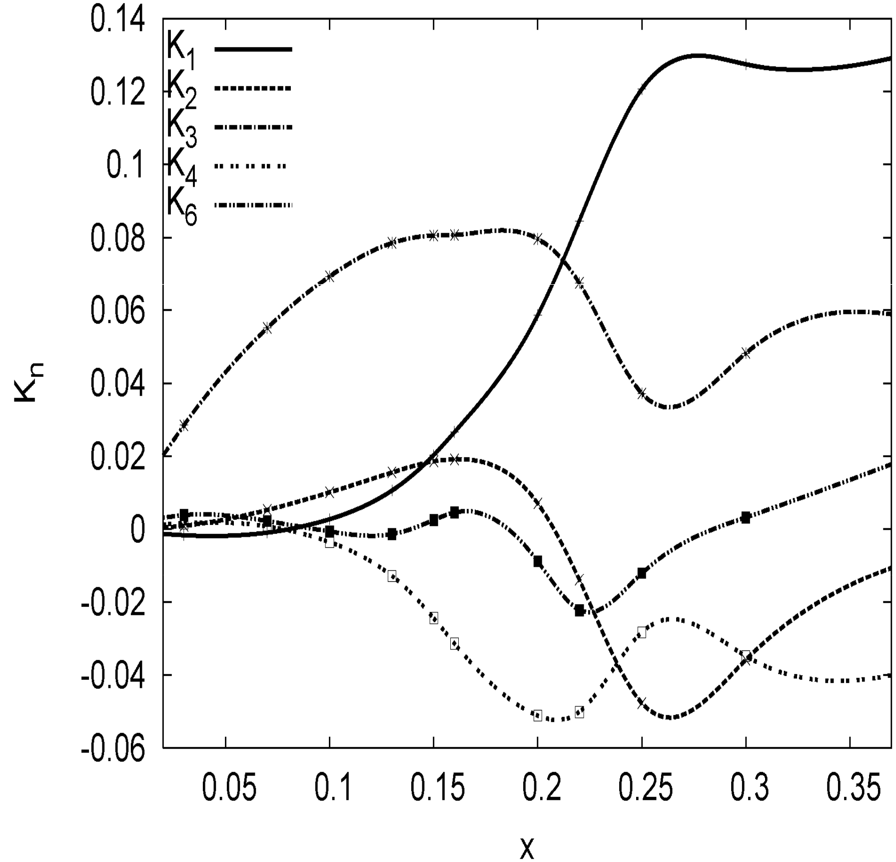
Self consistent spin and charge

Correlation functions in the t-J* model

$$C_n = 2\left\langle S_0^z S_n^z \right\rangle = \left\langle X_0^{\uparrow\downarrow} X_n^{\downarrow\uparrow} \right\rangle$$

$$K_n = \left\langle X_0^{\sigma 0} X_n^{0\sigma} \right\rangle$$





Lifshitz quantum phase transitions and change of Fermi surface topology with doping

Korshunov, Ovchinnikov Eur.Phys.J.B 2007

Xc1=0.15=Popt – maximum Tc(x)

Xc2=0.24=P* - critical point of the pseudogap formation

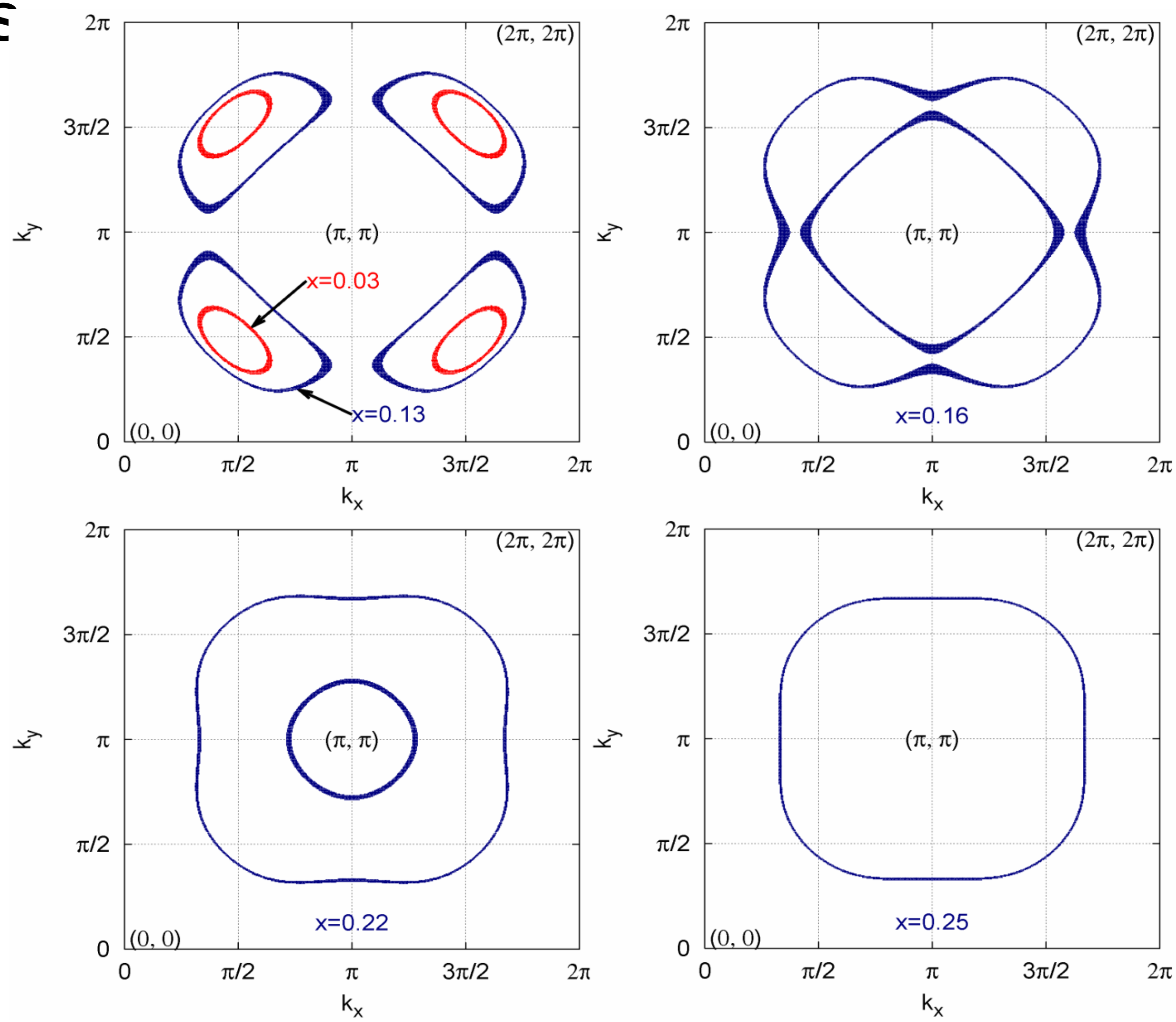


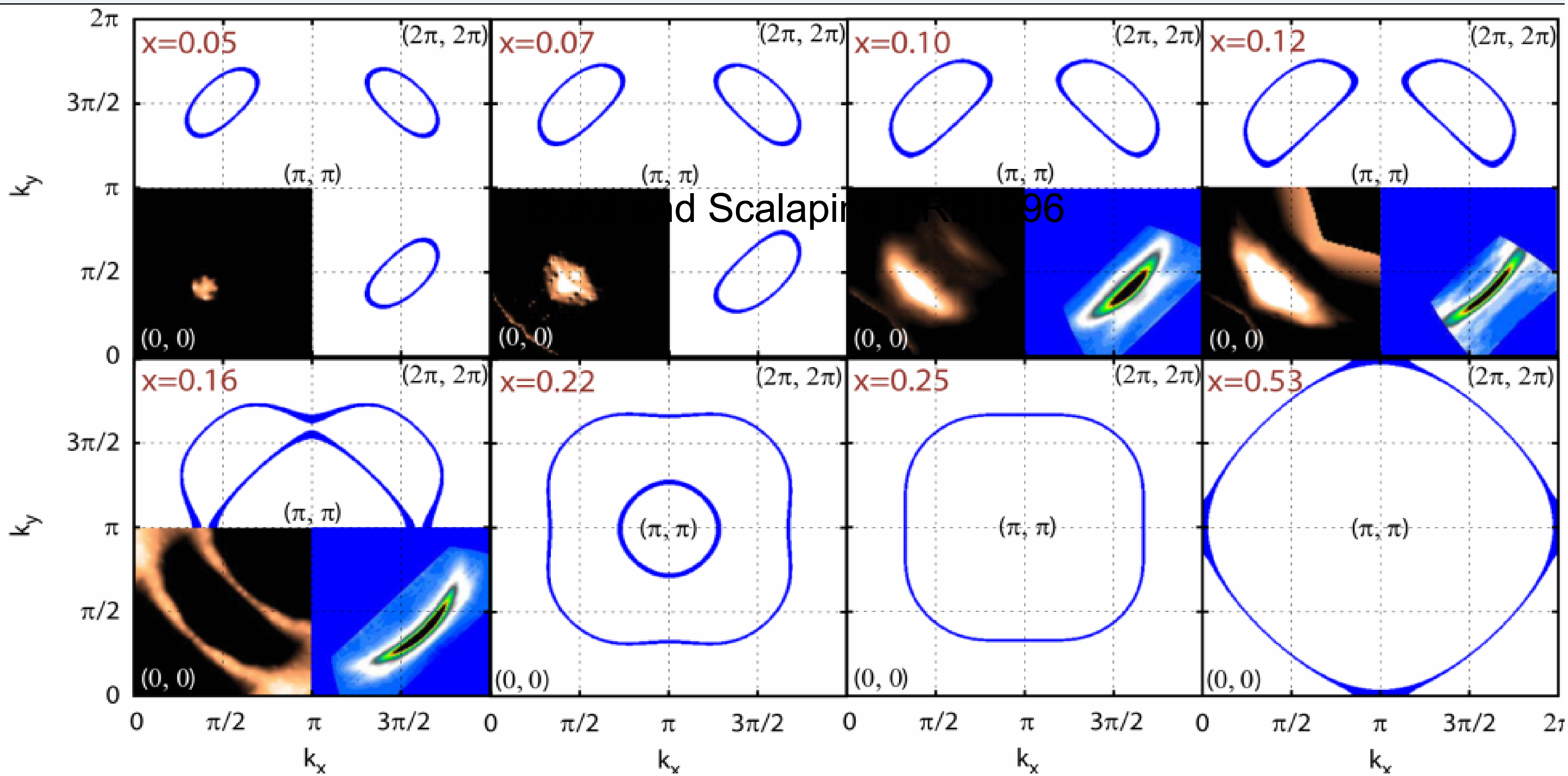
Fig. 1. Fermi surface evolution with doping (hole concentration) x.

Comparison ARPES and LDA+GTB calculations

Ovchinnikov, Korshunov, Shneyder, JETP 2009

ARPES data for Bi2201 Hashimoto etal, PRB77,2008 (left down),

and Meng etal, arXiv may 2009 (right down)



Effect of short range magnetic order on the electron dispersion

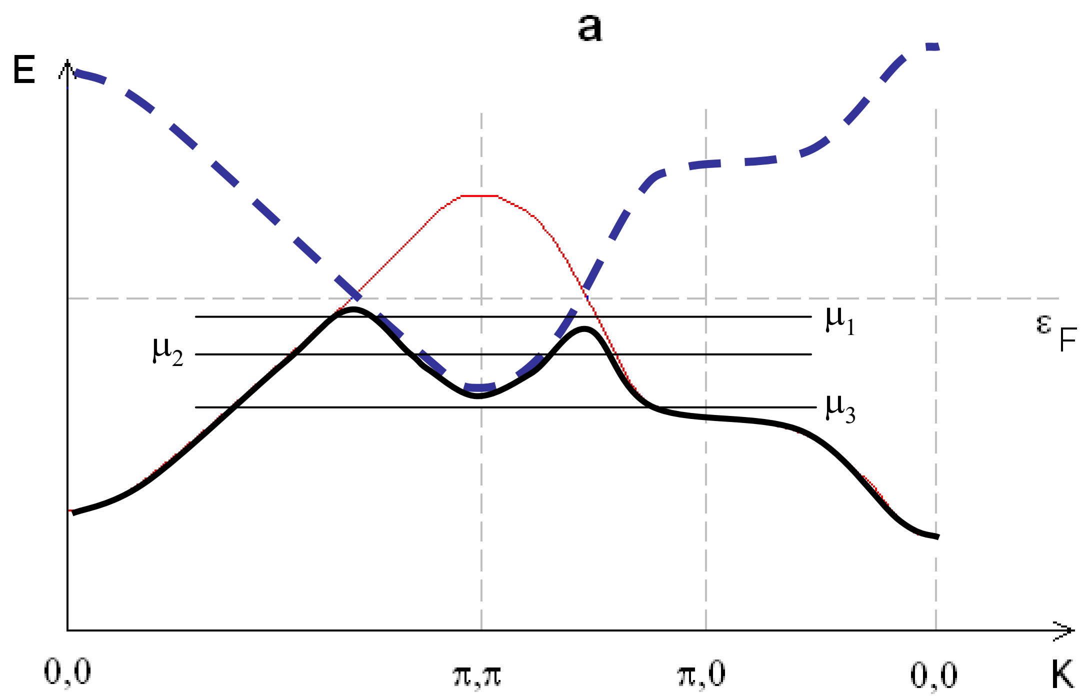
(Kuchinskii, Nekrasov, Sadovskii, JETP Lett. 2005,
Kuchinskii, Sadovskii, JETP 2006,
Kuchinskii, Sadovskii JETP Lett 88, 224, 2008)

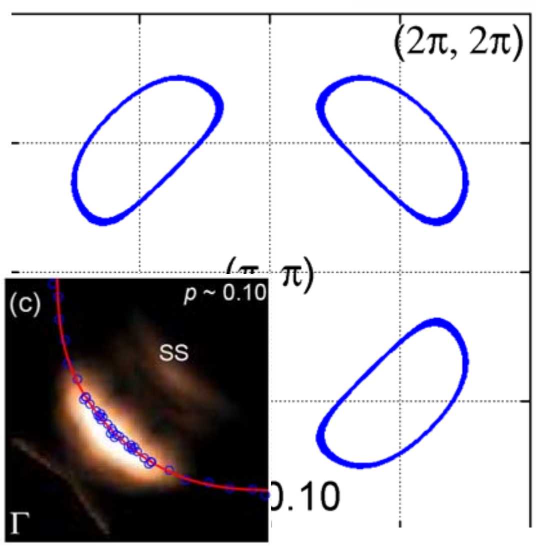
Green function of electron scattered by Gaussian fluctuating classical field is

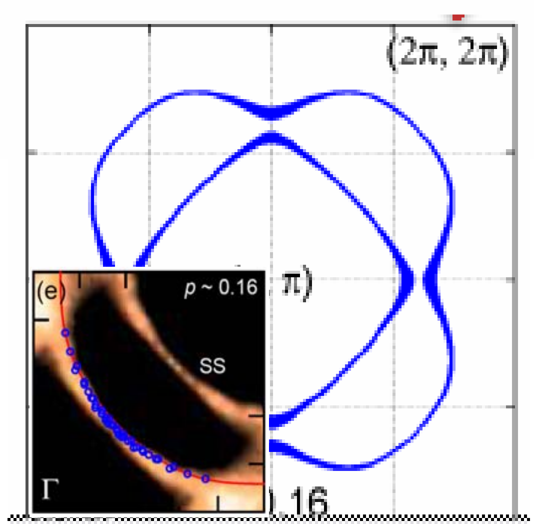
$$G_D(\mathbf{k},\varepsilon) = \frac{\varepsilon - \varepsilon(\mathbf{k}+\mathbf{Q}) + i\upsilon k}{\left(\varepsilon - \varepsilon(\mathbf{k})\right)\left(\varepsilon - \varepsilon(\mathbf{k}+\mathbf{Q}) + i\upsilon k\right) - |D|^2}$$

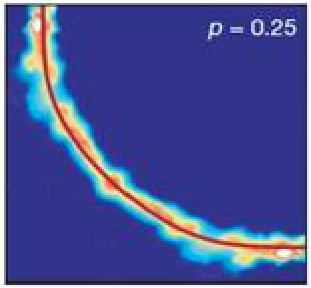
Here D is the amplitude of SDW, $\varepsilon(\mathrm{k})$ is bare paramagnetic dispersion

$$\upsilon = \left|\upsilon_x(\mathbf{k}+\mathbf{Q})\right| + \left|\upsilon_y(\mathbf{k}+\mathbf{Q})\right|, \quad \upsilon_{x,y}(\mathbf{k}) = \partial\varepsilon(\mathbf{k}) \big/ \partial k_{xy}$$


a
E
μ_1
μ_2
μ_3
ε_F
0,0
π,π
π,0
0,0
K


(2π, 2π)
π)
(c)
p ~ 0.10
SS
Γ


(2π, 2π)
π)
(e)
p ~ 0.16
SS
Γ


p = 0.25

Fermi surface analysis: Hole concentration Nh=1+x, Electron concentration Ne=1-x. Number of occupied electron states Ne(k), spectral weight F=(1+x)/2. then Ne=2*F*Ne(k)=1-x -> Ne(k)=(1-x)/(1+x)

Ovchinnikov, Korshunov, Shneyder, JETP 2009

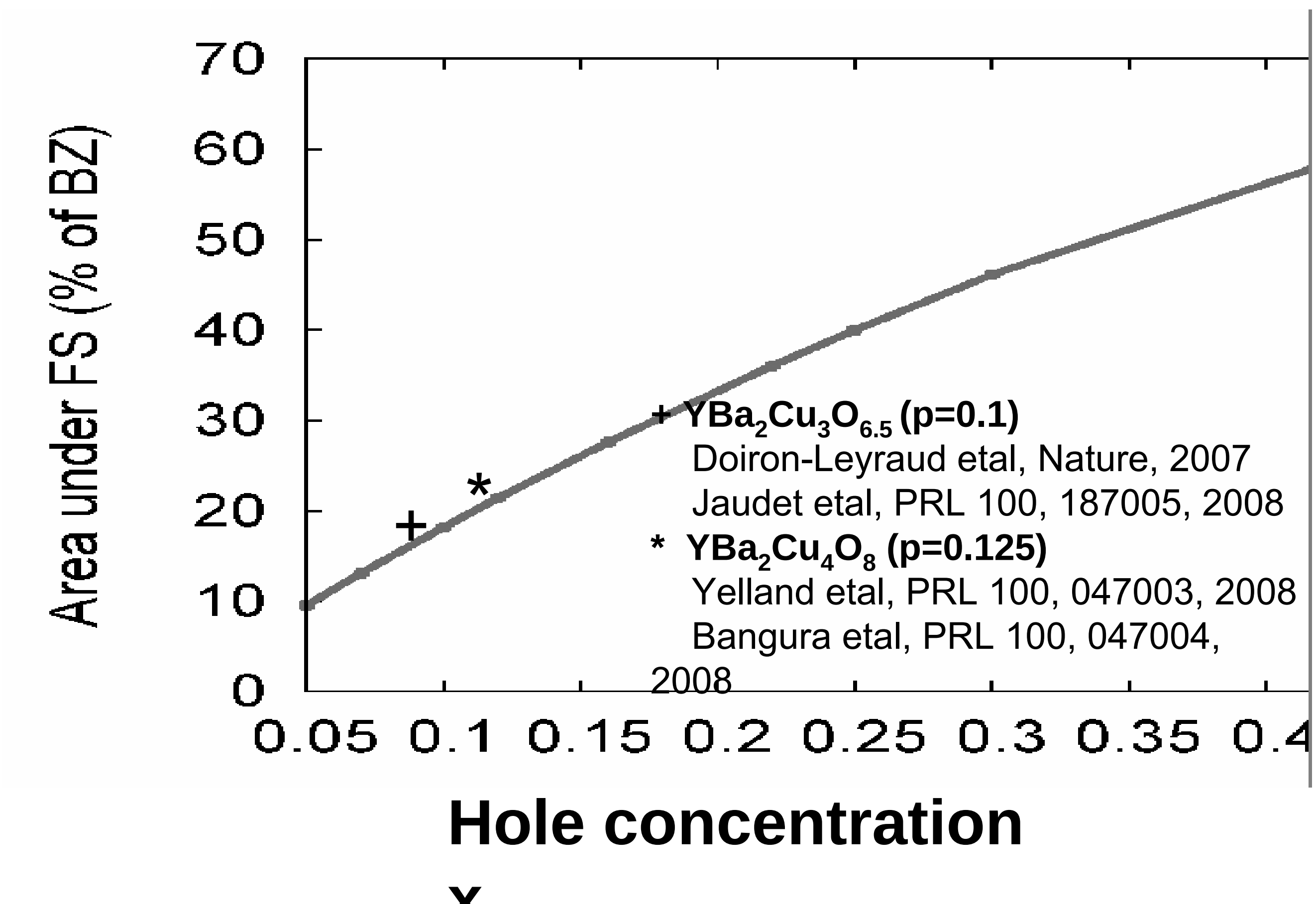
Hole occupied states

Nh(k)=1-Ne(k)

= 2x/(1+x)

Generalised Luttinger theorem: Korshunov, Ovchinnikov,

Sol.St.Phys 2003



Effective mass from quantum oscillations measurements:

+ $YBa_2Cu_3O_{6.5}$(p=0.1) Doiron-Leyraud I Nature,2007

* $YBa_2Cu_4O_8$ (p=0.125) Yelland etal, PRL 100, 2008

x $YBa_2Cu_4O_8$ Bangura etal, PRL 100, 047004, 2008

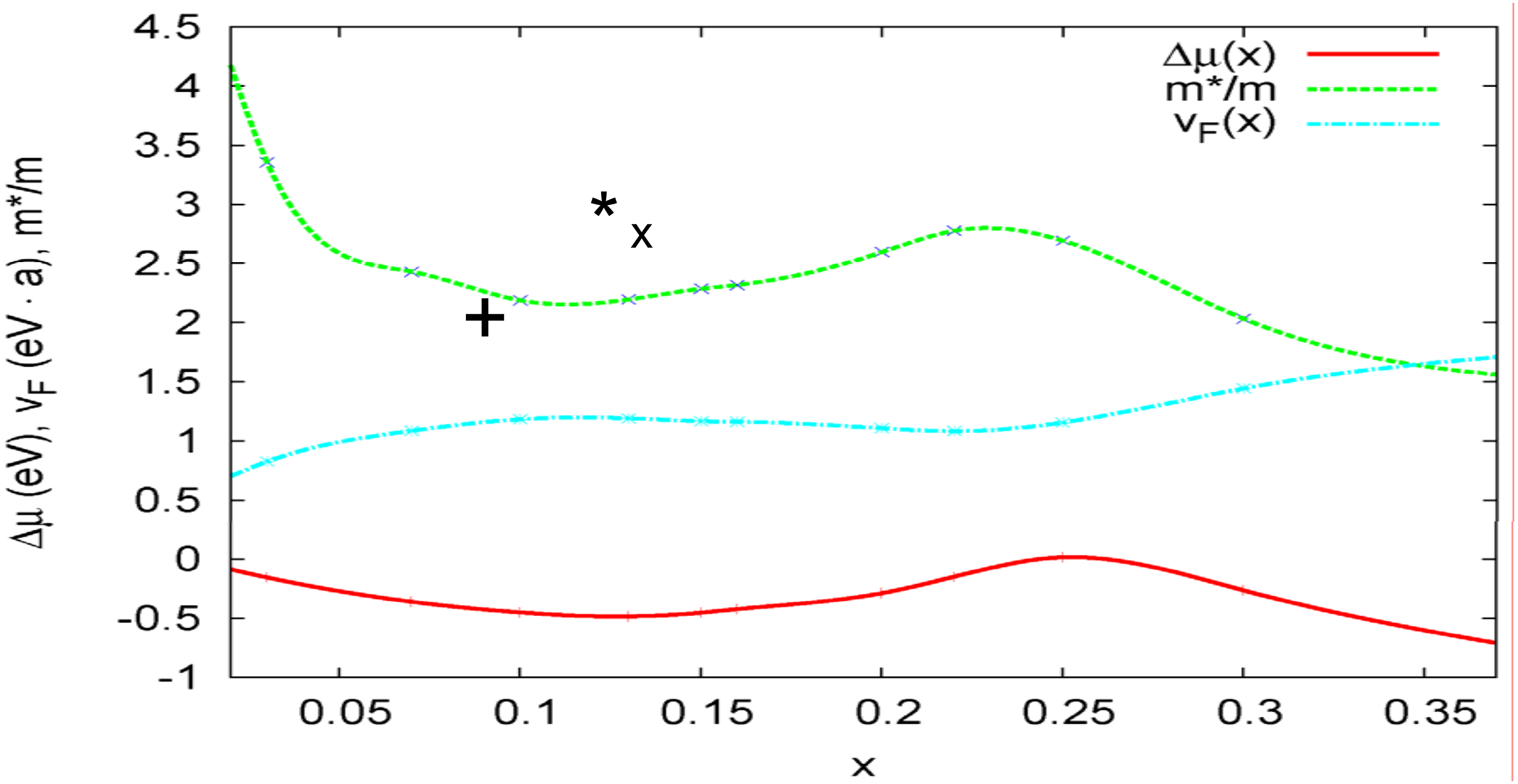
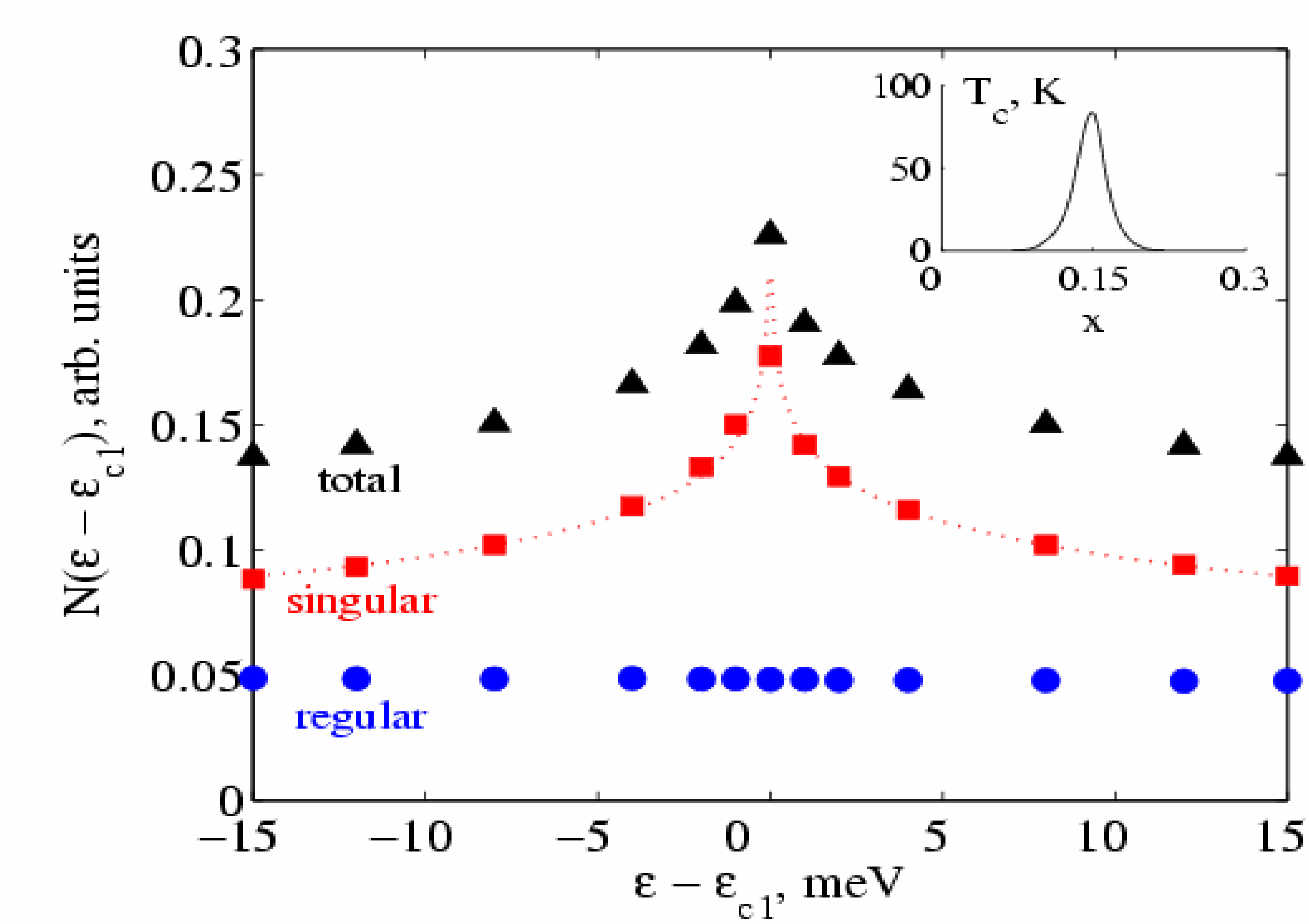


Fig. 2. Doping dependent evolution of the chemical potential shift, nodal Fermi velocity, and effective mass.

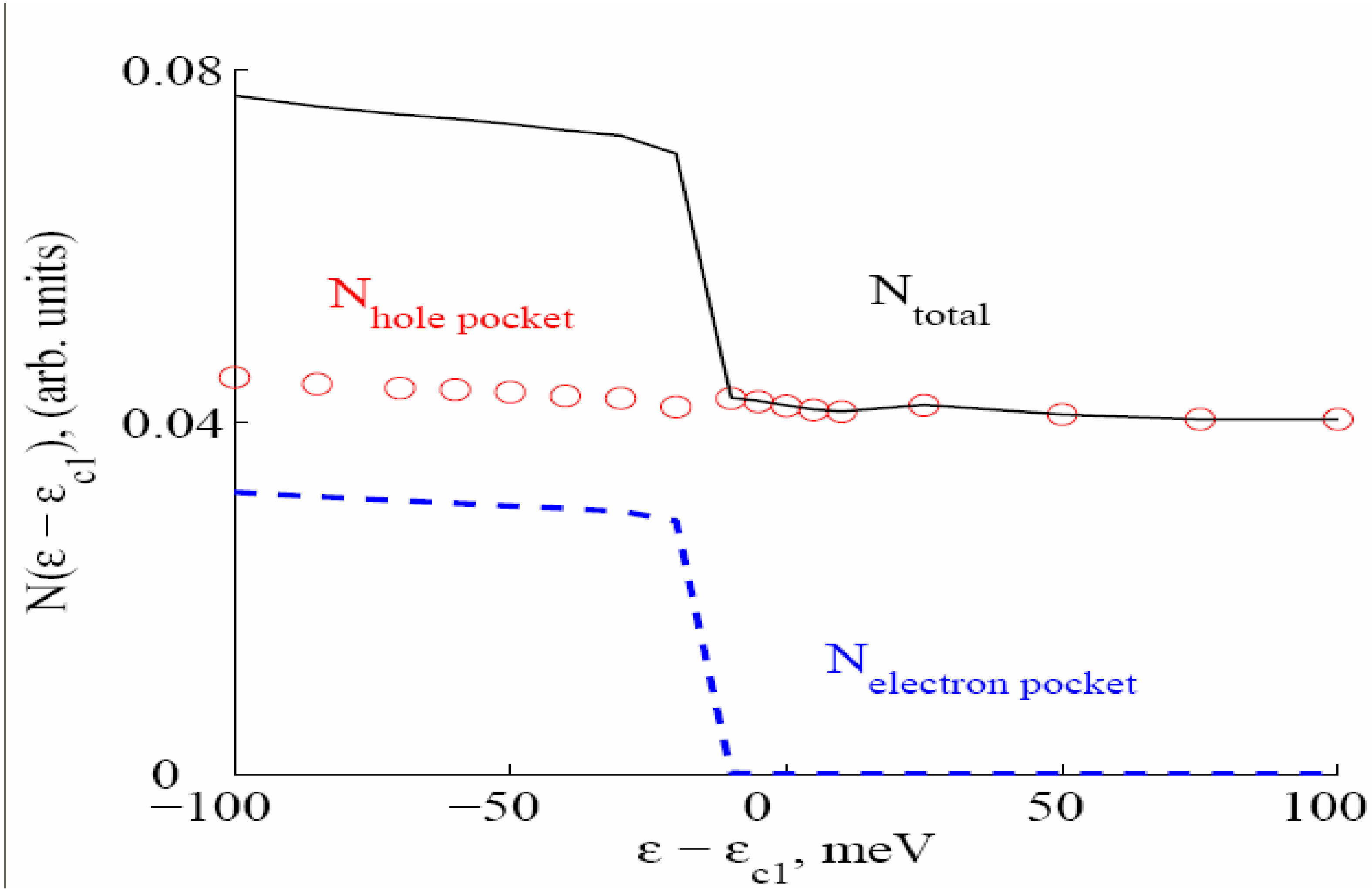
Density of states near optimal doping QPT,
N(E)=Nreg(E) + Nsing(E)

Ovchinnikov etal, arXiv 0908.0576



DOS near pseudogap critical point x=p*=0.24

Ovchinnikov etal, arXiv 0908.0576



Comparison of 3D and 2D Lifshitz transitions

- Two different transitions: Change of connection and Fermi pocket collapse
- In 3D for both Nsing(E) ~ (E-Ec)^0.5, Free energy Fsing ~z^2.5 → 2.5-order QPT, Ce/T~z^0.5 Here z=p-pcrit ~ Ef-Ec
- In 2D (S.S.Nedorezov, JETP,1966:
- Change of connection: Nsing(E) ~ Log|E-Ec|, Fsing ~z^2*Log|z|, Ce/T~Log|z|
- Collapse: Nsing(E) ~step, Fsing ~z^2, Ce/T~step

Pseudogap critical point and Fermi surface transformation in $La_{1.6-x}Nd_{0.4}Sr_xCuO_4$ *(R.Daou etal, Nat.Phys.2009)*

Tc(max)~20K, B up to 15T

P*<0.24

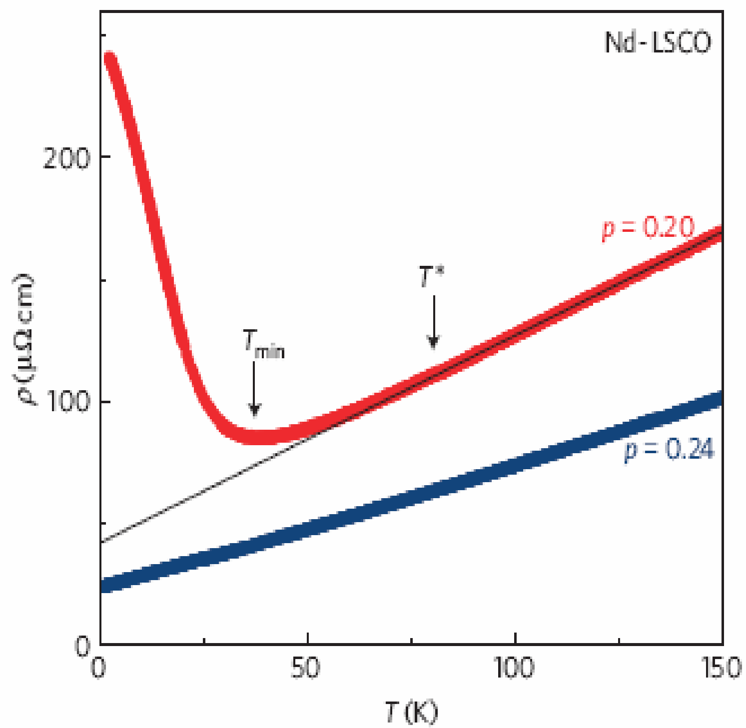


Figure 1 | Normal-state resistivity. In-plane electrical resistivity $\rho(T)$ of Nd-LSCO as a function of temperature, at $p = 0.20$ and 0.24, measured in a magnetic field strong enough to fully suppress superconductivity (see

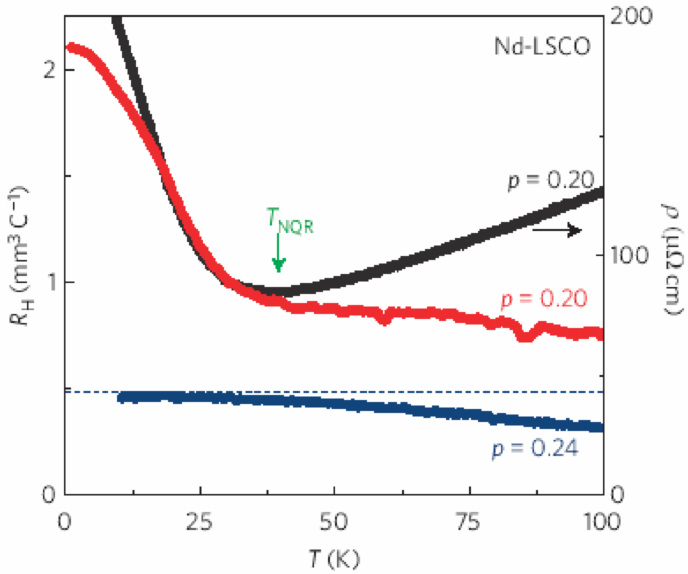
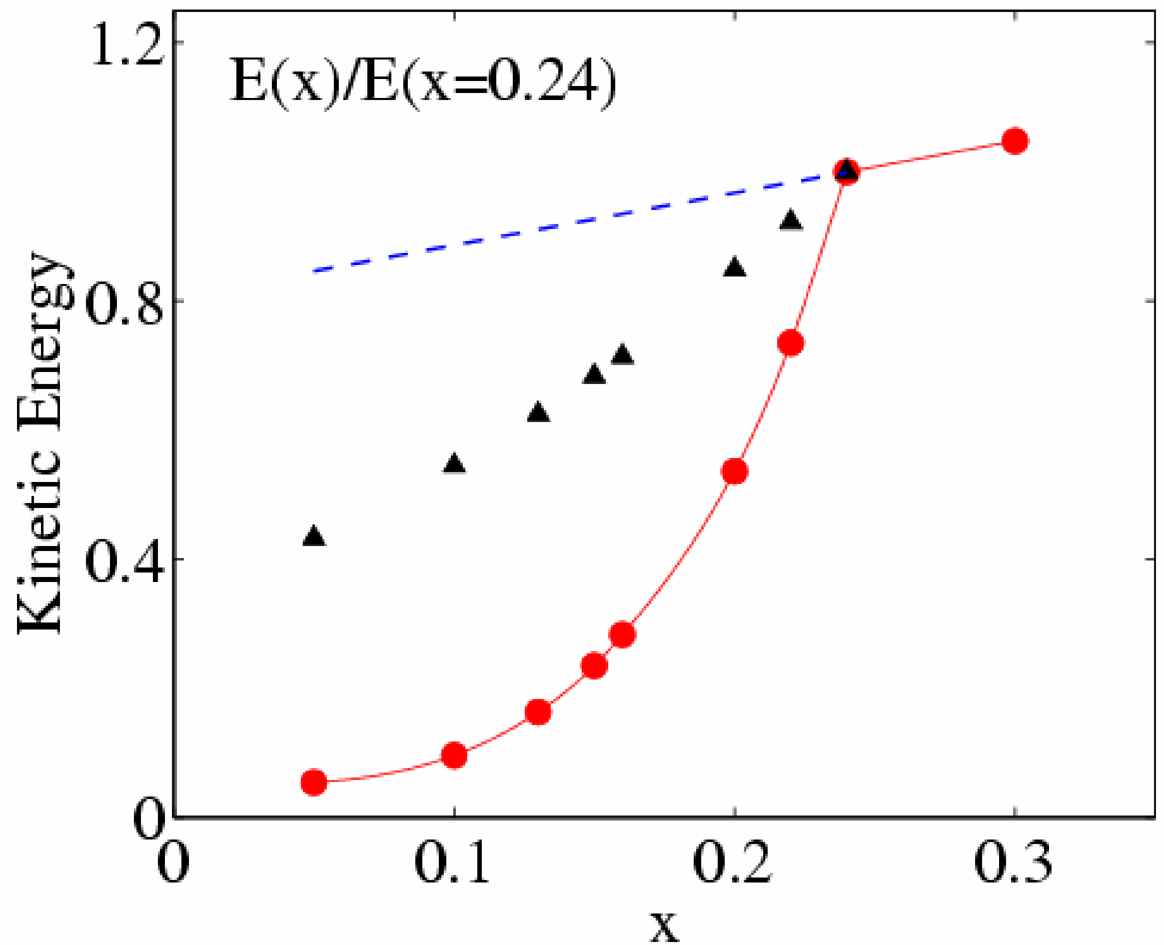


Figure 4 | Normal-state Hall coefficient. Hall coefficient $R_H(T)$ of Nd-LSCO as a function of temperature for $p = 0.20$ and 0.24, measured in a magnetic field of 15 T. Below 12 K, the 0.20 data are in 33 T, a magnetic field strong enough to fully suppress superconductivity (see Supplementary Information). The dashed blue horizontal line is the value of R_H calculated for a large cylindrical Fermi surface enclosing $1+p$ holes, namely $R_H = V/e(1+p)$, at $p = 0.24$. At $p = 0.20$, the rise in $R_H(T)$ at low temperature



Ovchinnikov, Korshunov, Shneyder,

arXiv 0908.0576

Eg(x)= J(1-x/p*)

Kinetic energy Ekin(x)/Ekin(p*) as function of doping. Above p* dependence ~(1+x) is expected for 2D electron gas. Below p* its extrapolation reveals the depletion of kinetic energy due to pseugogap. Black triangles-fitting with Loram-Cooper triangular pseudogap model. Red line – exponential fitting **E/E* ~ exp(-4Eg(x)/J)**

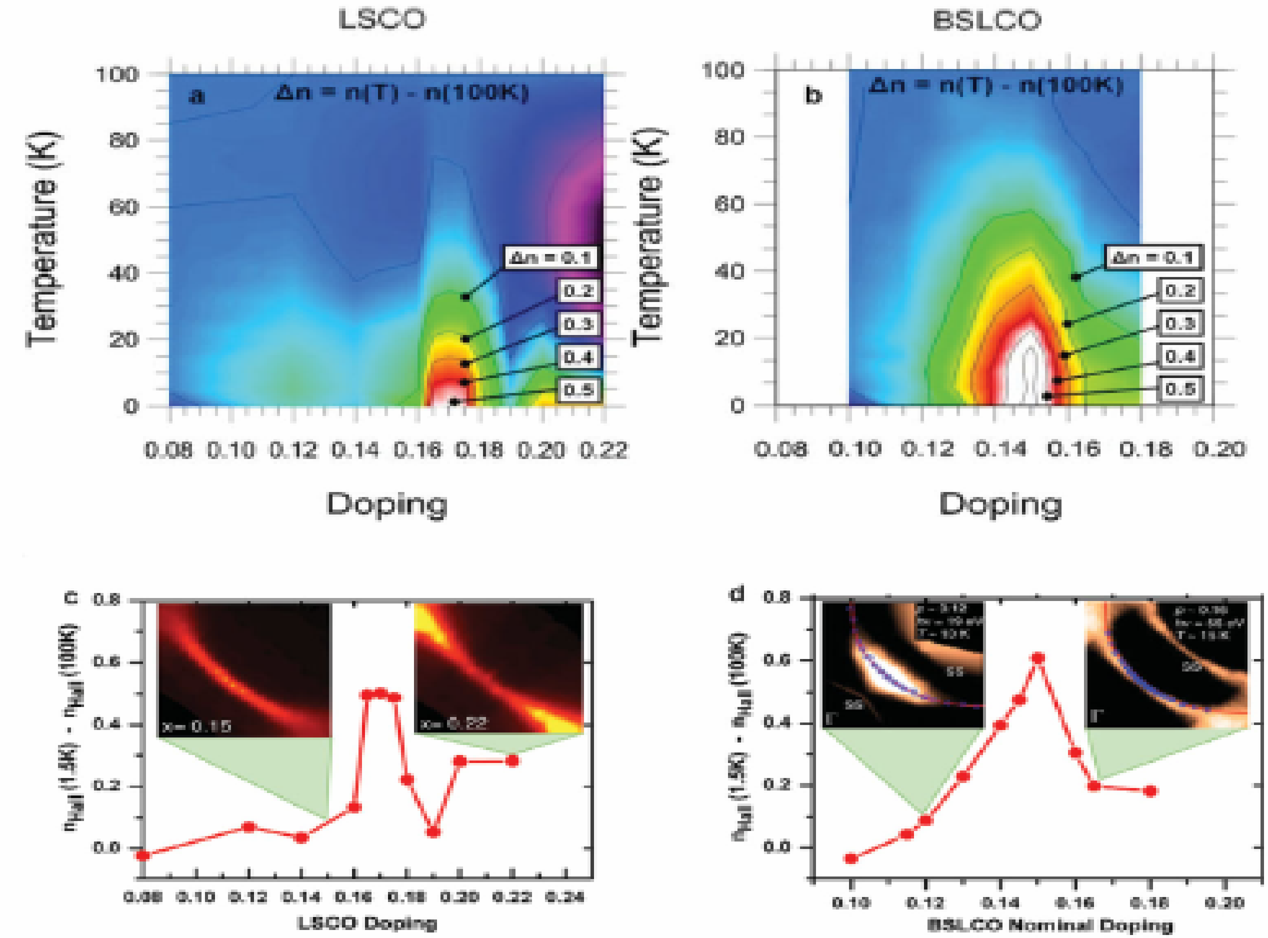


FIG. 4 (color). (a), (b) Contour plots of the Hall number variation, $\Delta n = n(T) - n(100\text{ K})$, as a function of doping and temperature in (a) LSCO and (b) BSLCO from the data of Fig. 3. (c), (d) The low-temperature ($T \sim 1.5$ K) value of the Δn versus doping in (c) LSCO and (d) BSLCO. The four insets show ARPES data for the dopings indicated, reproduced from (c) Ref. [29] and (d) Ref. [30].

Balakirev etal,
PRL 2009
QPT in strong
magnetic field 60T
SC is supressed

Thin films
La2-xSrxCu2O4

(LSCO)

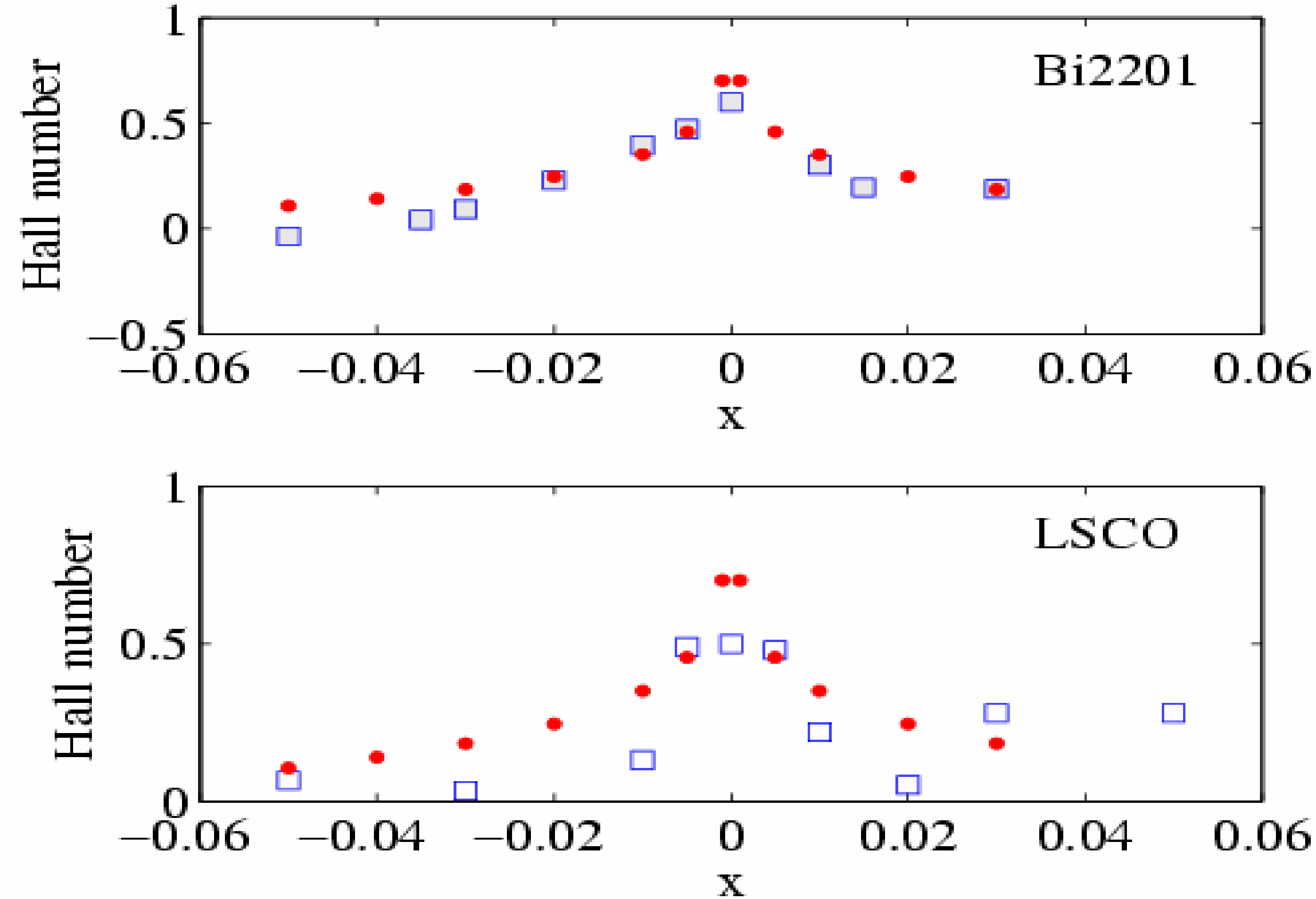
bulk single crystals

Bi2Sr2xLaxCuO6+y

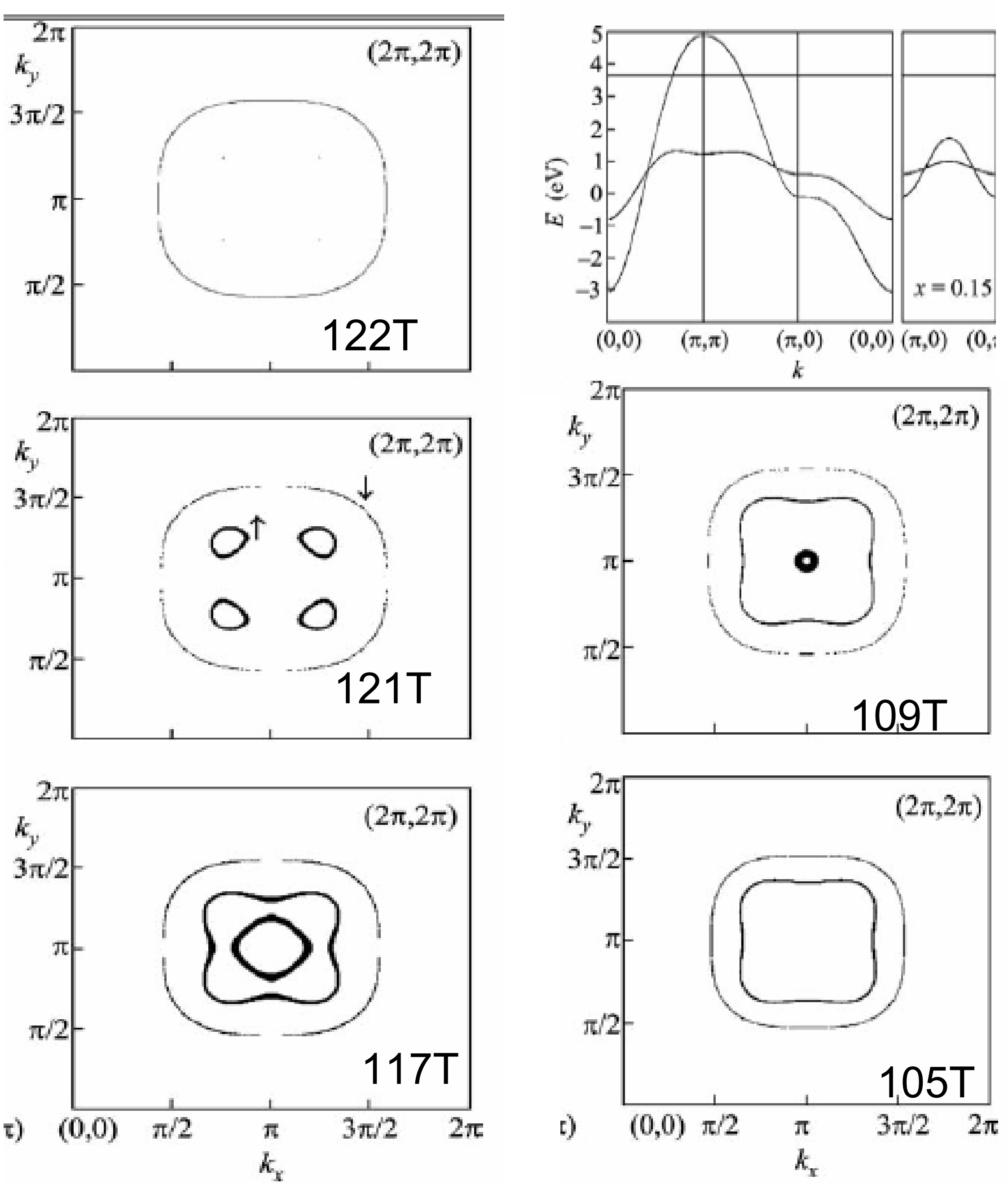
(Bi2201)

Comparison of Balakirev etal data for n(Hall) and our calculations for DOS at optimal doping
Near QPT Ef-Ec ~ z=x-xopt

Ovchinnikov etal, arXiv 0908.0576



Red circles- theory, squares- exper.



Fermi surface in the ultrastrong magnetic field

B>100T. All spins are parallel to field.

Makarov, Ovchinnikov, Shneyder,

JETP Lett.89, 632, 2009

For spin majority FS transforms with decreasing field similar to increasing doping

Magnetic pairing in the Hubbard and t-J models

- Anderson RVB 1987, Baskaran, Zhou, Anderson 1987
- QMC gives controversial conclusions: some pro (Scalapino etal) and some contra, f.e. Aimi and Imada, JPSJ 2007 by a new QMC reject d-type superconductivity. Is it the final answer? *M.Troyer: moderate optimism-bottle is more filled then empty*
- Cluster DMFT: Maier etal 2000; Lichtenstein and Katznelson 2000
- What is the superconducting glue: a combination of static and dynamical contributions (Scalapino).
- Dahm et al Nature Phys.2009: U and x(q,E) found from INS and ARPES, then Tc=150K for optimal doping
- Plakida et al, 1999: X-operators perturbation theory, Self energy in SCBA, both static J (85%) and dynamical x(q,E) (15%) contributions
- We will use Plakida-type formulation of the mean field theory with “no-double occupation” constraint and short AFM correlations +phonons

Electron-phonon interaction in GTB method

S.G.Ovchinnikov and E.I.Shneyder, JETP 101, 844 (2005)

- $H_{el} = \sum_{fnp} \left(E_n - n\mu \right) X_f^{p,p} + \sum_{fgmm'} t_{fg}^{mm'} \overset{+}{X}_f^{m} X_g^{m'}$ GTB Hamiltonian

- $Due\ to\ atomic\ displacements\ \vec{R}_f = \vec{R}_f^{(0)} + \vec{u}_f$

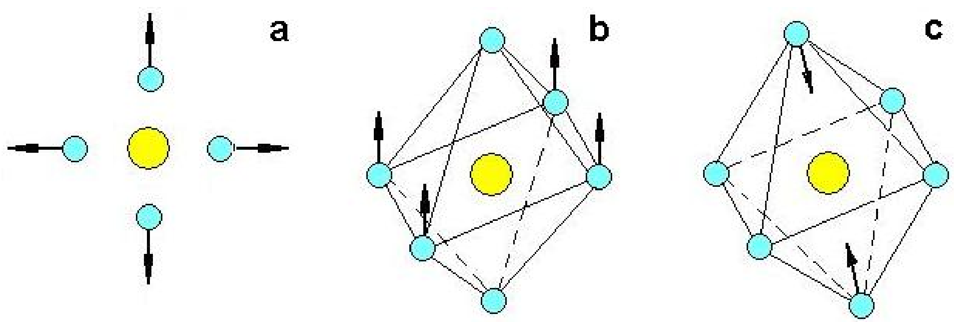
$$E_n \to E_n\left(f\right) = E_n\left(0\right) + \vec{g}_n \vec{u}_f, \qquad t_{fg}^{mm'} \to t_{fg}^{mm'} = t_{fg}^{mm'}\left(0\right) + \vec{V}^{mm'} \vec{u}_{fg}$$

- $Electron - phonon\ interaction$

$$H_{el-ph} = \sum_{kq\nu mm'} g_{mm'}^{(\nu)}\left(\vec{k},\vec{q}\right) \overset{+}{X}_k^{m} X_{k+q}^{m'} \left(b_{q,\nu} + b_{-q,\nu}^{+}\right),$$

$$g_{mm'}^{(\nu)}\left(\vec{k},\vec{q}\right) = \delta_{mm'} g_{m,dia}\left(q\right) + g_{mm',off}\left(\vec{k},\vec{q}\right)$$

Oxygen displacements



- Breathing mode (a),
- Buckling mode (b),
- Apical breathing mode (c).

Bulut and Scalapino PRB1996 __

N.S. Nunner et.al.,PRB, 8859 (1999).

Matrix

$$V^{(1)}_{dia,m}(q)=\frac{2ig^{(1)}_{dia,m}}{\sqrt{2M_O\omega_{q,\nu=1}}}\left(e_x(O)\sin\frac{q_xa}{2}+e_y(O)\sin\frac{q_ya}{2}\right),$$

$$V^{(1)}_{off,mm'}(\mathbf{k},\mathbf{q})=\frac{8ig^{(1)}_{off,mm'}}{\sqrt{2M_O\omega_{\mathbf{q},1}}}\left[\mathrm{e}_x(O_x)\sin\frac{q_xa}{2}+\mathrm{e}_y(O_y)\sin\frac{q_ya}{2}\right]\left[\gamma(\mathbf{k})+\gamma(\mathbf{k}+\mathbf{q})\right],$$

$$где\ \gamma(\mathbf{q})=\left(\cos q_xa+\cos q_ya\right)/2.$$

Sumio Ishihara and Naoto Nagaosa, PRB,144520 (2004).

Mean field theory of d-type superconductivity with magnetic and phonon pairing with "no-double occupation" constraint

(E.Shneyder, S.Ovchinnikov, JETP Lett. 83,394(2006))

$$\Delta_{\mathbf{k}} = \frac{2\varphi_{\mathbf{k}}}{N} \sum_{\mathbf{q}} \left\{ \frac{1-x}{2} J + \lambda \theta\left(\left| \xi_{\mathbf{q}} - \mu \right| - \omega_D \right) \right\} \frac{2\Delta_{\mathbf{q}} \varphi_{\mathbf{q}}}{\xi_{\mathbf{q}} - \mu} \tanh\left(\frac{\xi_{\mathbf{q}} - \mu}{2\tau} \right)$$

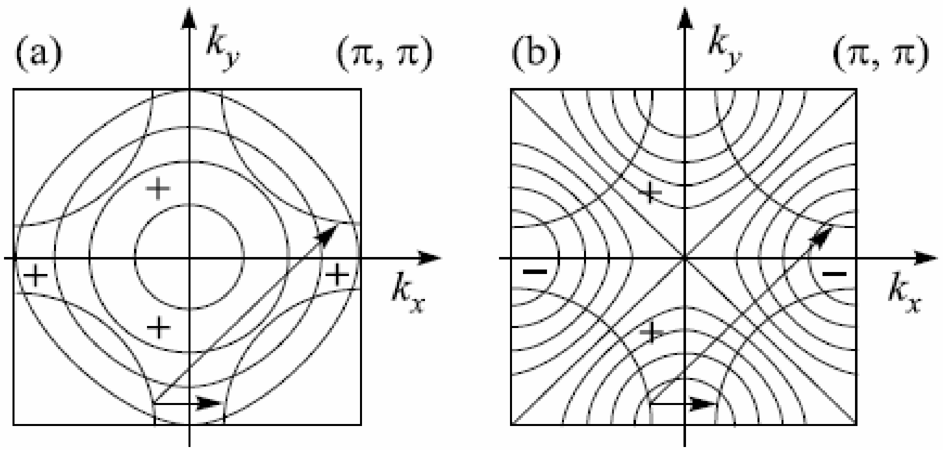
$$\Delta_{\mathbf{q}} = \Delta_0 \varphi_{\mathbf{q}} \qquad \varphi_{\mathbf{q}} = (\cos q_x a - \cos q_y a)/2$$

$$\lambda = f(x) \cdot G \qquad f(x) = (1+x)(3+x)/8 + 3(-c_{01})/4$$

$$G = \left(g_{buck}^2 / \omega_{buck} - g_{breath}^2 / \omega_{breath} \right)$$

Effect of Buckling and breathing modes EPI on superconductivity

(Bulut and Scalapino PRB1996,
Shneyder and OvchinnikovJETP LETT2006
Honerkamp etal PRB 2007)



1. Buckling mode has the large EPI at small q, breathing mode at q~pi/a
2. EPI with large q does not change a phase of the order parameter for s-pairing (a), and changes it to the opposite for d-pairing (b).
3. The total EPI parameter G may be G>0 (support) or G<0 (supress) magnetic mechanism
4. No contribution of the strong EPI with apical O in parameter G agrees with the absence of the site-selective isotope effect (Khasanov etal PRB 2003)

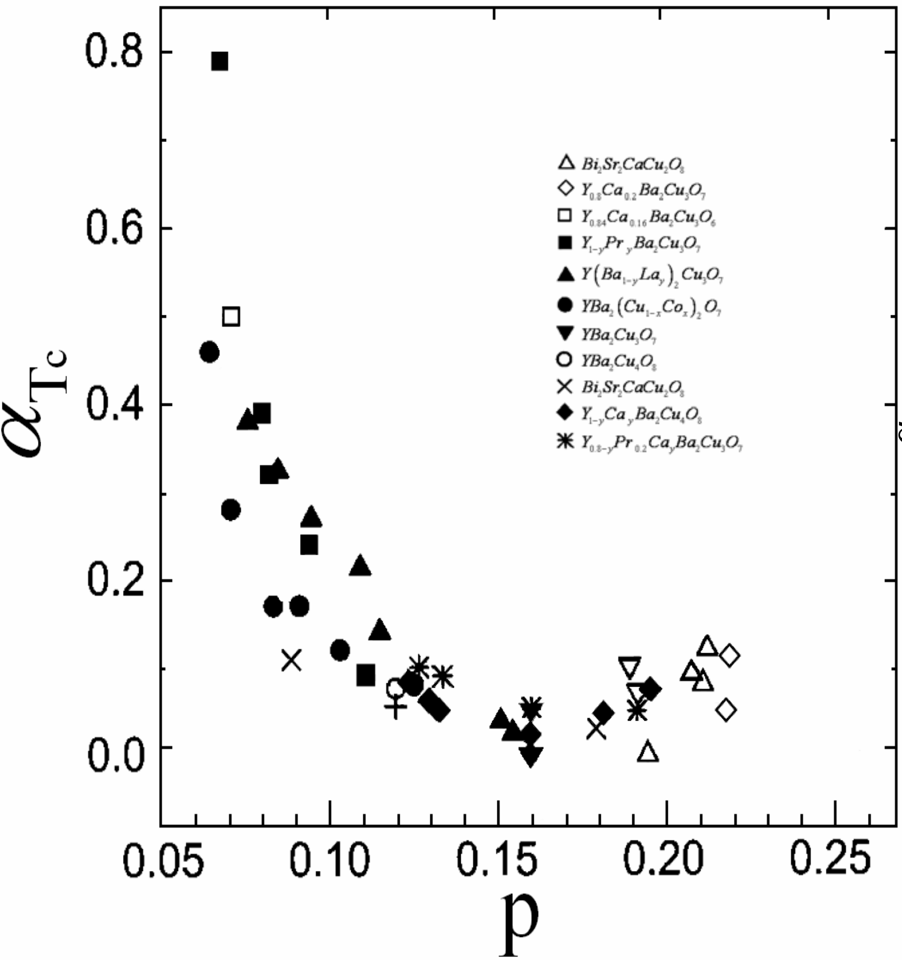
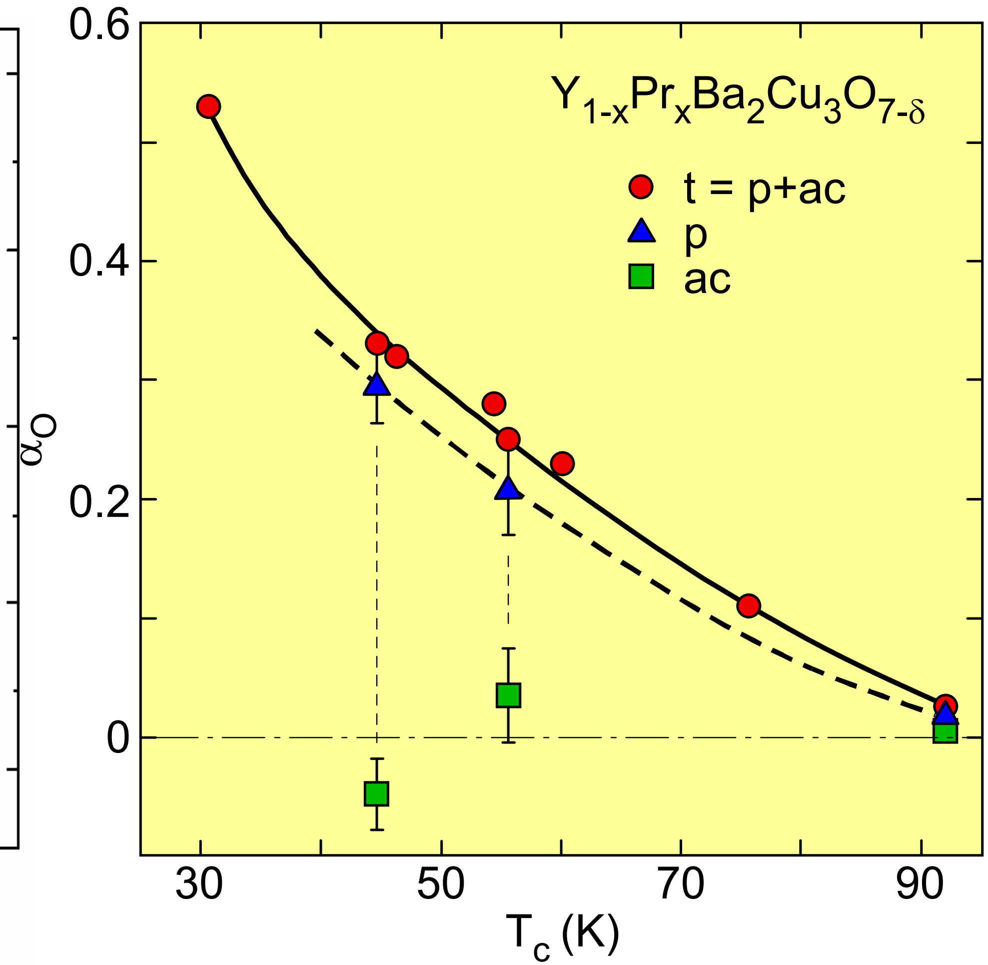
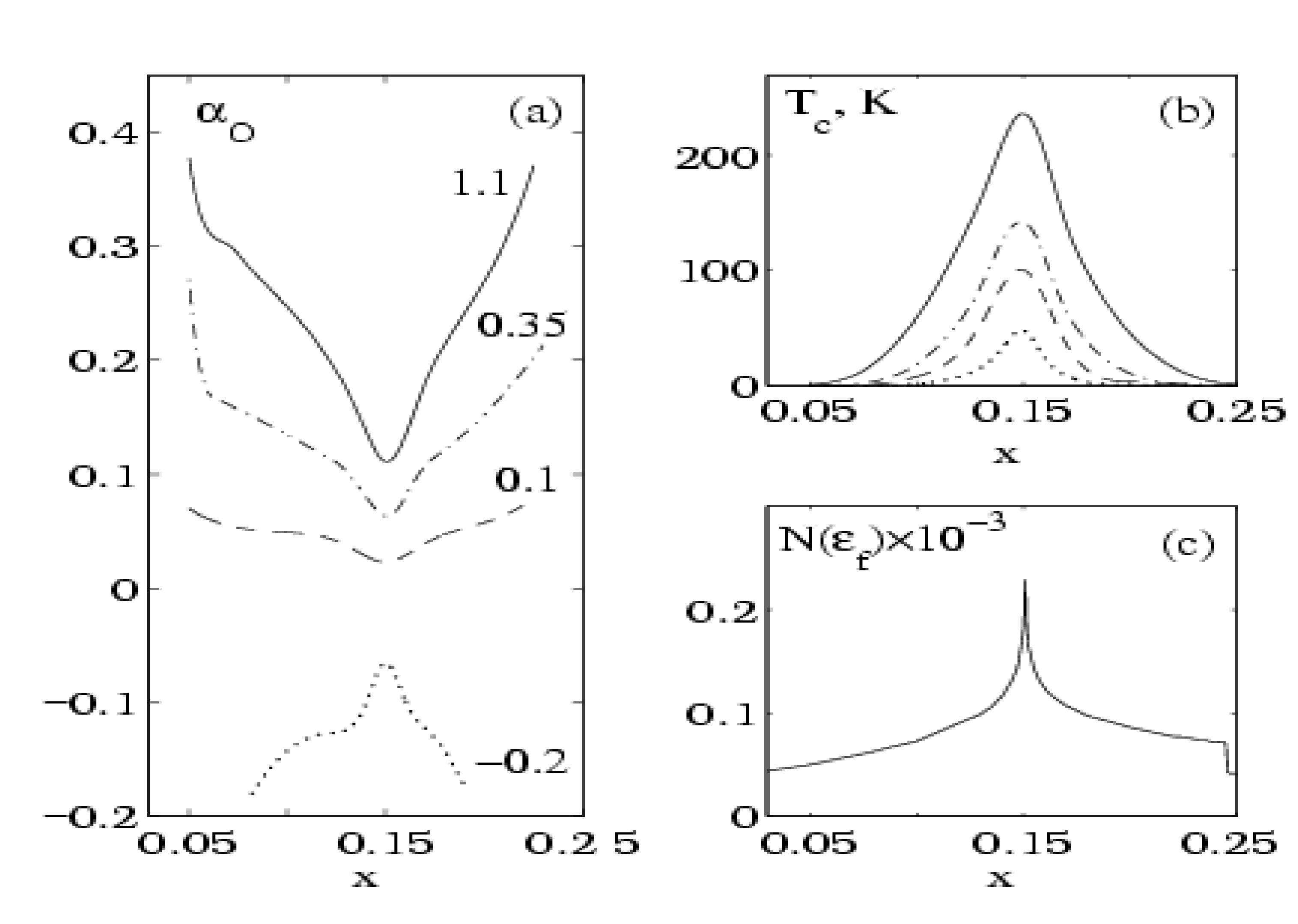


Fig. 11. Plot of the oxygen isotope effect coefficient in Tc against hole concentration for various SC cuprates (D.J. Pringle et al., PRB 62 and references therein).



Site selective substituton reveals no isotope effect (Khasanov et al. Phys. Rev. B 68, 220506 (2003))

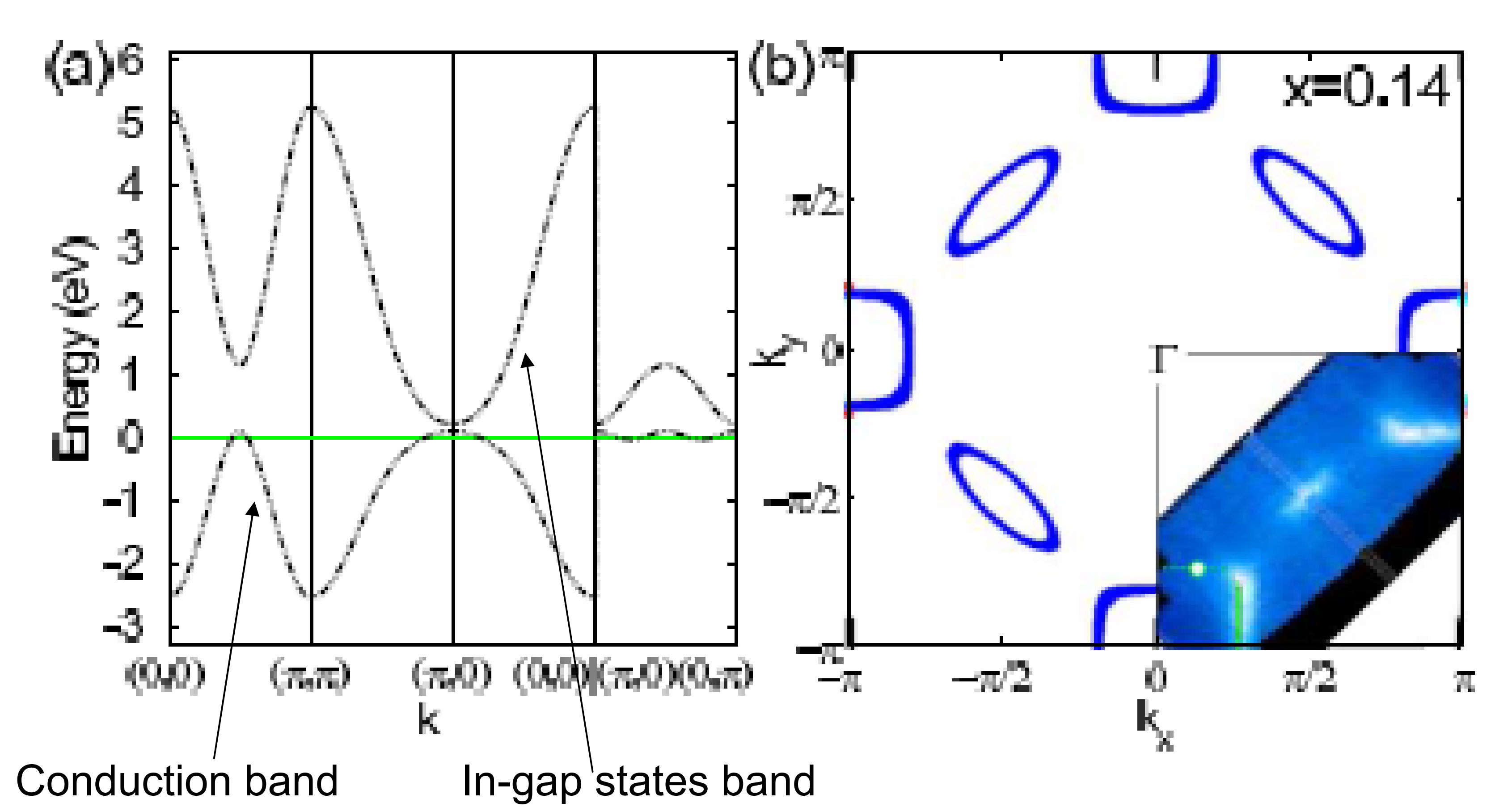
Isotope effect and critical temperature at different values G/J (Shneyder, Ovchinnikov, JETP 2009)



Conclusion

- Both “normal” and d-type superconducting state can be obtained from hole dynamics at the short range AFM background in the self consistent 2D electronic and spin systems in the strong electron correlation regime
- Doping results in two QPT with Fermi surface topology changes at optimal doping p_c=0.15 and p^*=0.24
- Phonon contribution to pairing increase magnetic one. The only fitting parameter G>0 of the EPI was found from the isotope effect. The EPI and magnetic mechanism support each other and are of the same order of magnitude

Band structure of holes in AFM by LDA+GTB and Fermi surface in $Sm_{1.86}Ce_{0.14}CuO_4$ n-type



Korshunov etal, arXiv 0901.2650, ARPES S.Park etal PRB 75, 060501 (2007)

Small phonon contribution to ARPES kink

F.Giustino, M.Cohen, S.Louie, NATURE 06874, 2008

(GGA+DF perturbation theory)

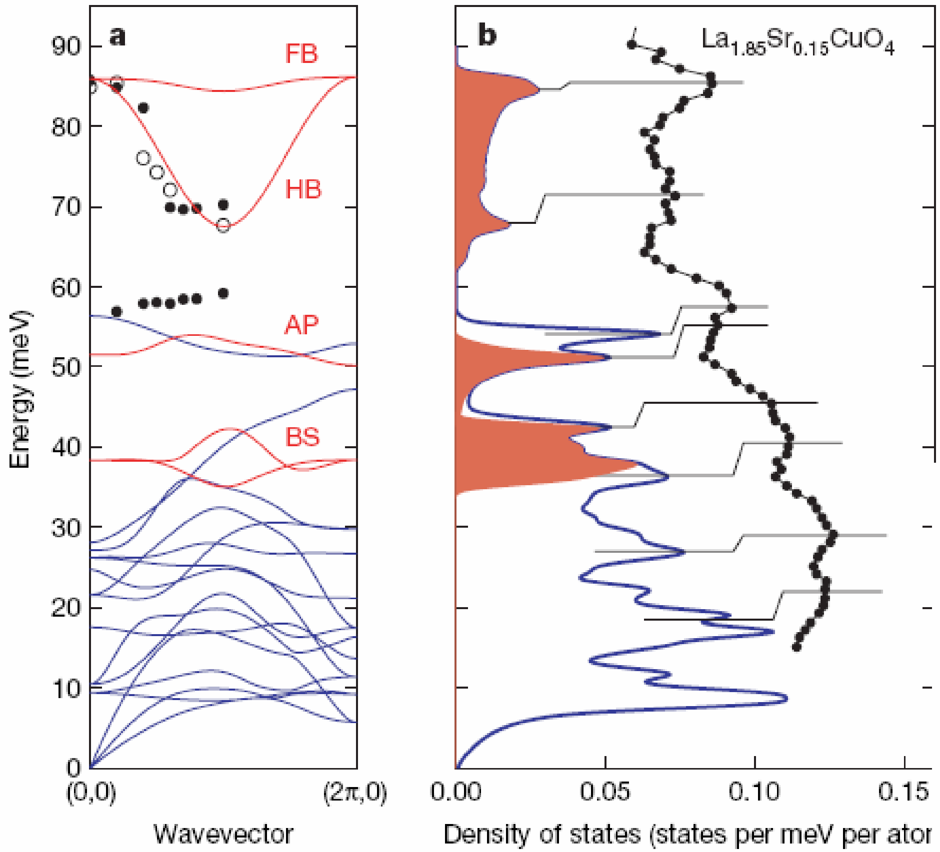


Figure 1 | Phonons of $La_{2-x}Sr_xCuO_4$ at optimal doping ($x = 0.15$).

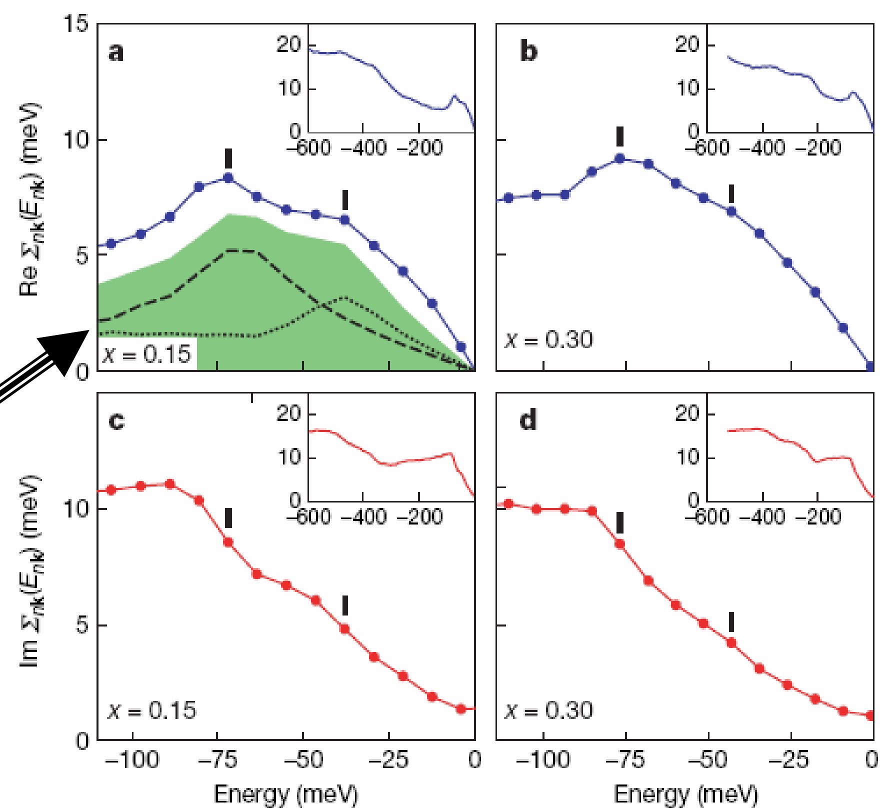
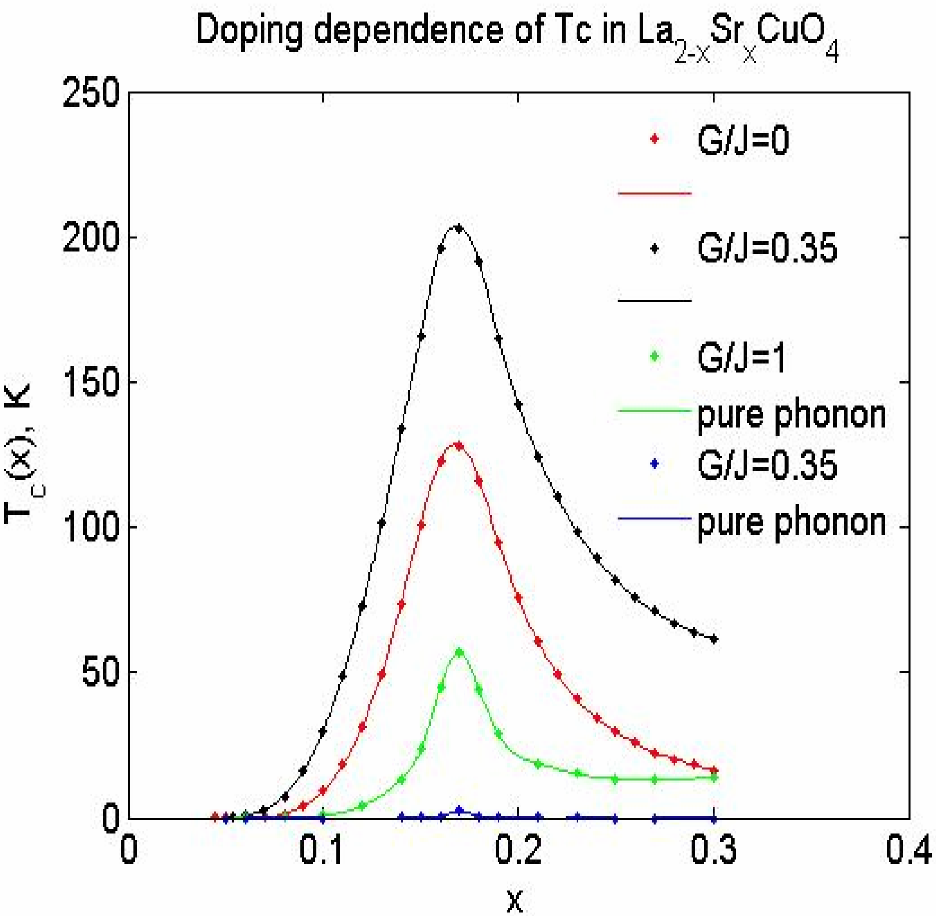
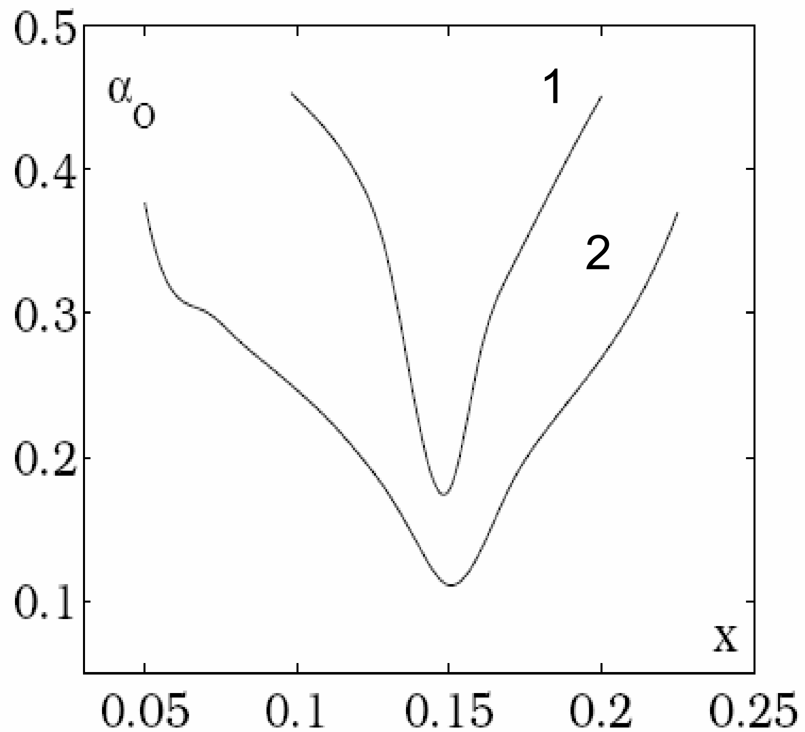


Figure 2 | Calculated electron self-energy in LSCO due to the electron–phonon interaction. a, b, Real parts of the self-energy for optimally

Breathing modes 70meV + buckling / stretching in plane O-O modes 40meV provide 80% (green) of the total self-energy

What would be if to switch off magnetic pairing?





1) Phonon, 2) Phonon +J

Any non-phonon mechanism reduce IE