ISOTOPE EFFECT, PHONON AND MAGNETIC MECHANISM OF PAIRING IN HIGH-TC CUPRATES IN STRONG ELECTRON CORRELATION LIMIT

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Outline

- Microscopically derived t-t’-t”-J* model from ab initio muliband 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

Hybrid LDA+GTB scheme without fitting parameters

(in collaboration with prof.V.I.Anisimov group, Ekaterinburg,
(Korshunov, Ovchinnikov, etal, Phys.Rev.B 2005))

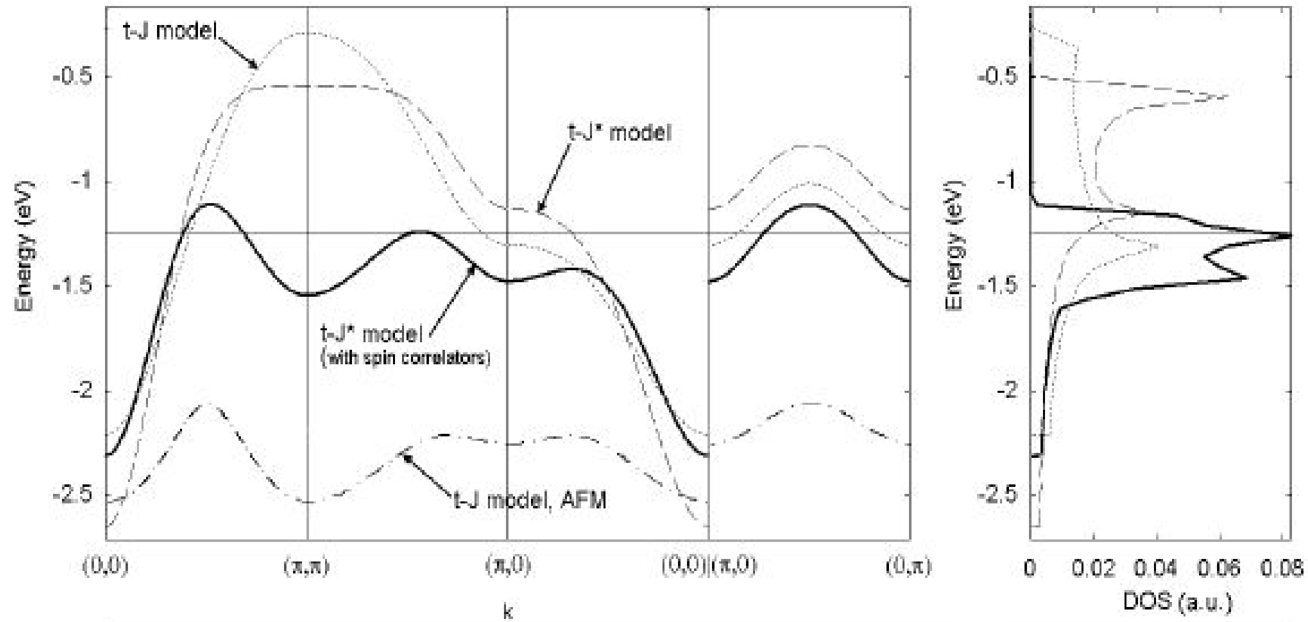
- Projection of LDA band structure and construction the Wannier functions for the multiband p-d –model

- *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

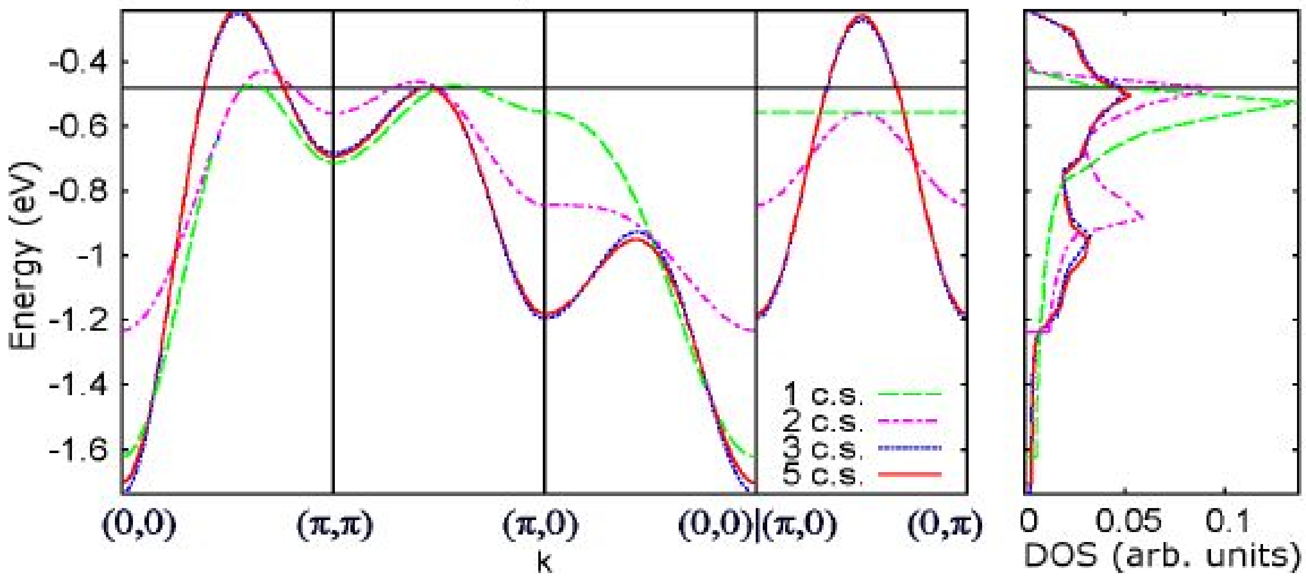
Quasiparticle dispersion in the t-J and t-J* models



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)*]



*v*F 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

Low energy effective model is obtained to be the t-t'-t"-J* model with all parameters calculated from LDA+GTB method

- Restriction to a single *t* or two *t* and *t'* hopping is not enough
- Negligible difference between 3 (t,t',t") and more hoppings is found

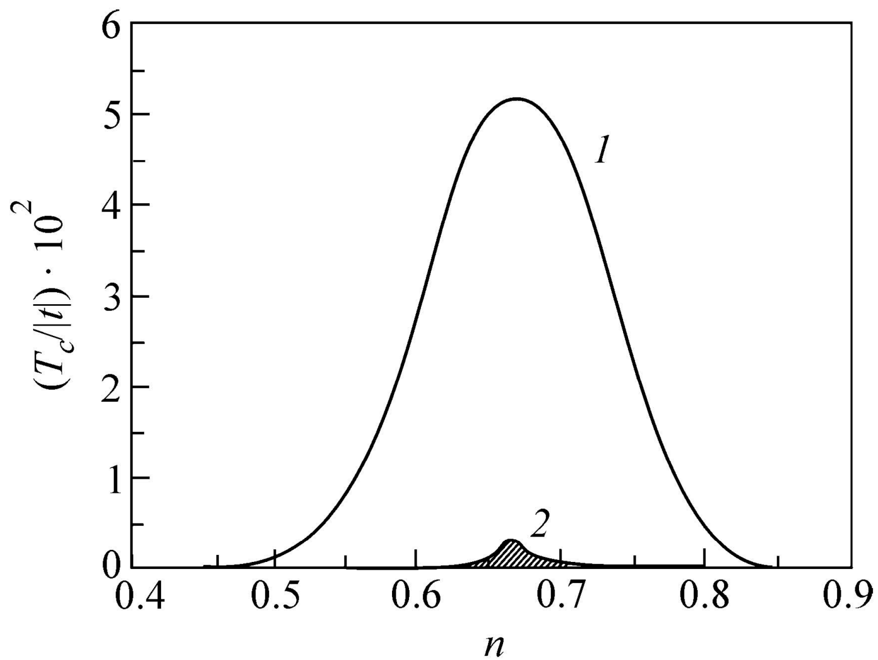
Korshunov etal, PRB 72, 165104 (2005)

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)

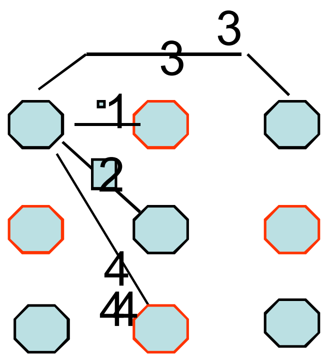
Hole dynamics in SCES at the short range order antiferromagnetic background. SCBA for Self-energy. At low T correlations are static (Barabanov et al, JETP 2001, Valkov and Dzebisashvili, JETP 2005, Plakida and Oudovenko JETP 2007, Korshunov and Ovchinnikov Eur.Phys.J.B, 2007)

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

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

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

Correlation functions are calculated follow Valkov and Dzebisashvili, JETP 2005



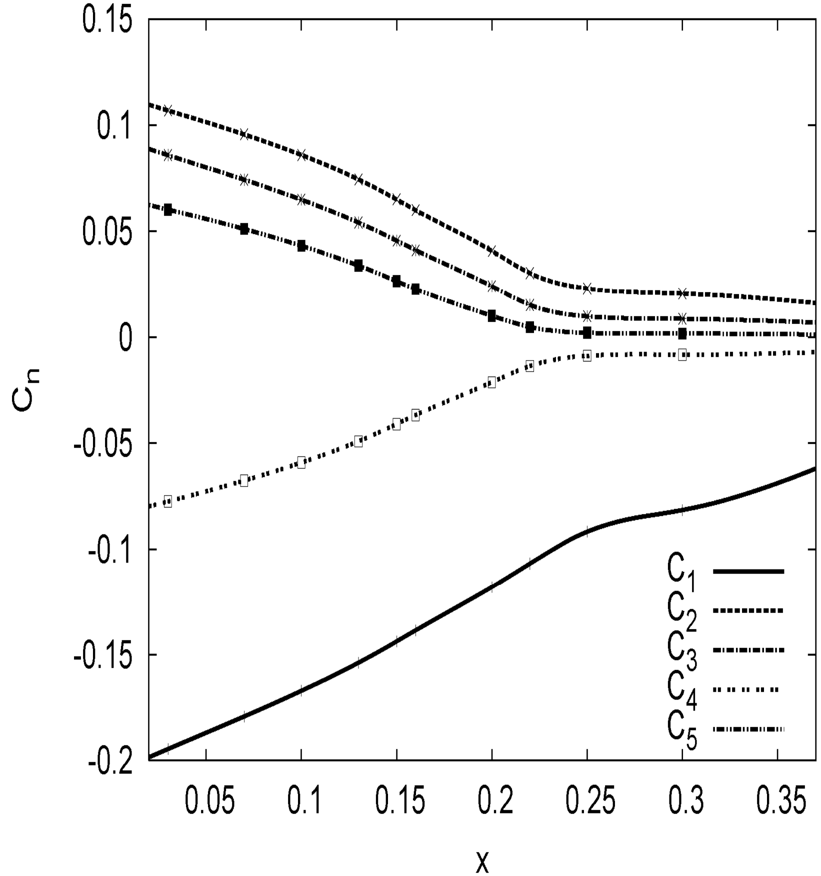
Beyond the Hubbard 1: short range magnetic order in spin liquid state up to 9-th neighbor

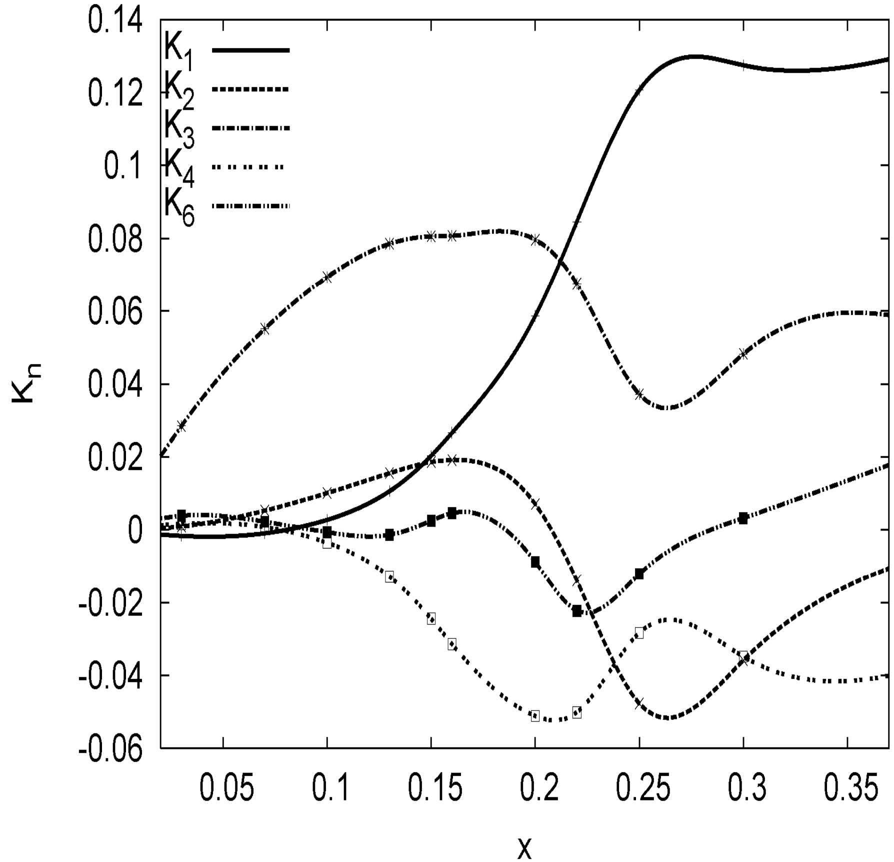
Self consistent spin and charge

Correlation functions in the t-J* model

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

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





Change of Fermi surface topology with doping

Korshunov, Ovchinnikov Eur.Phys.J.B 2007

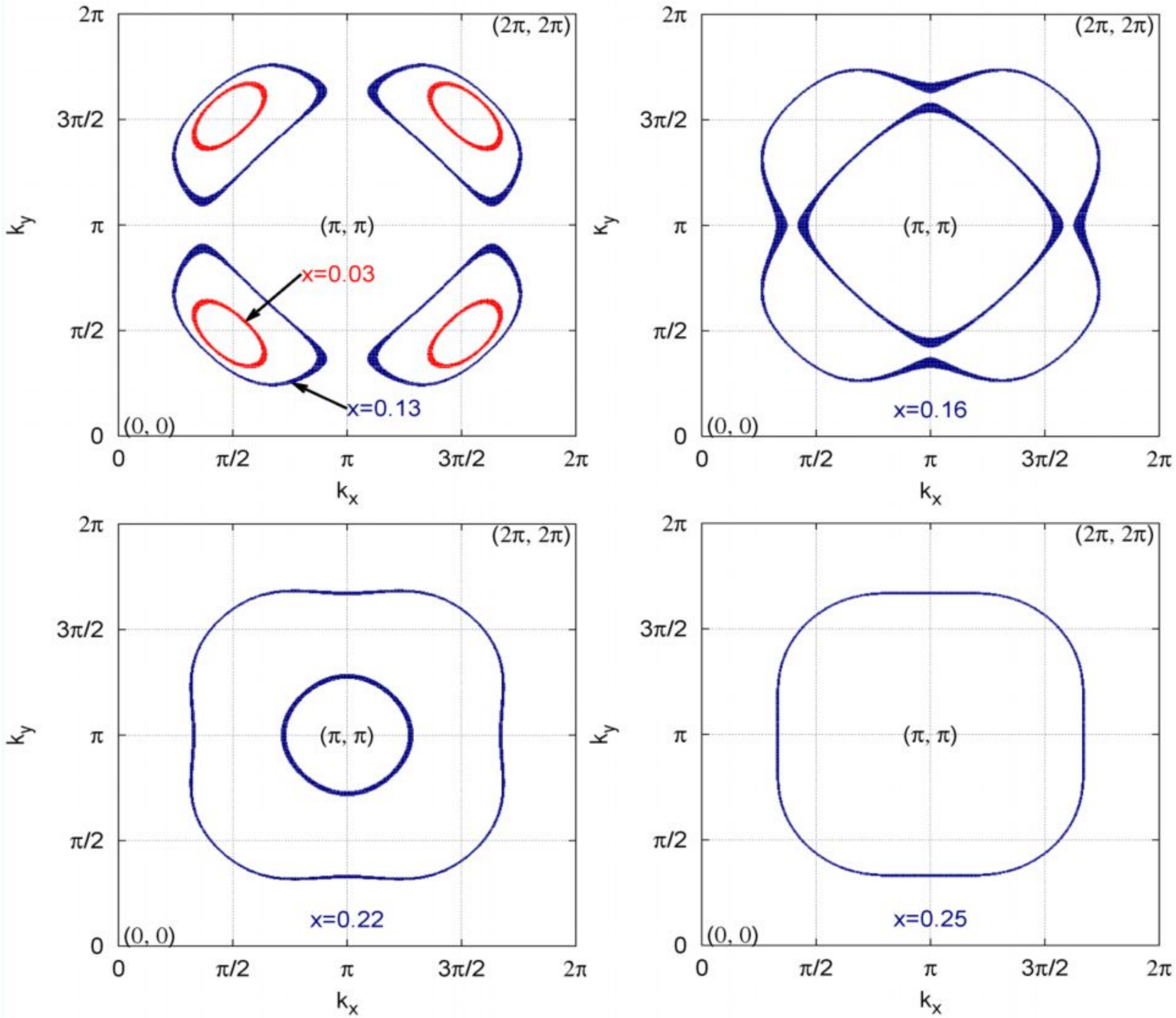


Fig. 1. Fermi surface evolution with doping (hole concentration) x.

Xc1=0.15=Popt – maximum Tc(x)

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

Effective mass from quantum oscillations measurements:

+ YBa2Cu3O6.5(p=0.1) Doiron-Leyraud l Nature,2007

* YBa2Cu4O8 (p=0.125) Yelland etal, PRL 100, 2008

x YBa2Cu4O8 Bangura etal, PRL 100, 047004, 2008

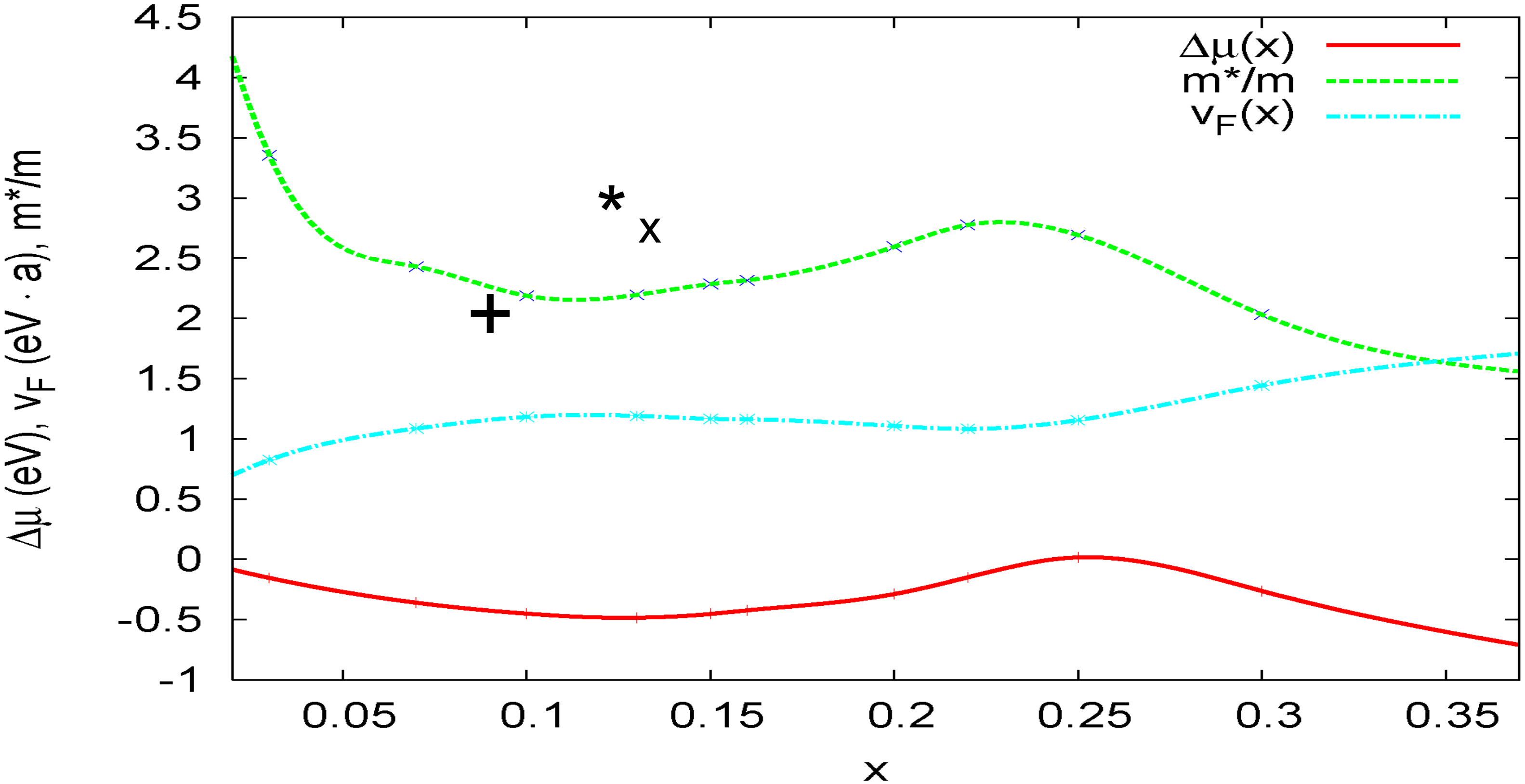


Fig. 2. Doping dependent evolution of the chemical potential shift, nodal Fermi velocity, and effective mass.

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)

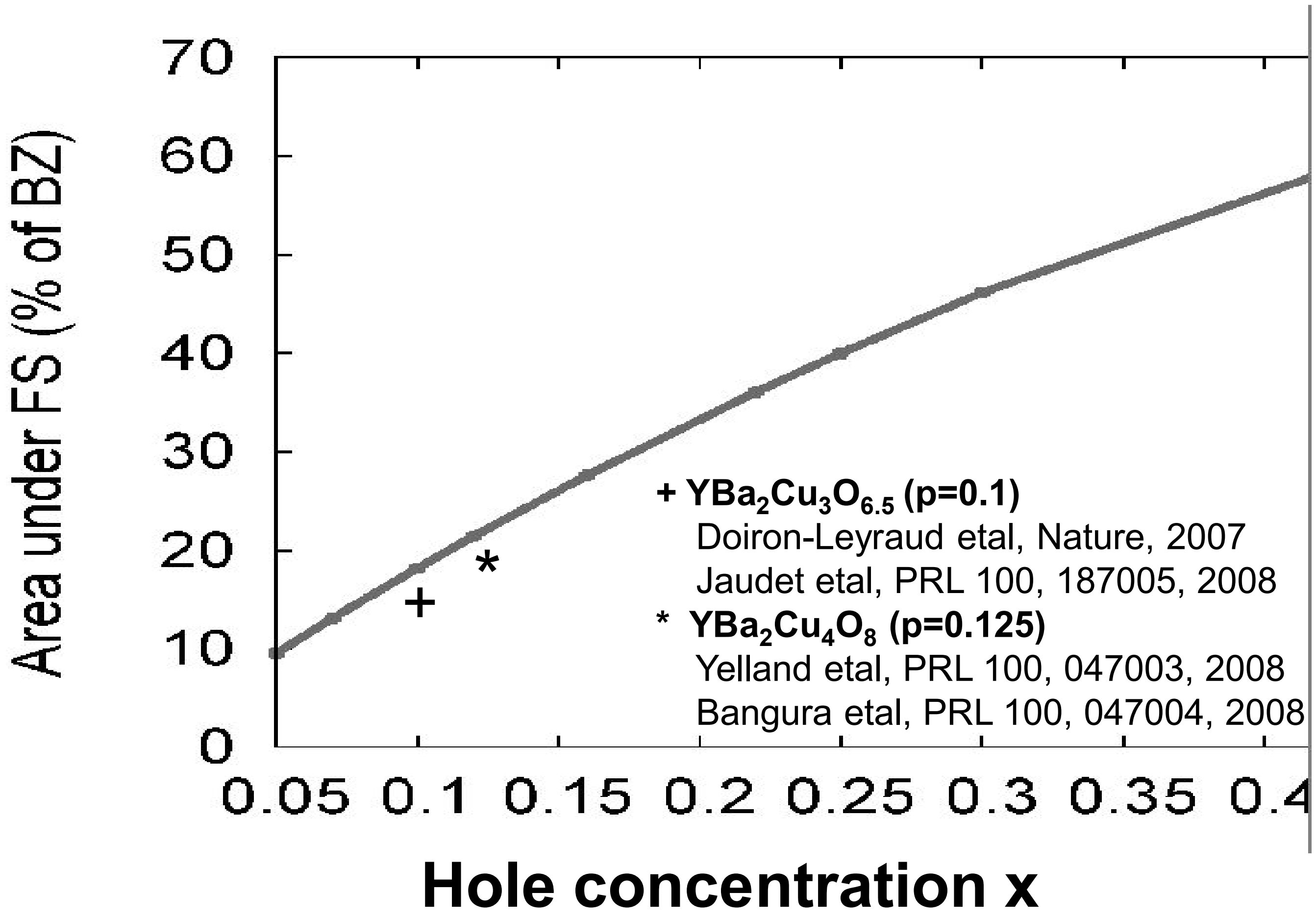
Hole occupied states

Nh(k)=1-Ne(k)

= 2x/(1+x)

Generalised Luttinger theorem: Korshunov, Ovchinnikov,

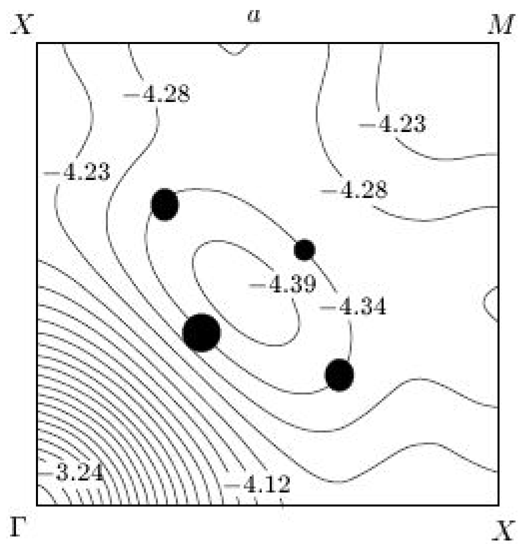
Sol.St.Phys 2003

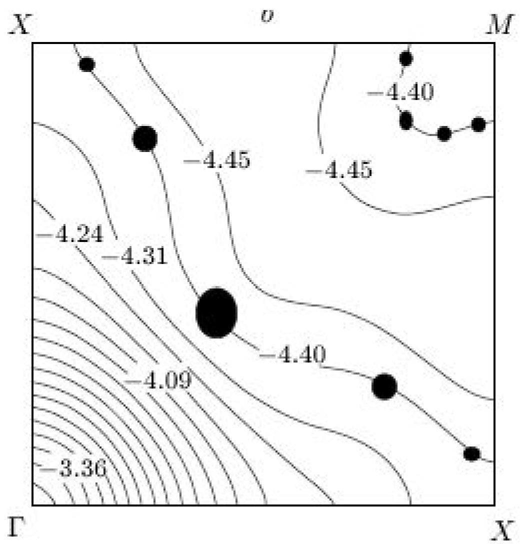


Barabanov et al, JETP 119, вып.4 (2001)

Spin-polaron approach, *Mori-type projection method for spin-fermion model*

X=0.06



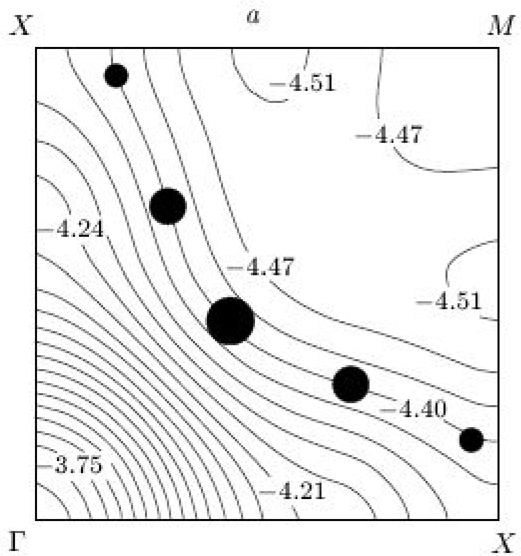


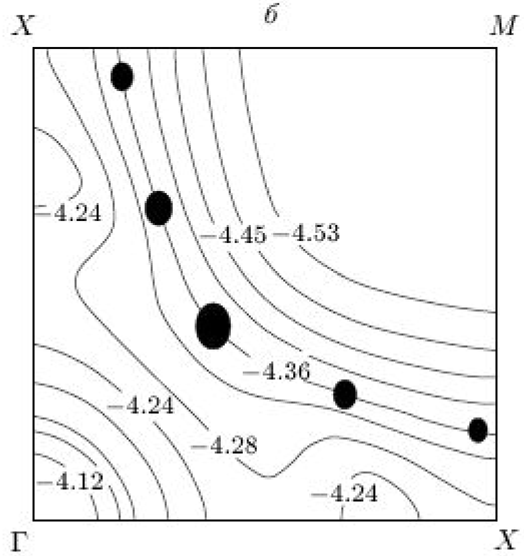
X=0.11

Shadow band intensity is smaller due to spectral weight redisribution.

No QP damping

X=0.14





X=0.19

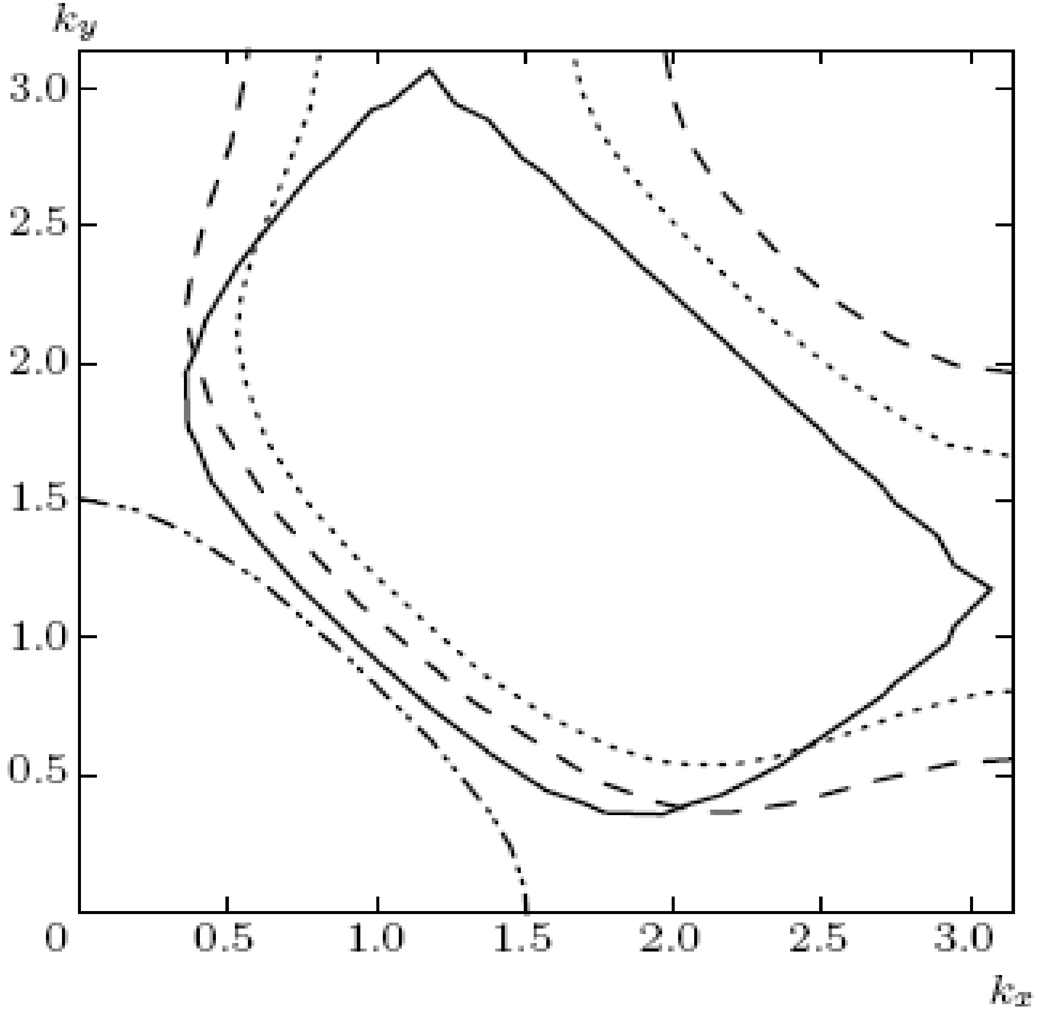


Fig. 15. Doping dependence of the FS for $\delta = 0.1$ (solid line at $T = 0.03t$ and dotted line at $T = 0.3t$), $\delta = 0.2$ (dashed line), and $\delta = 0.3$ (dot-dashed line) for $\Delta = 4t$

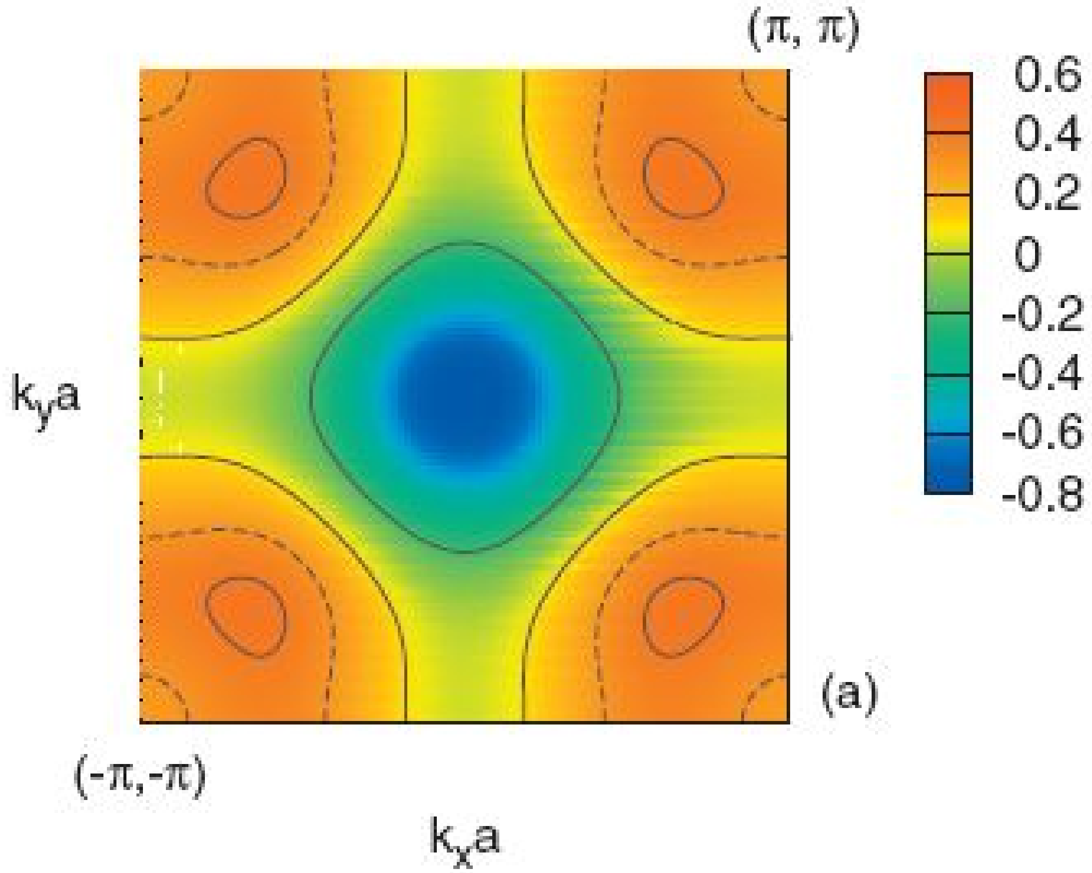
Fermi surface
in the p-d Hubbard
model,

SCBA (non crossing
approximation) for the
self-energy,
$\Sigma(\kappa,\omega) = \Sigma_{Re} + \iota\Sigma_{Im}$

Plakida, Oudovenko
JETP 131, 259 (2007)

Ab initio variational CASSSF method gives similar results for the doping evolution of the Fermi surface: from small hole pockets to large hole FS with both hole and electron FS in the intermediate region

(Hozoi, Laad, Fulde, PRB 2008)



Effect of short antiferromagnetic order on the electron spectrum

(Kuchinskii, Nekrasov, Sadovskii,

JETP Lett. 2005, JETP 2006, JETP Lett. 88, 224, 2008)

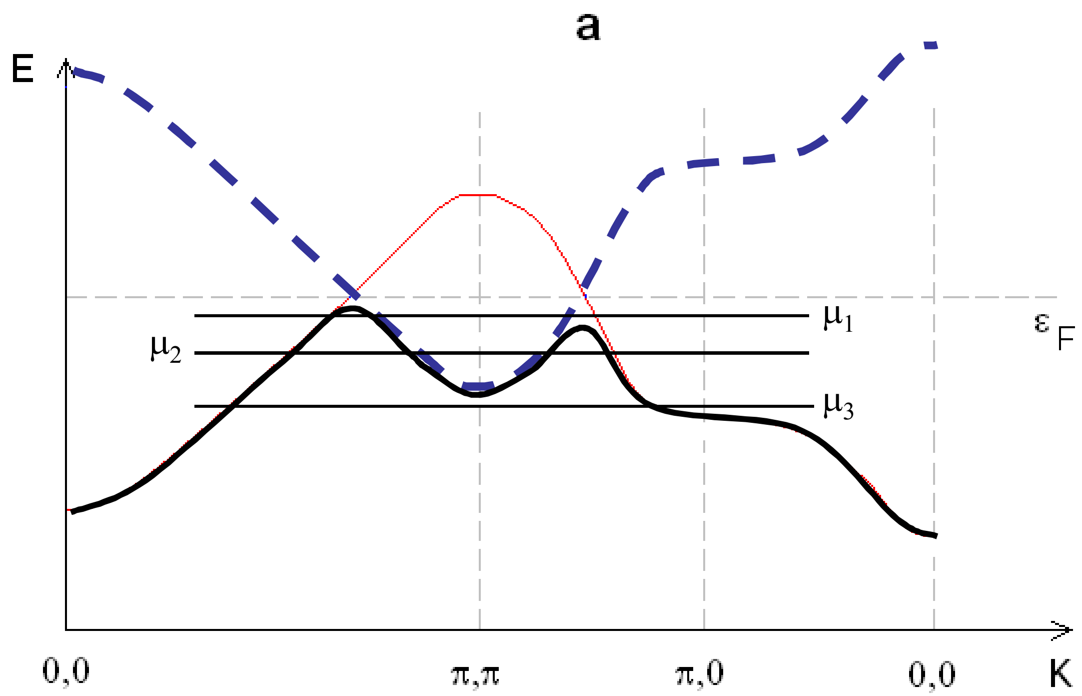
Green function for electron interacting with a random
Gaussian spin fluctuation field is given by

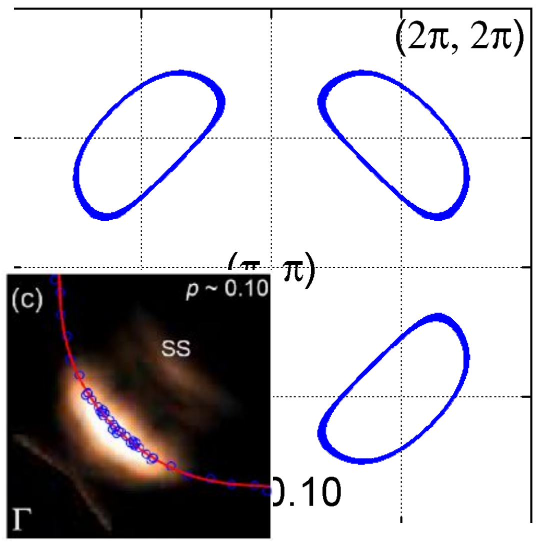
$$G_D(\mathbf{k},\varepsilon) = \frac{\varepsilon - \varepsilon(\mathbf{k}+\mathbf{Q}) + i\upsilon k}{\left(\varepsilon - \varepsilon(\mathbf{k})\right)\left(\varepsilon - \varepsilon(\mathbf{k}+\mathbf{Q}) + i\upsilon k\right) - |D|^2}$$

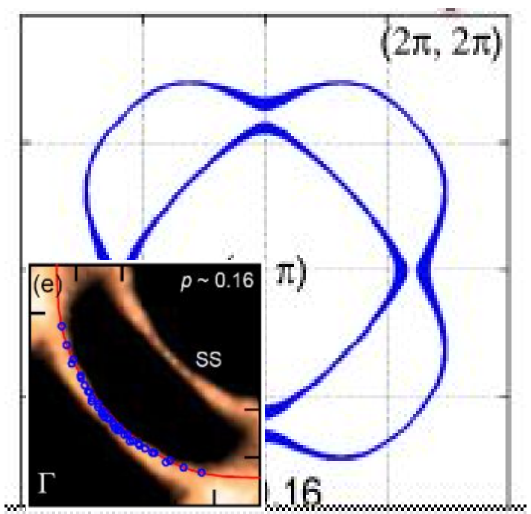
Here D is the amplitude of the fluctuating AFM order , $\varepsilon(\mathrm{k})$ is the electron dispersion in the paramagnetic state

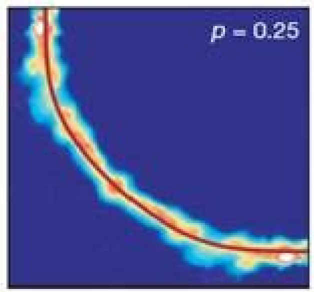
$$\upsilon = \left|\upsilon_x(\mathbf{k}+\mathbf{Q})\right| + \left|\upsilon_y(\mathbf{k}+\mathbf{Q})\right|, \quad \upsilon_{x,y}(\mathbf{k}) = \partial\varepsilon(\mathbf{k})\big/\partial k_{xy}$$

In the limit of zero Im part the long range AFM (SDW) is restored



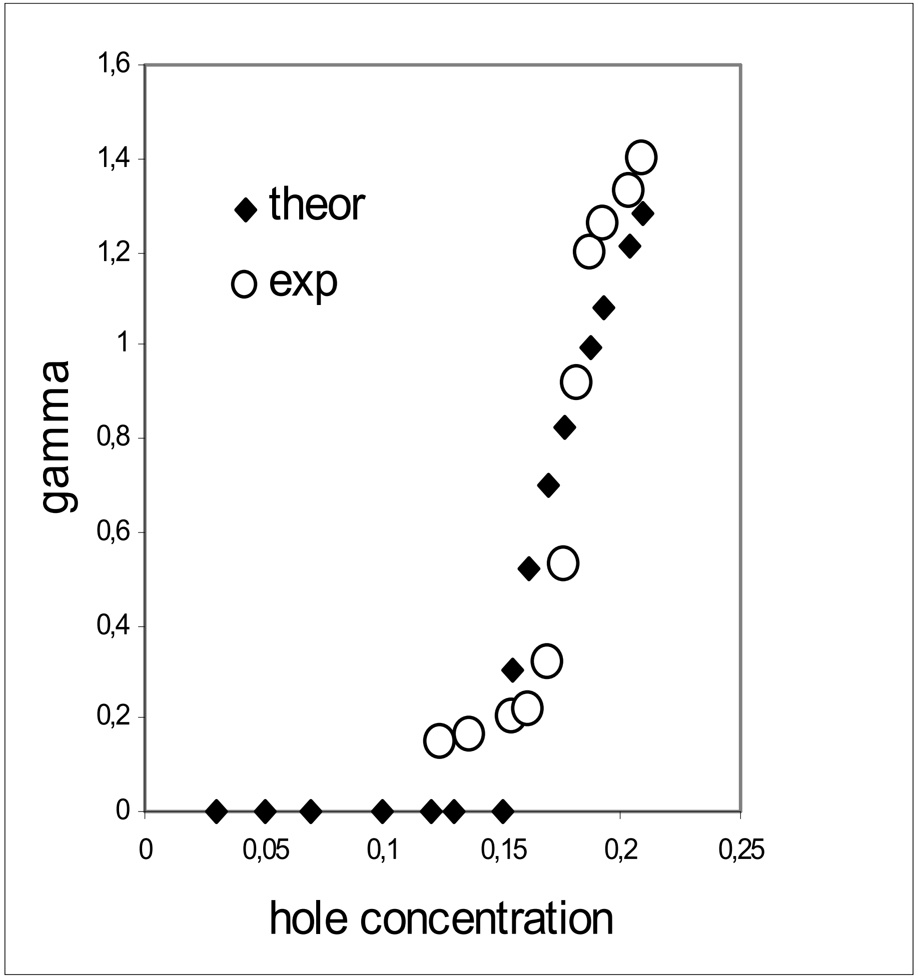






ARPES *Hashimoto etal, PRB 2008*

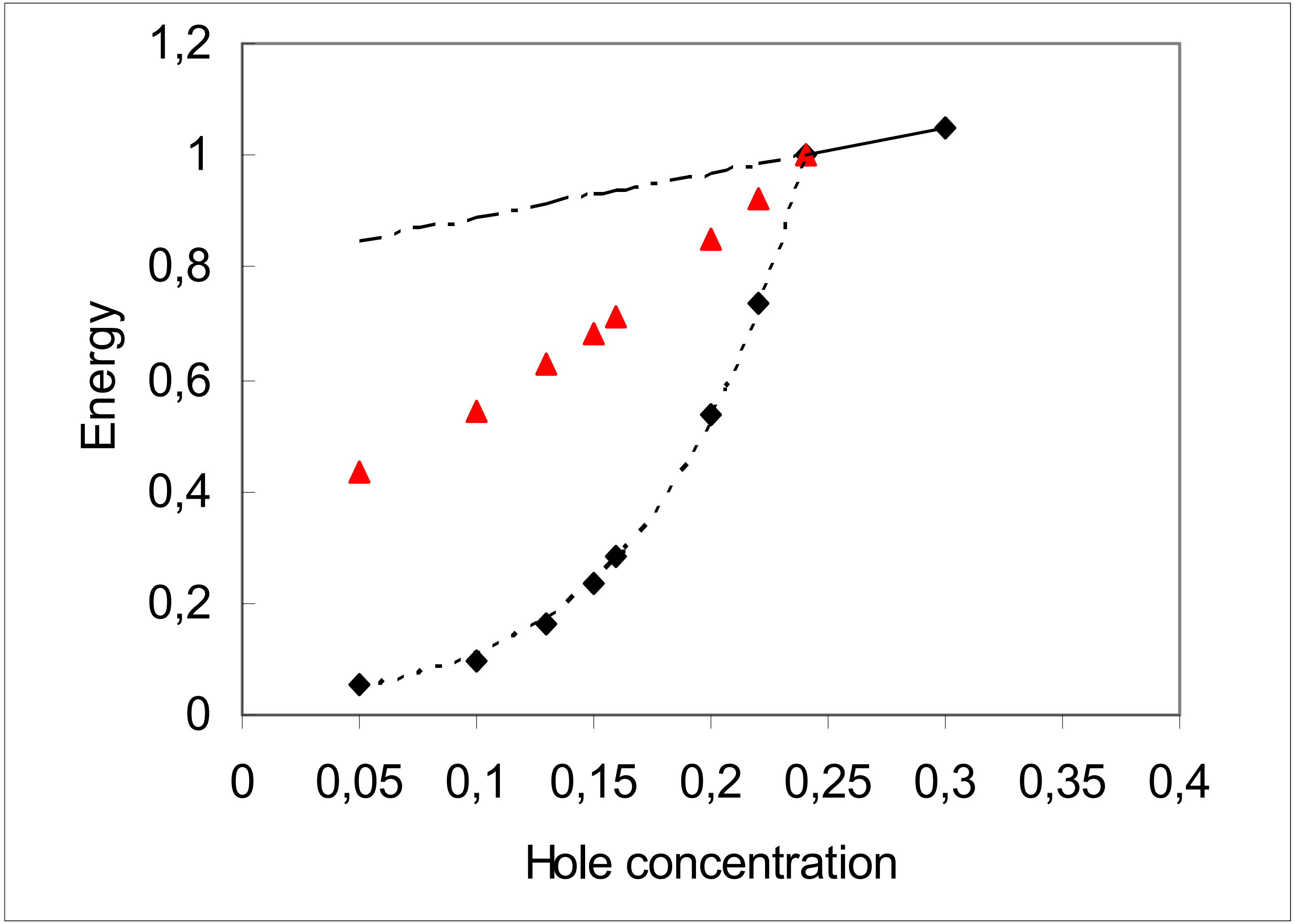
Electronic heat capacity near the Lifshitz QPT



$$\delta\gamma = \delta(C_e/T) \sim (x - x_{c1})^{0.5}$$

Experiment from Loram etal, J.Phys.Chem.Sol.2001, T=10K

$$\gamma_{exp} = \gamma_0 + \delta\gamma$$



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. Red triangles-fitting with Loram-Cooper triangular pseudogap model. Dash line – exponential fitting **E/E* ~ exp(-4Eg(x)/J)**

Magnetic mechanism of superconductivity in the Hubbard and t-J models

- Anderson RVB 1987, Baskaran, Zhou, Anderson 1987
- 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
- QMC gives controversial conclusions some pro and some contra, the well-known paper by Aimi and Imada, JPSJ 2007 by a new QMC reject d-type superconductivity. Is it the final answer?
- We will use Plakida-type formulation of the mean field theory with "no-double occupation" constraint and short AFM correlations

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

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

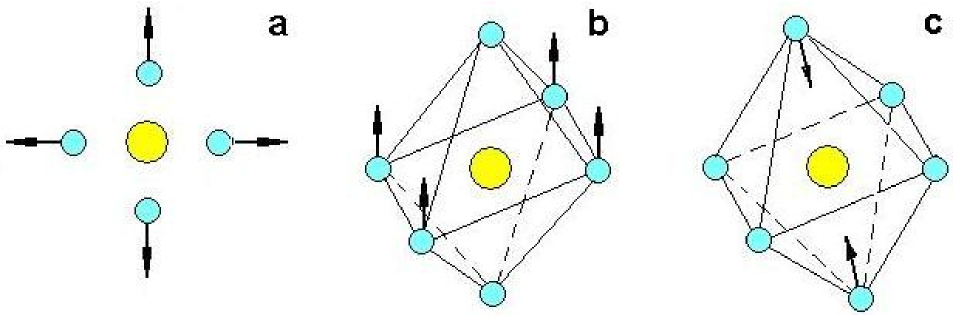
$$E_n \to E_n\left(f\right) = E_n\left(0\right) + \vec{g}_n \vec{u}_f, \qquad t_{fg}^{mm'} \to t_{fg}^{mm'} = t_{fg}^{mm'}\left(0\right) + \vec{V}^{mm'} \vec{u}_{fg}$$

- $Electron - phonon\ interaction$

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

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

Oxygen displacements



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

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

Matrix

$$V_{dia,m}^{(1)}(q) = \frac{2ig_{dia,m}^{(1)}}{\sqrt{2M_O\omega_{q,\nu=1}}}\left(e_x(O)\sin\frac{q_x a}{2} + e_y(O)\sin\frac{q_y a}{2}\right),$$

$$V_{off,mm'}^{(1)}(\mathbf{k},\mathbf{q}) = \frac{8ig_{off,mm'}^{(1)}}{\sqrt{2M_O\omega_{\mathbf{q},1}}}\left[\mathrm{e}_x(O_x)\sin\frac{q_x a}{2} + \mathrm{e}_y(O_y)\sin\frac{q_y a}{2}\right]\left[\gamma(\mathbf{k}) + \gamma(\mathbf{k}+\mathbf{q})\right],$$

$$\text{где } \gamma(\mathbf{q}) = \left(\cos q_x a + \cos q_y a\right)/2.$$

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))

Electronic contribution to pairing in t-J* model

$$\Delta_{\mathbf{k}}^{tJ*} = \frac{1}{N}\sum_{\mathbf{q}}\left(-\frac{4}{1+x}t_{\mathbf{q}} - \frac{1-x}{1+x}\left(J_{\mathbf{k}+\mathbf{q}} + J_{\mathbf{k}-\mathbf{q}}\right) - -4t_{\mathbf{k}}t_{\mathbf{q}} + \frac{1-x}{1+x}\frac{t_{\mathbf{q}}^2}{E_{ct}}\right)B_{\mathbf{q}},$$

Phonon contribution

$$\Delta_{\mathbf{k}}^{el-ph} = \frac{1}{N}\sum_{\mathbf{q}}\frac{1+x}{4}\{V_{-\mathbf{q},\mathbf{q},\mathbf{q}+\mathbf{k}} + V_{-\mathbf{q},\mathbf{q},\mathbf{q}-\mathbf{k}}\}B_{\mathbf{q}} - -\frac{1}{N^2}\sum_{\mathbf{q},\mathbf{p}}\frac{3}{2(1+x)}\{V_{-\mathbf{q},\mathbf{q},\mathbf{p}+\mathbf{k}} + V_{-\mathbf{q},\mathbf{q},\mathbf{p}-\mathbf{k}}\}B_{\mathbf{q}}c_{\mathbf{q}-\mathbf{p}}.$$

$$B_{\mathbf{q}} = \left\langle X_{-\mathbf{q}}^{0,-\sigma}X_{\mathbf{q}}^{0,\sigma}\right\rangle$$

c_q - spin correlation function,

$$\Delta_{\mathbf{k}}^{tot} = \Delta_{\mathbf{k}}^{tJ*} + \Delta_{\mathbf{k}}^{el-ph}.$$

$$\Delta_{\mathbf{k}}^{(d_{x^2-y^2})} = = -\frac{1}{N}\varphi(\mathbf{k})\sum_{\mathbf{q}}\left\{\frac{1-x}{1+x}J + \left(\frac{3(-c_{01})+0.5(1+x)^2}{2(1+x)}\right)\times \times\theta\left(|\xi_{\mathbf{q}}-\mu| - \omega_D\right)G\right\}\times B_{\mathbf{q}}\varphi(\mathbf{q}),$$

$$G = \left(\frac{v_{\mathrm{dia},\nu=2}^2}{\omega_{\nu=2}} - \frac{v_{\mathrm{dia},\nu=1}^2}{\omega_{\nu=1}}\right)$$

$$\varphi(\mathbf{k}) = (\cos(k_x) - \cos(k_y)),\ \theta(x) = 0$$

G =Buckling- Breathing modes EPI, no contribution from the apical breathing mode

Oxygen isotope effect: experiment and theory

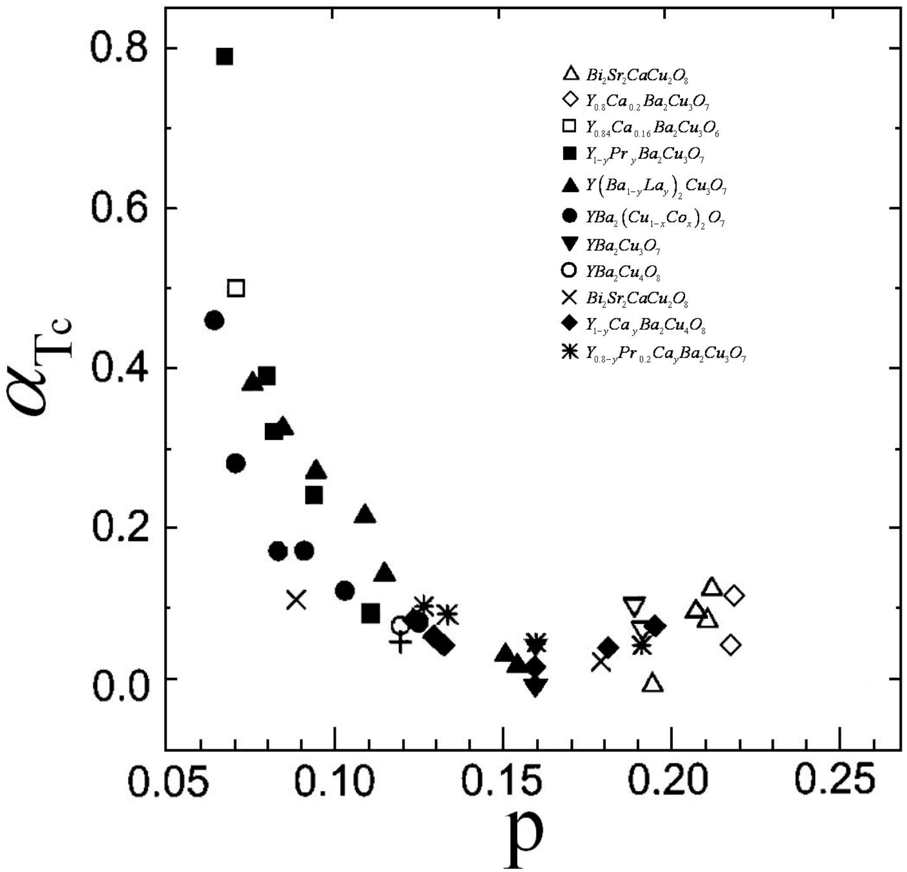
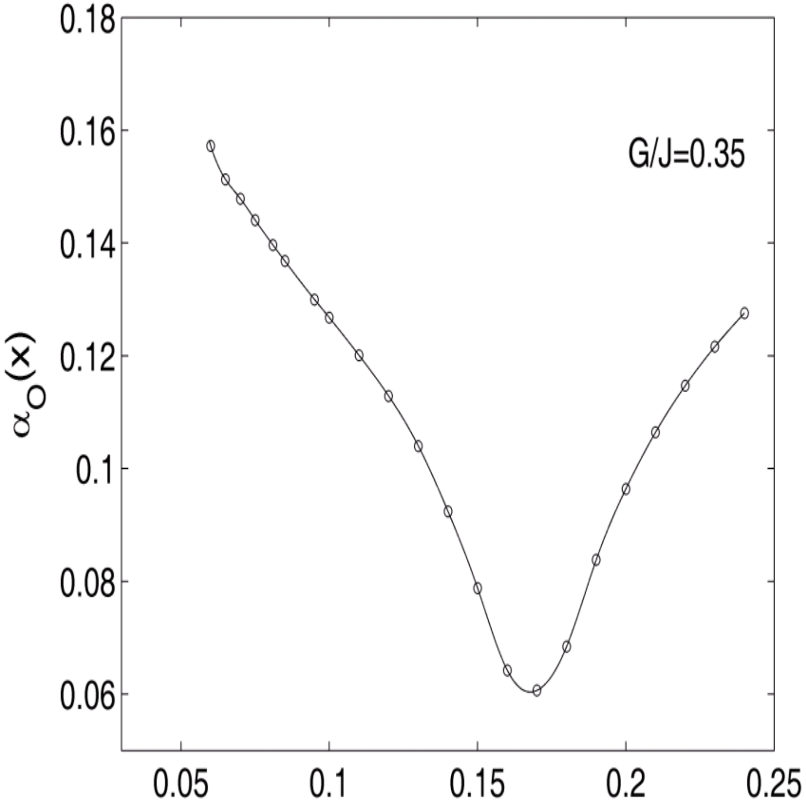


Fig. 11. Plot of the oxygen isotope effect coefficient in Tc against hole concentration for various SC cuprates (D.J. Pringle et al., PRB 62 and references therein).



E.Shneyder, S.Ovchinnikov

FPS, 2008

S.Ovchinnikov,
E.Shneyder, 2008

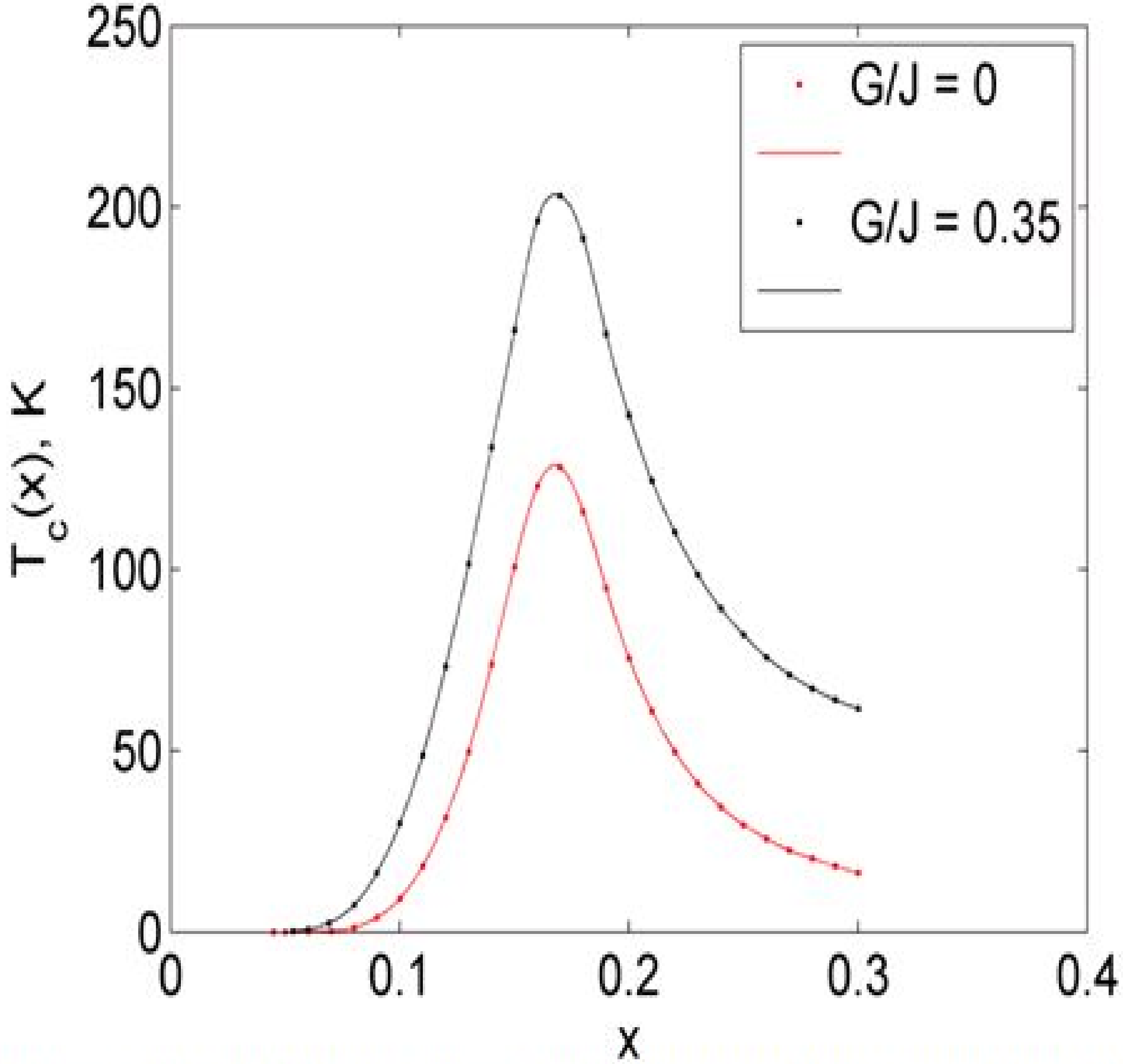


Figure 2. The critical temperature as function of the doping concentration in $La_{2-x}Sr_xCuO_4$. The maximum corresponds to the optimal doping x=0.17. The pure magnetic mechanism takes place at G=0 and both magnetic and phonon mechanisms are considered with parameter G/J=0.35 detemined from the isotope effect. The phonon-mediated pairing works together with the magnetic one increasing each other.

Conclusion

- Both “normal pseudogapped”, 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
- Fermi surface topology changes result in QPT with doping
- Phonon contribution to pairing may decrease or 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

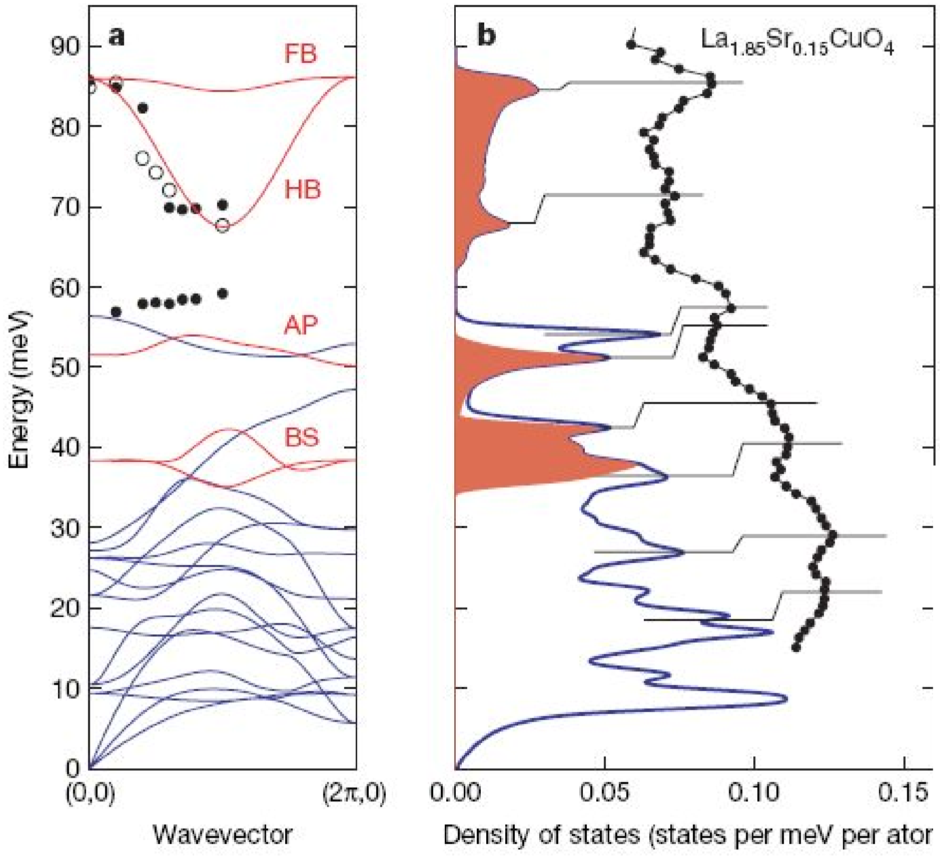


Figure 1 | Phonons of $La_{2-x}Sr_xCuO_4$ at optimal doping ($x = 0.15$).

Small phonon contribution to ARPES kink

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

(GGA+DF perturbation theory)

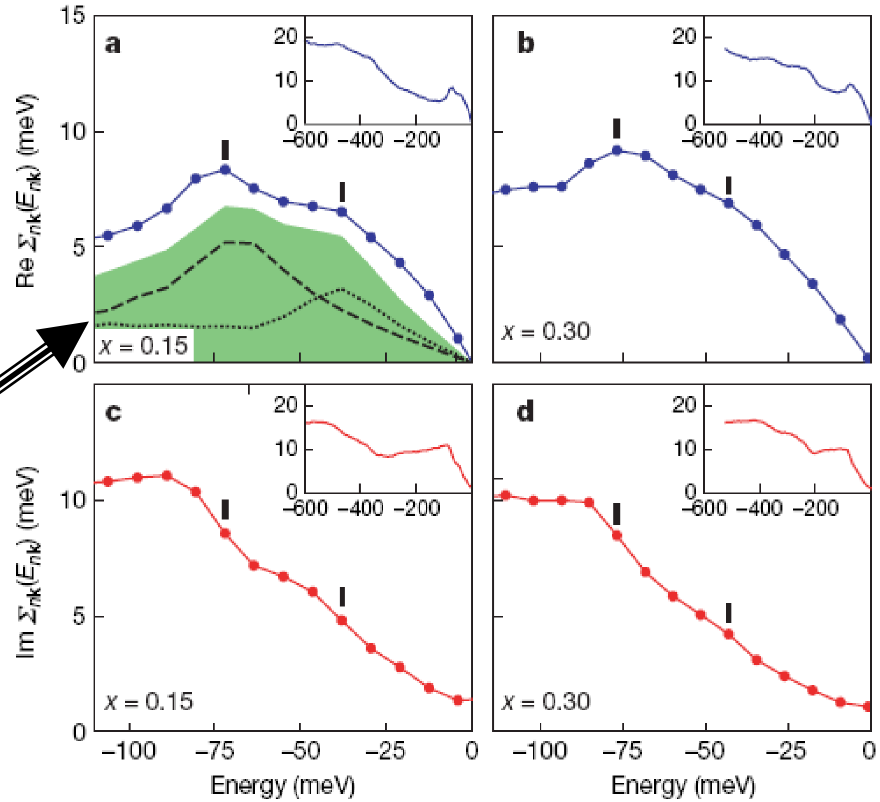


Figure 2 | Calculated electron self-energy in LSCO due to the electron–phonon interaction. a, b, Real parts of the self-energy for optimally

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