XV Конференция молодых ученых
"Проблемы физики твердого тела и высоких давлений"

Влияние межузельных кулоновских корреляций на условия реализации высокотемпературной сверхпроводимости с d- и s-типом симметрии параметра порядка

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пос.Вишневка, пансионат МГУ "Буревестник" 16-26 сентября 2016г.

Outline

I. Contradiction between theory and experiment

II . Fundamental interactions in CoO_2 – plane of cuprate HTSC;

III. Emery model → Spin-fermion model;

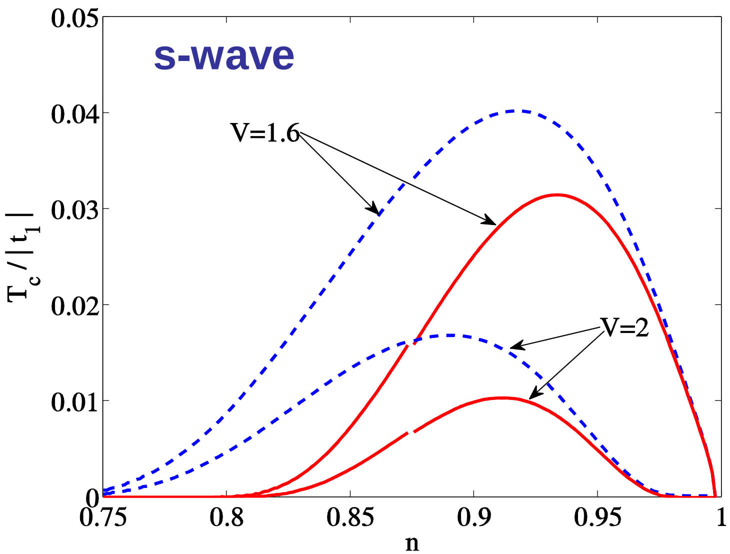
IV. Spin-polaron nature of Fermi quasiparticles in HTSC;

V. Cooper instability in the ensemble of spin-polarons;

VI. Stability of the d-wave pairing with respect to the intersite Coulomb repulsion in cuprates;

VII. Conclusion

Effect of the intersite Coulomb repulsion on the s- and d-wave coupling in Hubbard model (t<<U) and in the t-J – model



Equation for Tc in s-wave phase

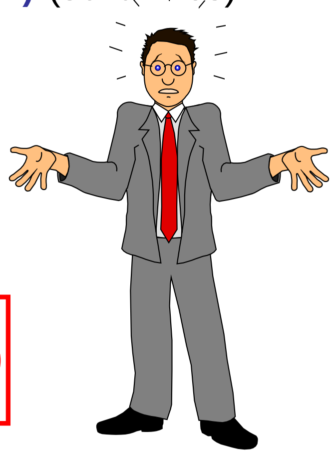
$$1=\frac{4t}{N}\sum_q\left(\cos q_x+\cos q_y\right)\Phi(q)-\frac{V}{N}\sum_q\left(\cos q_x+\cos q_y\right)^2\Phi(q)$$

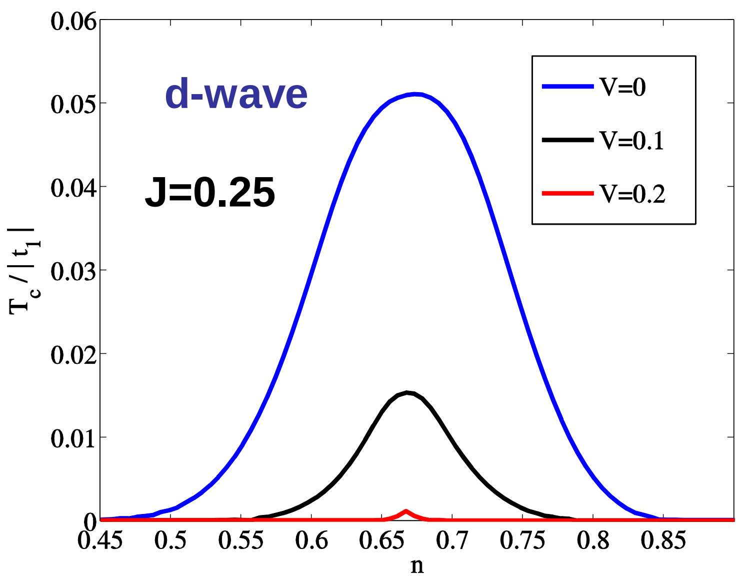
$$\Phi(q)=\frac{1}{2E_q}\tanh\left(\frac{E_q}{2T}\right)$$

R.O. Zaitsev, JETP (2004) (dashed line)

At account for band of fluctuation states

V.V. Val'kov, M.M. Korovushkin, JETP (2011) (solid lines)





Equation for T_c in d-wave phase

$$1=\frac{J}{N}\sum_q\left(\cos q_x-\cos q_y\right)^2\Phi(q)$$

$$1=\frac{(J-V)}{N}\sum_q\left(\cos q_x-\cos q_y\right)^2\Phi(q)$$

$$1=\frac{\left(J-V+A_{el-ph}+A_{sf+cf}\right)}{N}\sum_q\left(\cos q_x-\cos q_y\right)^2\Phi(q)$$

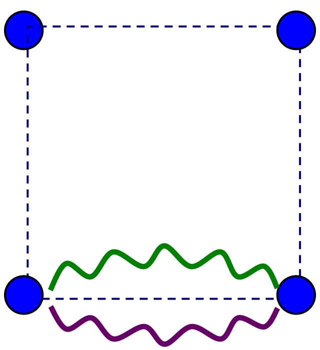
A_{el-ph} - **E.I. Shneider, S.G. Ovchinnikov, JETP (2009)**

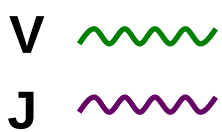
A_{sf+cf} - **N.M. Plakida, V.S. Oudovenko, EPJB (2013); JETP (2014)**

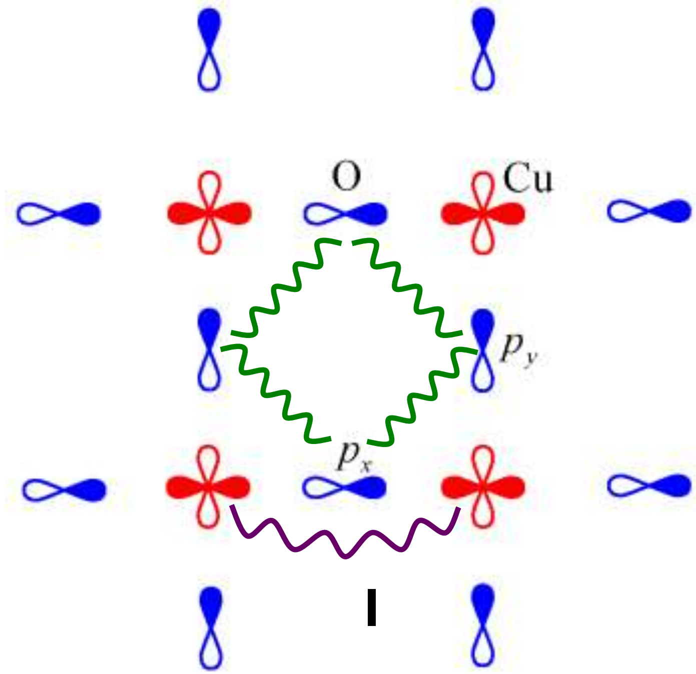
Contradiction between theory and experiment

There is a contradiction between the theory and experiment: account for the intersite Coulomb repulsion suppresses the d-wave pairing that occurs in reality, but does not effect the s-wave phase.

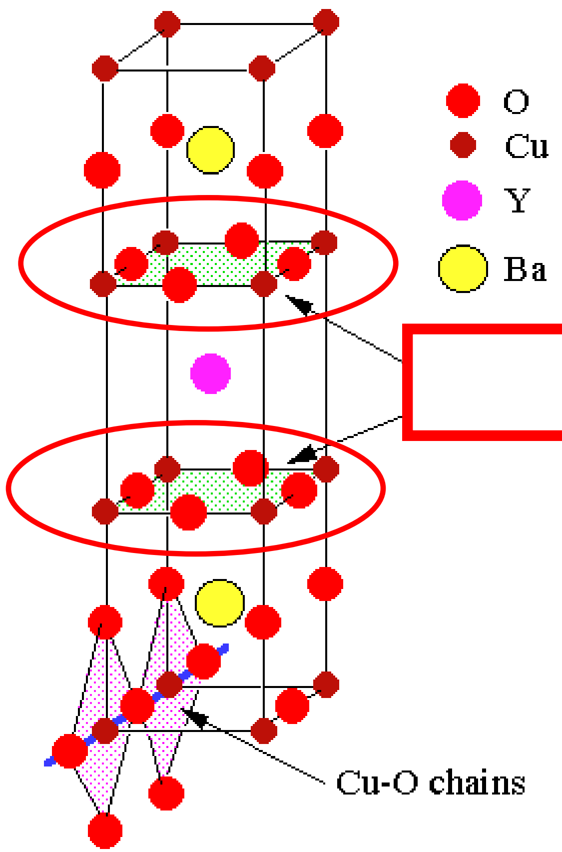
An account for the real structure of the CuO_2-plane described by the Emery model eliminates the mentioned contradiction, because in the proposed theory the Coulomb potential of holes at the neighboring sites does not contribute to the solution of the integral equation for the d-wave pairing for symmetry reasons.



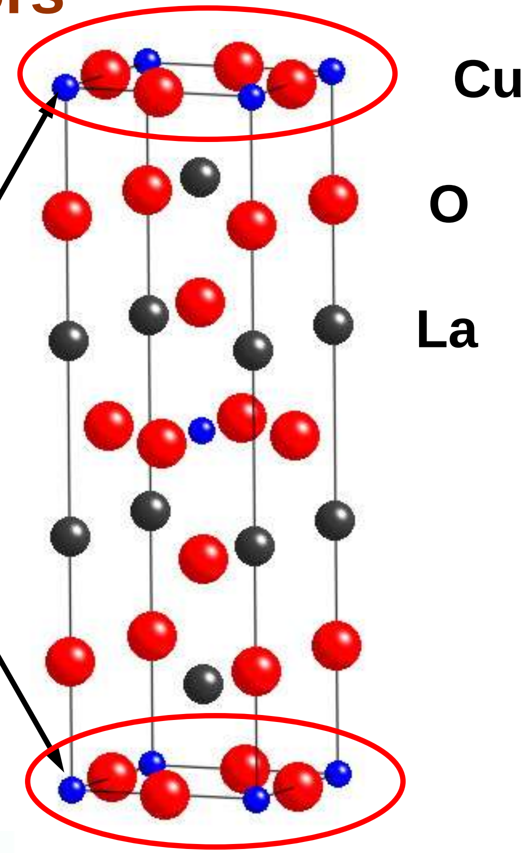




Crystal structure and phase diagram of cuprate high-temperature superconductors

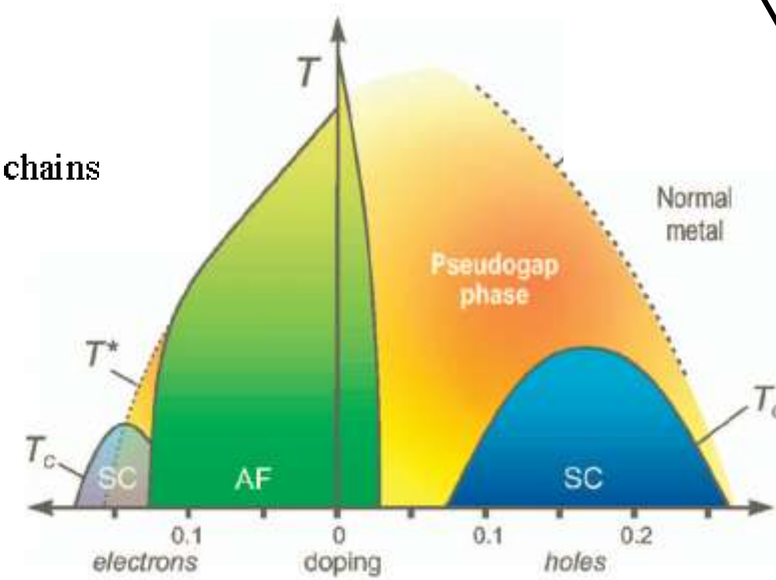


Cu-O-plane



$YBa_2Cu_30_7$

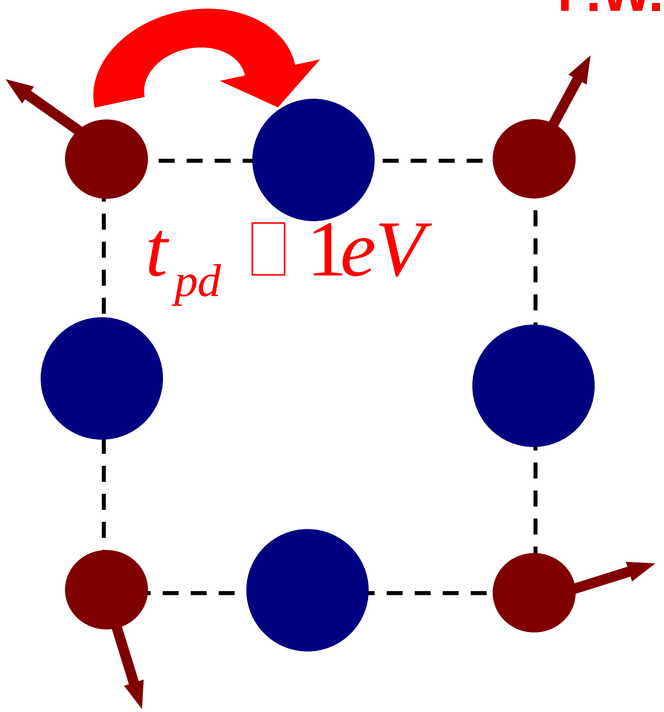
La_2Cu0_4

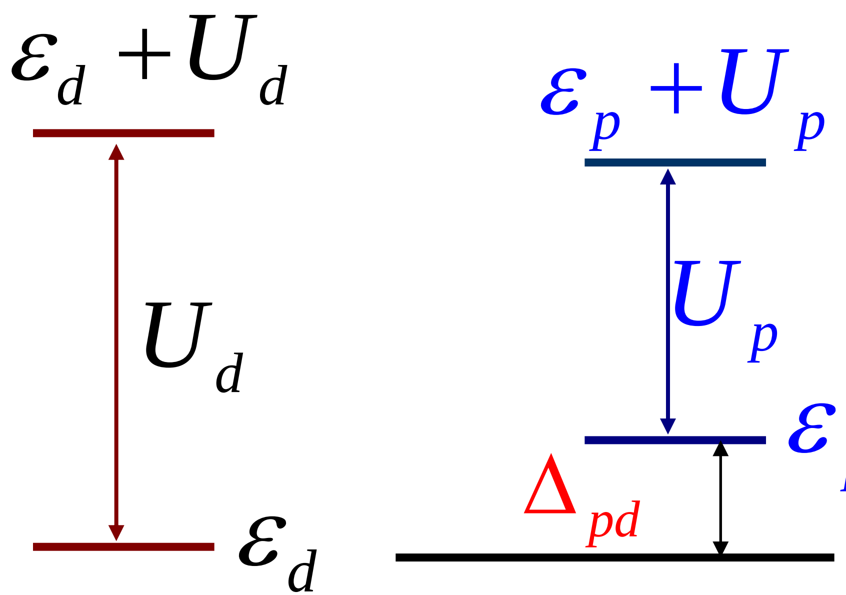


$YBa_2Cu_30_6$

Strong on-site Coulomb interactions of Cu 3d levels of oxide superconductors:

P.W.Anderson, Science, 235, 1196 (1987)





$O^{2-} \rightarrow \left(p^6\right)$

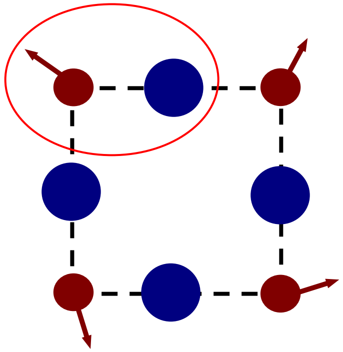
$Cu^{2+} \rightarrow \left(3d^9\right)$

$$\Delta_{pd} = \varepsilon_p - \varepsilon_d = 3.6eV$$

$$t_{pd} = 1.3eV$$

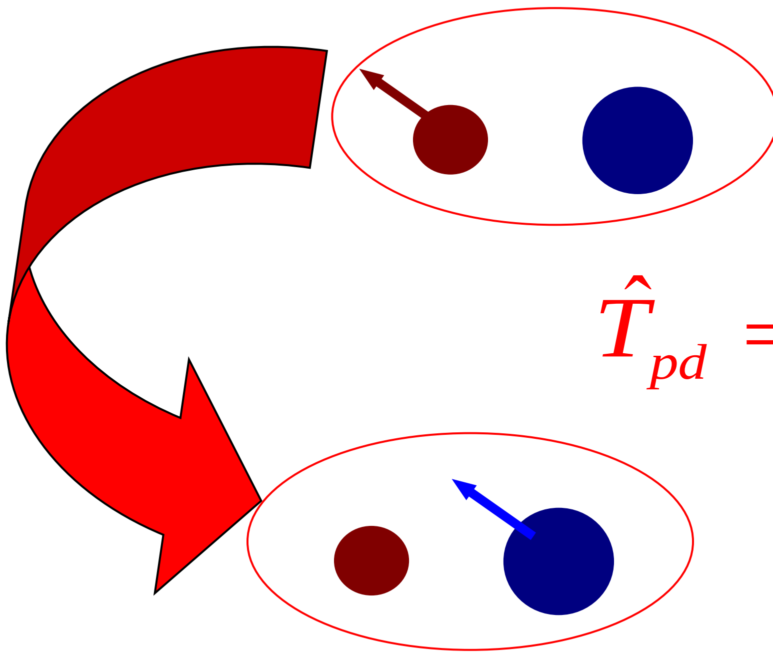
$$t_{pd} \;\square\; \Delta_{pd} \;!!$$

Hybridization effects



$$O^{2-} \rightarrow \left(p^{6}\right)$$

$$Cu^{2+} \rightarrow \left(3d^{9}\right)$$



$$\hat{T}_{pd} = t_{pd} \sum_{\sigma} \left(p_{\sigma}^{+} d_{\sigma} + d_{\sigma}^{+} p_{\sigma} \right)$$

$$O^{1-} \rightarrow \left(p^{5}\right)$$

$$Cu^{1+} \rightarrow \left(3d^{10}\right)$$

$$E\left(d^{10} p^{5}\right) - E\left(d^{9} p^{6}\right) = \Delta_{pd} = 3.6eV$$

Three-band p-d-model (Emery model)

V. J. Emery, PRL 58, 2794 (1987)
C.M. Varma et.al. Solid State Commun. 62 681 (1987)
J.E. Hirsch, PRL 59, 228 (1987)

Hamiltonian of the three-band p-d-model:

$$H = \varepsilon_p \sum_l c_l^+ c_l + \varepsilon_d \sum_f d_f^+ d_f + U_d \sum_f n_{f\uparrow}^{(d)} n_{f\downarrow}^{(d)} + \\ + \sum_{f\delta} \left(t_{pd}(\delta) d_f^+ c_{f+\delta} + t_{pd}(\delta) c_{f+\delta}^+ d_f \right),$$

$$c_l^+ = (c_{l\uparrow}^+, c_{l\downarrow}^+),$$

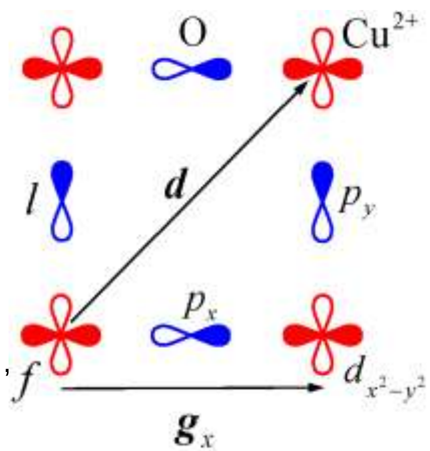
$$d_l^+ = (d_{l\uparrow}^+, d_{l\downarrow}^+),$$

$$n_{l\sigma}^{(p)} = c_{l\sigma}^+ c_{l\sigma},$$

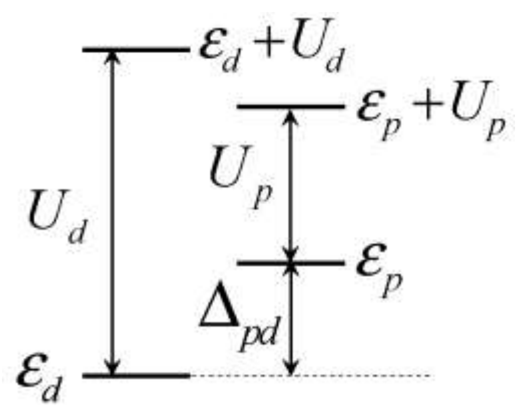
$$n_{f\sigma}^{(d)} = d_{f\sigma}^+ d_{f\sigma},$$

$$\Delta_{pd} = \varepsilon_p - \varepsilon_d,$$

$$\delta = \{\pm a_x, \pm a_y\} = \\ = \{\pm g_x, \pm g_y\}/2.$$



The unit cell of CuO_2-planes



Energy diagram for model’s parameters

Parameters of the model:

ε_d (ε_p) - binding energy of a hole in the copper (oxygen) ion;

U_d (U_p) - the energy of Coulomb repulsion of two holes in the copper (oxygen) ion;

V_{pd} - the energy of the Coulomb repulsion between nearest copper and oxygen ions;

t - O-O-hopping integral;

t_δ^{pd} - hybridization of p- and d-orbitals.

$$H = H_0 + V,$$

Операторная форма теории возмущений
(теория возмущений для вырожденного уровня)
Боголюбов Н.Н. Лекции по квантовой статистике, Харьков, 1936
(можно воспользоваться методом унитарного преобразования)

$$H_{eff} = PH_0P + PVP + PV\left(H_0 - E_0\right)^{-1}\left(PVP - VP\right) + H_{(3)} + H_{(4)} + \ldots$$

$$H_{(4)} = PV\left(\frac{1}{H_0 - E_0}\right)\left(PV - V\right)\left(\frac{1}{H_0 - E_0}\right)\left(PV - V\right)\left(\frac{1}{H_0 - E_0}\right)\left(PVP - VP\right)$$

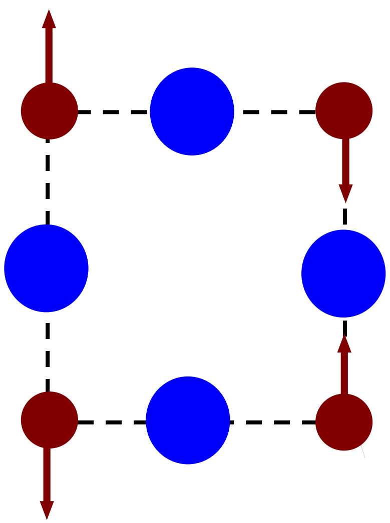
$$P = \prod_l X_l^{00}$$

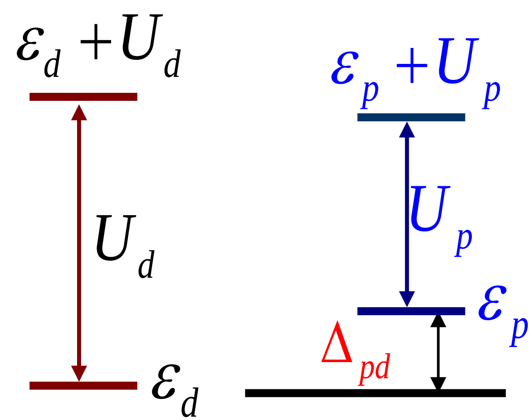
$$H_{exch} = \frac{1}{2}\sum_{\langle fm \rangle} I\left(\vec{S}_f \cdot \vec{S}_m\right)$$

Exchange interaction

$$I = 4\left(t_{pd}\right)^4 \left(\frac{1}{\Delta_{pd} + V_{pd}}\right)^2 \left(\frac{1}{U_d} + \frac{2}{U_p + 2\Delta_{pd}}\right)$$

Mott-Hubbard insulator antiferromagnetic state





$t_{pd} = 1.3eV;$

$\Delta_{pd} = 3.6eV;$

$U_d = 10eV;$

$U_p = 3eV;$

$V_{pd} = 1eV,$

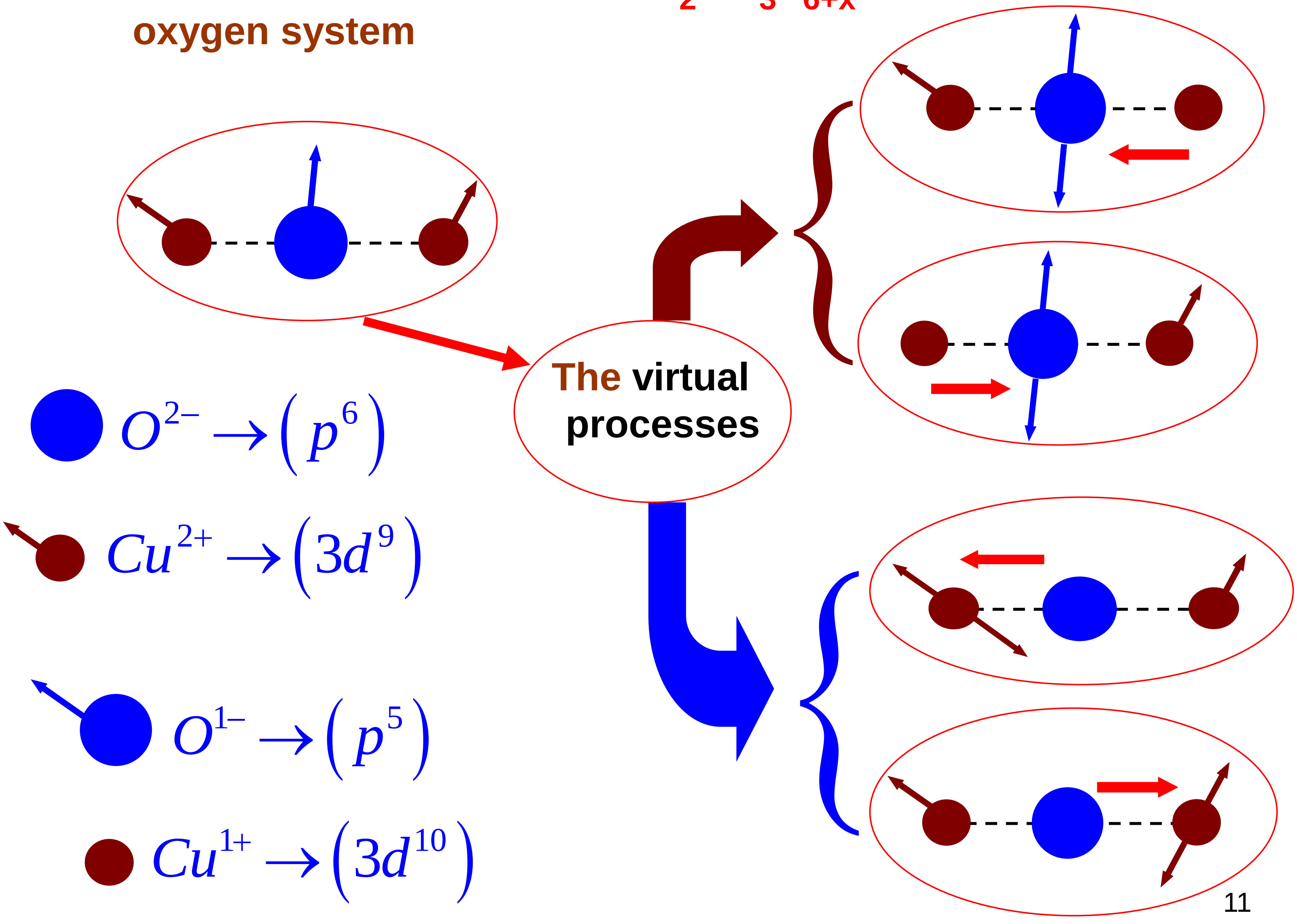
$I = 1600K$

$O^{2-} \rightarrow \left(p^6\right)$

$Cu^{2+} \rightarrow \left(3d^9\right)$

There are holes in the oxygen system

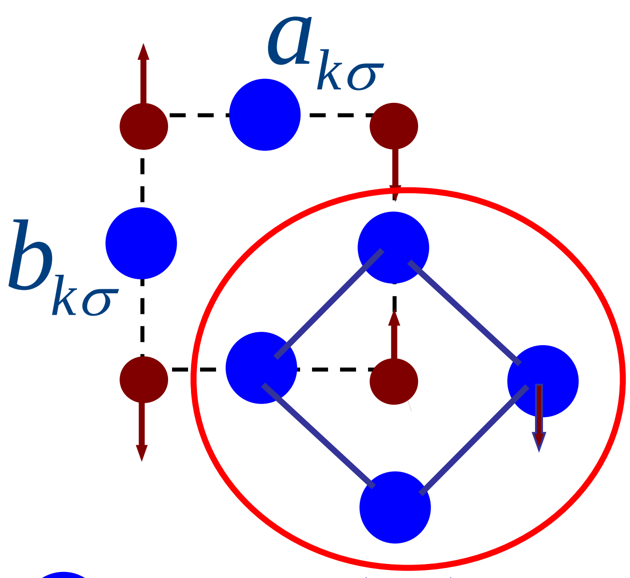
$YBa_2Cu_3O_{6+x}$

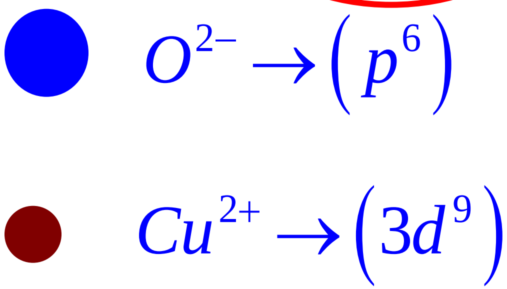


$$\varphi_{k\sigma} = \frac{\sin(k_x/2)}{\nu_k} a_{k\sigma} + \frac{\sin(k_y/2)}{\nu_k} b_{k\sigma},$$

$$\psi_{k\sigma} = \frac{\sin(k_y/2)}{\nu_k} a_{k\sigma} - \frac{\sin(k_x/2)}{\nu_k} b_{k\sigma},$$

$$\nu_k = \sqrt{\sin^2(k_x/2) + \sin^2(k_y/2)}.$$





- F.C.Zhang and T.M.Rice, PRB, **37**, 3759 (1988);
- B.S.Shastry, PPL, **63**, 1288, (1989);
- S.Lovtsov and V.Yushankhai, Physica C: Supercond., **179**, 159 (1991);
- J.H.Jefferson, H.Eskes and L.F.Fener, PRB, **45**, 7959, (1992);
- В.А.Гавричков, С.Г.Овчинников, ФТТ, **40,** 184 (1998);
- В.А.Гавричков, С.Г.Овчинников, А.А.Борисов, Е.Г.Горячев, ЖЭТФ 118, 422 (2000)

The strong exchange interaction between localized spin of the ion Cu and spin of the fermion in oxygen subsystem is determined

$$H_{sp-f} = \sum_{k\sigma} \varepsilon_p \psi^+_{k\sigma} \psi_{k\sigma} + \sum_{k\sigma} \xi_k \varphi^+_{k\sigma} \varphi_{k\sigma} +$$

$$\frac{J}{N} \sum_{fkq\sigma\sigma'} \nu_k \nu_q e^{-i(k-q)f} \varphi^+_{k\sigma} \left(\vec{S}_f \frac{1}{2} \vec{\tau}_{\sigma\sigma'} \right) \varphi_{q\sigma'} + \frac{1}{2} \sum_{fm} I_{fm} \left(\vec{S}_f \vec{S}_m \right)$$

$$J = 8 \left[\frac{t^2_{pd}}{\Delta_{pd} + V_{pd}} + \frac{t^2_{pd}}{U_d - \Delta_{pd} - 2V_{pd}} \right] \square\, 5.7eV\,!!$$

Energy diagram of the spin-fermion model

Parameters of the Emery model: $\Delta_{pd} = 3.6\ eV, \quad t_{pd} = 1.3\ eV, \quad U_d = 10.5\ eV$

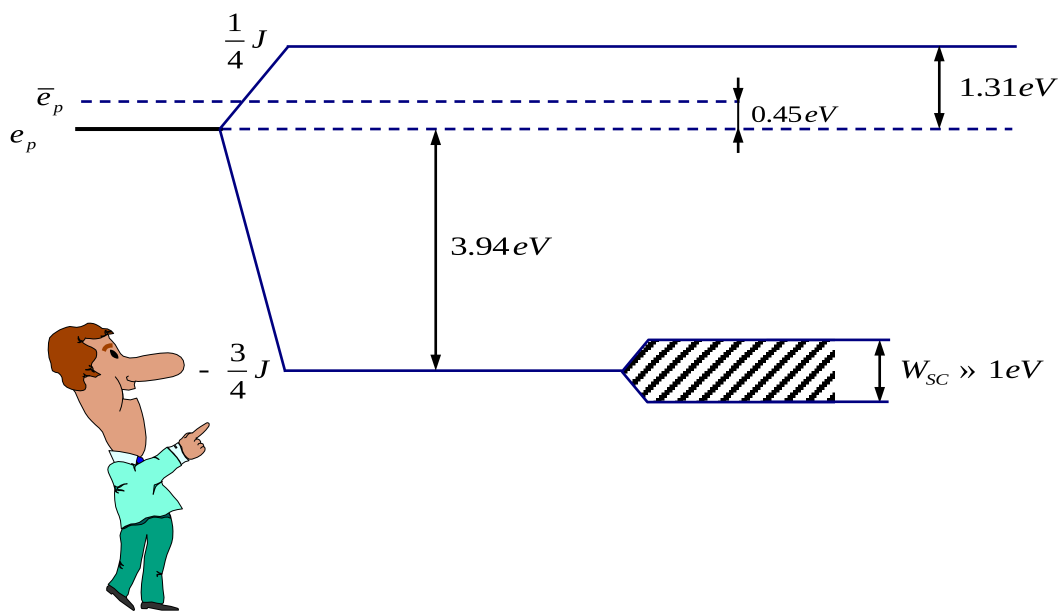
Parameters of the effective Emery model: $\tau = \frac{t_{pd}^2}{\Delta_{pd}} = 0.47\ eV \qquad \eta = \frac{\Delta_{pd}}{U_d - \Delta_{pd}} = 0.52$

Parameters of the exchange interaction J: $J = 8\tau(1+\eta)(\sigma_0 \sigma_0^*) = 5.26\ eV$

Energy of spin-correlated hoppings: $t^{SC} = 4\tau(1+\eta)(\sigma_0 \sigma_\Delta^*) = -0.389\ eV$

Energy of non-correlated hoppings: $t = \frac{\tau}{2}(1-\eta) = 0.112\ eV$

Width of the spin-polaron band $W_{SC} \equiv 8 t^{SC} C_1 \sim 8 \times 0.389 \times 0.3 = 0.93 \sim 1\ eV$



Effective Hamiltonian of the three-band p-d-model
(spin-fermion model)

In the regime of strong electron correlations $U_d > \Delta_{pd} >> t^{pd}$ the low energy effective Hamiltonian is:

J. Zaanen, A.M. Oles, PRB 37, 9423 (1988)

$$H = \varepsilon_p \sum_l c_l^+ c_l - t \sum_{l\rho} c_l^+ c_{l+\rho} + \frac{\tau_-}{2} \sum_{f\delta\delta'} c^+_{f+\delta} c_{f+\delta'} + \tau_+ \sum_{f\delta\delta'} c^+_{f+\delta} \tilde{S}_f c_{f+\delta'} + H_{exch},$$

where:

$$\tau_\pm = \tau(1 \pm \eta),\ \tau = \frac{(t^{pd})^2}{\Delta_{pd}},\ \eta = \frac{\Delta_{pd}}{U_d - \Delta_{pd} - 2V_{pd}},\ \tilde{S}_f = \vec{S}_f \vec{\sigma}.$$

Pauli matrices $\vec{\sigma} = (\sigma^x, \sigma^y, \sigma^z)$

In the fourth order on the parameter τ the exchange interaction emerges:

$$H_{exch} = \tfrac{1}{2} I_1 \sum_{fg} \vec{S}_f \vec{S}_{f+g} + \tfrac{1}{2} I_2 \sum_{fd} \vec{S}_f \vec{S}_{f+d},$$

$I_1 = (1-p)I,$
$I_2 = pI,$
- exchange integrals for the interactions within two coordination spheres.

I - Effective exchange

p - frustration parameter related to the holes concentration x.

Generally accepted values for the Emery model parameters are:

$$t^{pd} = 1.3(eV), \Delta_{pd} = 3.6(eV),$$
$$t = 0.1(eV), U_d = 10.5(eV),$$
$$I = 0.34\ (eV), U_p = V_{pd} = 0.$$

Spin-fermion model parameters:

$$\tau = 0.47(eV),\ \eta = 0.52$$
$$\tau_+ = 0.71(eV),\ \tau_- = 0.22(eV)$$

Spin-polaron concept

2D Kondo Lattice

N - phase

A.F. Barabanov, A.V. Mikheenkov, A.M. Belemouk, JETP Letters **75**, 118 (2002) (review);

A.M. Belemouk, A.F. Barabanov, L.A. Maksimov, JETP Letters **79**, 195 (2004) (Hall effect);

A.F. Barabanov, A.M. Belemouk, JETP Letters **87**, 725 (2008) (pseudogap);

SC - phase

A.F. Barabanov, A.V. Mikheenkov, JETP Letters **74**, 362 (2001);

V.V. Val'kov, M.M, Korovushkin, A.F. Barabanov, JETP Letters **88**, 426 (2008) ;

Spin-fermion model

N – phase

P.Prelovsek, Physics Letters A **126,** 287 (1988);

A.Ramsak and P.Prelovsek, PRB, **40**, 2239 (1989);

A.Ramsak and P.Prelovsek, PRB, **42**, 10415 (1990);

A.F. Barabanov, R.O. Kuzian, L.A. Maksimov, Phys. Rev. B **55**, 4015 (1997);

R.O.Kuzian, R.Hayn, A.F.Barabanov, L.A.Maksimov, Phys. Rev. B **58**, 6194 (1998);

A.F. Barabanov, A.A. Kovalev, O.V.Urazaev et al. JETP **119**, 777 (2001);

D.M. Dzebisashvili, V.V. Val'kov, A.F. Barabanov, JETP Letters, **98**, 596 (2013);

V.V. Val'kov, D.M. Dzebisashvili, A.F. Barabanov, JETP, **145**, 1087 (2014);

SC - phase

V.V. Val'kov, D.M. Dzebisashvili, A.F. Barabanov, Physics Letters A, **379**, 421 (2015);

V.V. Val'kov, D.M. Dzebisashvili, M.M. Korovushkin, A.F. Barabanov, JETP Lett. **103**, 385 (2016).

On the spin-polaron nature of Fermi quasiparticles in the Emery model (variational method, one hole)

$|G\rangle$ - singlet ground state of the undoped Emery model.

In the spin-liquid phase:

$$\vec{S}^{2}_{tot}|G\rangle = 0|G\rangle, \quad \langle G|\vec{S}^{x,y,z}_{f}|G\rangle = 0, \;\; \vec{S}_{tot} = \sum_{f}\vec{S}_{f}.$$

Operator basis required to describe the spin-polaron in the normal phase can not be limited by two operators:

$$|\psi_{k\sigma}\rangle = \alpha_{1k}\cdot\left(a^{+}_{k\sigma}|G\rangle\right) + \alpha_{2k}\cdot\left(b^{+}_{k\sigma}|G\rangle\right) + \alpha_{3k}\cdot\left(L^{+}_{k\sigma}|G\rangle\right).$$

of fundamental importance is accounting of the third operator:

$$L_{k\sigma} = \frac{1}{2\sqrt{N}}\sum_{f\delta\sigma'} e^{-ikR_f}\left(\vec{S}_f\vec{\tau}_{\sigma\sigma'}\right)c_{f+\delta,\sigma'}$$

Spectrum of a spin-polaron quasiparticle in the spin-fermion model

Dispersion equation:

$$\det_k(\omega) = \left(\omega - \varepsilon_p\right)^3 - A_k\left(\omega - \varepsilon_p\right)^2 + B_k\left(\omega - \varepsilon_p\right) + R_k$$

$$A_k = 2\tau_-(1+\gamma_{1k}) + \Lambda_k,$$

$$B_k = \left(2\tau_-\Lambda_k - 16\tau_+^2 K_{33}\right)(1+\gamma_{1k}) + 4t\left(\tau_- - t\right)\chi_k,$$

$$R_k = 4t\chi_k\left[8\tau_+^2 K_{33} - \Lambda_k(\tau_- - t)\right],$$

$$\Lambda_k = \frac{D_{33}(k)}{K_{33}} - \varepsilon_p, \quad \chi_k = 1 + 2\gamma_{1k} + \gamma_{2k}.$$

Analytical formula for the spectrum:

$$\mathrm{T}_{1k} = \varepsilon_p + x_k,$$

$$x_k = \frac{A_k}{2} - \sqrt{\frac{A_k^2}{4} - B_k - \frac{R_k}{x_{k0}}},$$

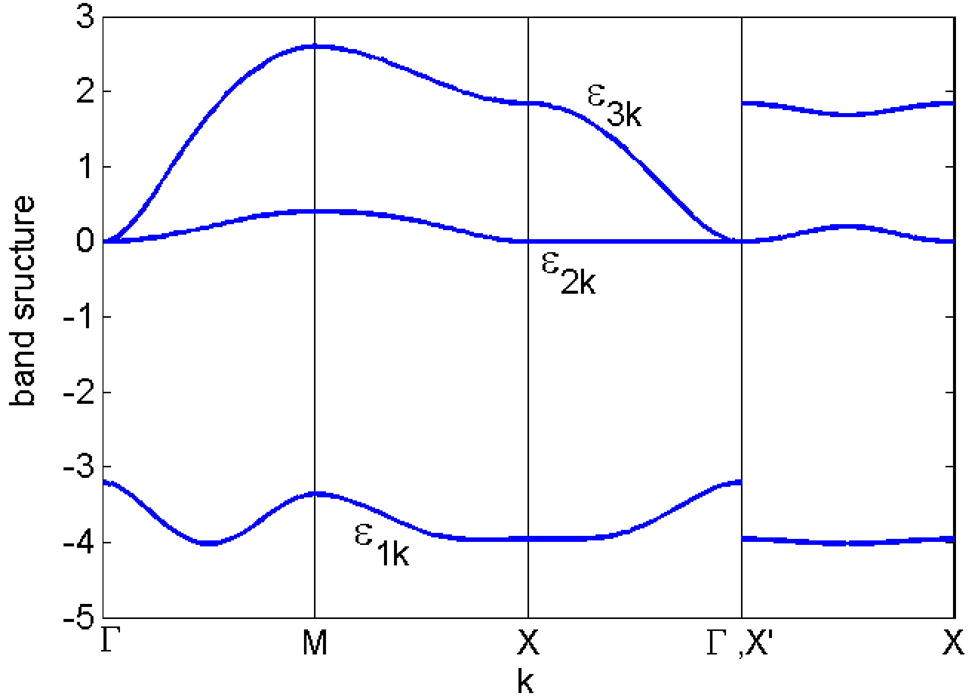
$$x_{k0} = A_k/2 - \sqrt{A_k^2/4 - B_k}$$

$$\mathrm{T}_{2k} = \varepsilon_p + \frac{A_k - x_k}{2} - v_k,$$

$$\mathrm{T}_{3k} = \varepsilon_p + \frac{A_k - x_k}{2} + v_k,$$

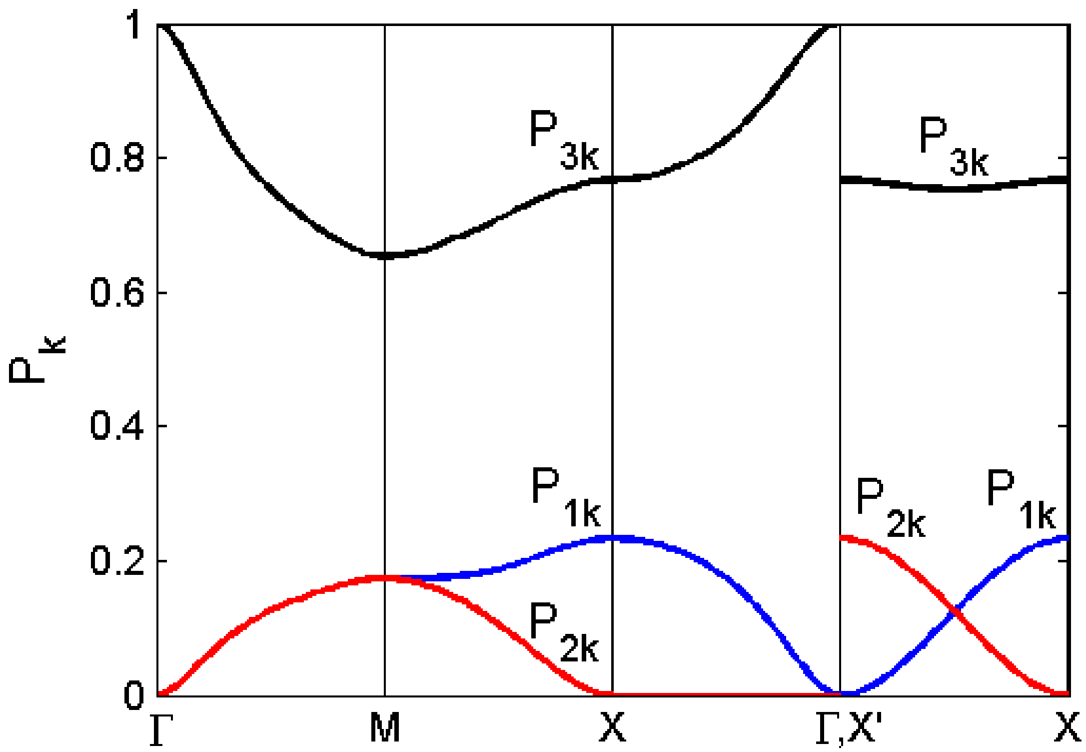
$$v_k = \sqrt{(A_k - x_k)^2/4 + R_k/x_k}.$$

Three branches of the Fermi excitations in the Emery model. The lower branch corresponds to the spin-polaron excitations.



D.M. Dzebisashvili, V.V. Val’kov, A.F. Barabanov, JETP Letters 98, 596 (2013);

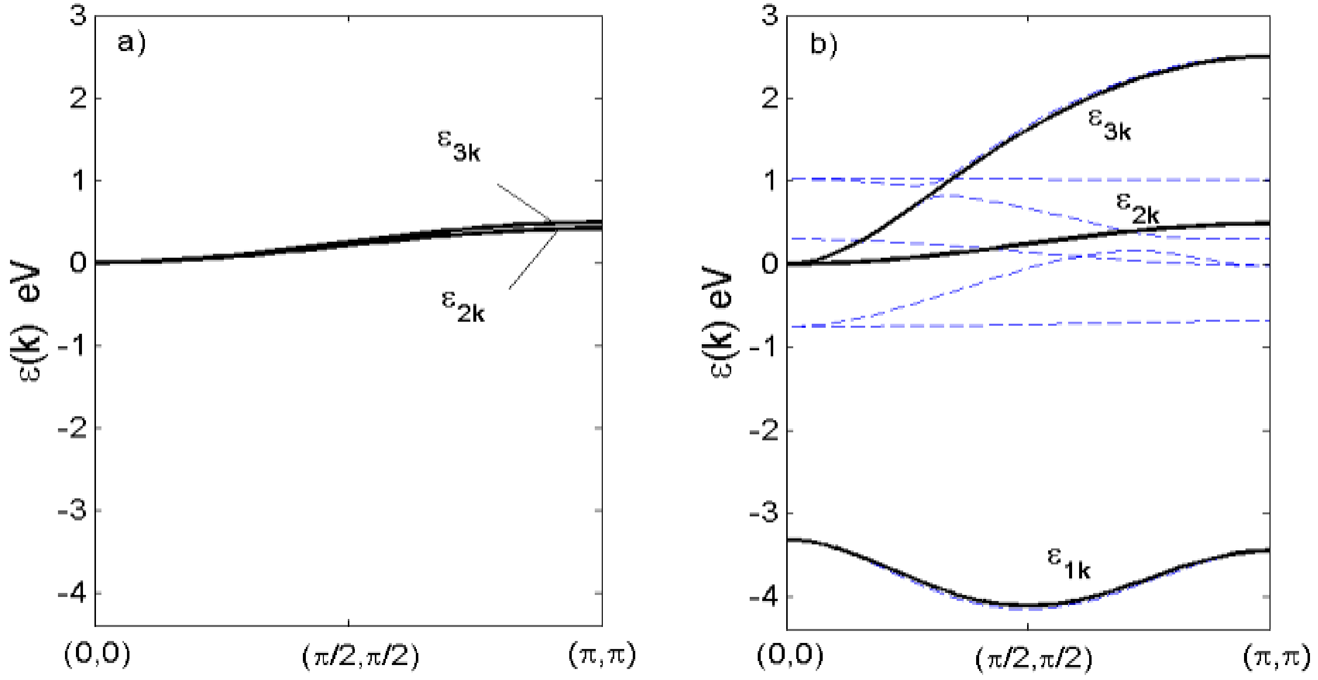
Partial contributions of the basis states to the one-hole state corresponding to the lower branch of the spectrum



$$P_{1k} = |\alpha_{1k}|^2, \quad P_{2k} = |\alpha_{2k}|^2$$ – weight contributions of bare hole states $A^{+}_{1(2)k\sigma}|G\rangle$

$$P_{3k} = K_{33}|\alpha_{3k}|^2$$ – weight contribution of spin-polaron state $A^{+}_{3k\sigma}|G\rangle$

Spin polaron spectrum in the spin-fermion model



a) k-dependence of the energy of one-hole states when only two operators are taken into account in the basis:

$$A_{1f\sigma} = c_{f+a_x,\sigma},$$

$$A_{2f\sigma} = c_{f+a_y,\sigma}$$

b) Emergence of the bottom, split-off spin-polaron band when operator $A_{3f\sigma} = \frac{1}{2}\sum_{\delta}\left(\tilde{S}_f c_{f+\delta}\right)_\sigma$

is added in the basis.

Eight dashed lines are calculated using the basis of eight operators:

Spin-correlation functions

Spin subsystem is considered in SU(2)-invariant spin-liquid phase.
J. Kondo, K.Yamaji, PTP 47, 807 (1972).

$$C_r = 3\left\langle \vec{S}_f^{x(y,z)} \vec{S}_{f+r}^{x(y,z)} \right\rangle, \ \left\langle \vec{S}_f^{\alpha} \right\rangle = 0, \ (\alpha = x, y, z), \ r = (g, d, 2g).$$

Spin correlators:

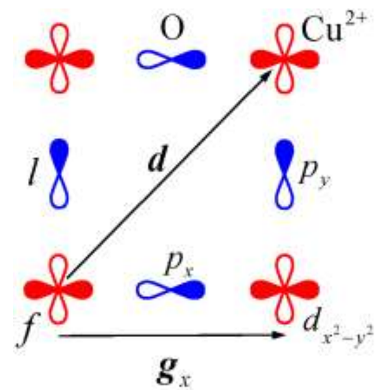
$$C_r = \left\langle \vec{S}_f \vec{S}_{f+r} \right\rangle$$

Method of calculating the spin correlators

$$x \ \Rightarrow \ \xi^{-1} \sim \Delta \ \Rightarrow \ p \text{ and } (C_g, C_d, C_{2g})$$

For each x the magnetic correlation length $\xi \sim \Delta^{-1}$ is determined from experiment.

The gap Δ in the spectrum of magnetic excitations in the vicinity of the point (π, π) of the Brillouin zone and the spin correlation functions are determined on the basis of spherically symmetric approach to a frustrated 2D Heisenberg antiferromagnet **[A.F. Barabanov *et al.* JETP 119, 777 (2001)]** for each p.



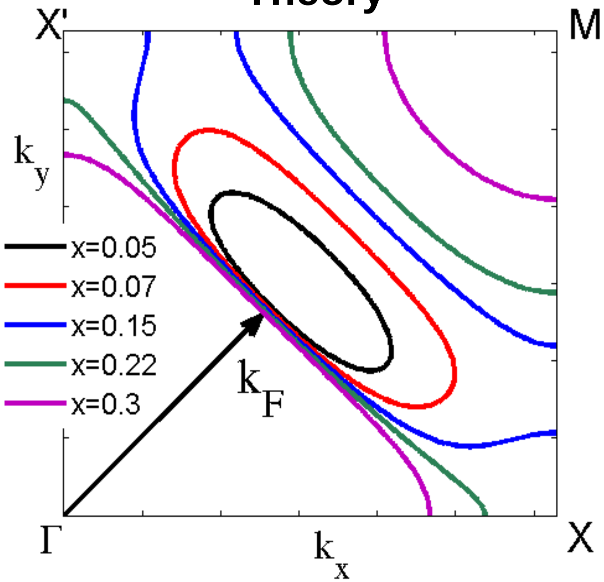
As a result, a correspondence between the values of doping x, frustration parameter p and spin correlation functions for the Emery model is established.

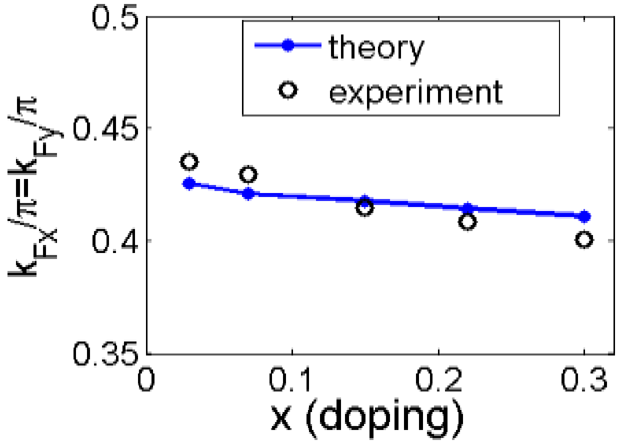
x	p	C_g	C_d	C_{2g}
0.03	0.16	-0.276	0.124	0.095
0.07	0.21	-0.255	0.075	0.064
0.15	0.25	-0.238	0.036	0.051
0.22	0.275	-0.224	0.009	0.045
0.3	0.3	-0.200	-0.0222	0.0457

$t_{pp} = 0.1eV$

Fermi surface evolution in $La_{2-x}Sr_xCuO_4$ with doping within the spin-fermion model

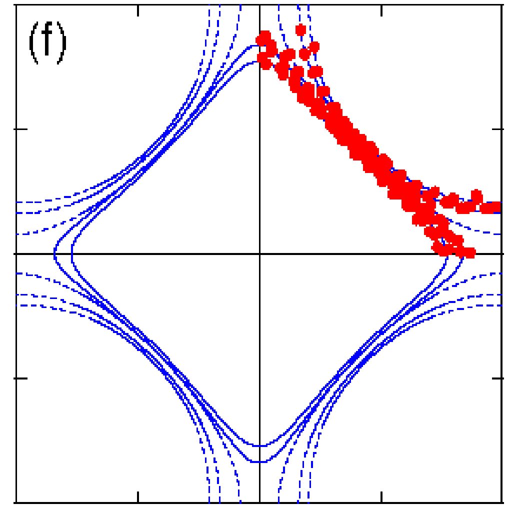
Theory

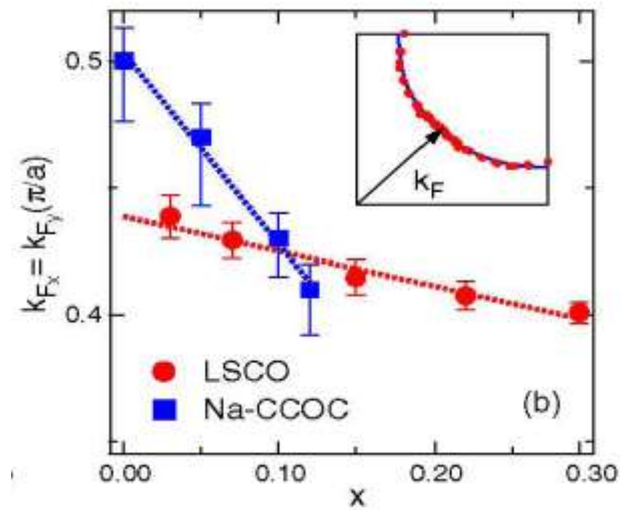




D.M. Dzebisashvili, V.V. Val'kov, A.F. Barabanov, JETP Lett. (2013)

Experiment





T. Yoshida *et al.* J. Phys.: Cond. Mat. 19, 125209 (2007)

Basis operators and elements of the matrices K and D in the superconducting phase

Minimal operator basis required to describe superconducting phase:

$$a_{k\uparrow},\quad b_{k\uparrow},\quad L_{k\uparrow} = \frac{1}{N}\sum_{fq\beta}\exp\left[if\left(q-k\right)\right]\cdot\left(\vec{S}_f\vec{\tau}_{\uparrow\beta}\right)\cdot u_{q\beta},$$

$$a^{+}_{-k\downarrow},\quad b^{+}_{-k\downarrow},\quad L^{+}_{-\downarrow}.$$

$$u_{q\beta} = \sin\left(\frac{q_x}{2}\right)\cdot a_{q\beta} + \sin\left(\frac{q_y}{2}\right)\cdot b_{q\beta}$$

Equation for the superconducting order parameter and critical temperature T_c

The equation for the superconducting order parameter has a d-wave solution:

$$E_k = \sqrt{(\varepsilon_{1k} - \mu)^2 + \Delta^2(k)}$$

$$\Delta(k) = \Delta_0(\cos k_x - \cos k_y).$$

Equation for the order parameter amplitude:

$$1 = \frac{I_1}{N}\sum_k \frac{(\cos k_x - \cos k_y)^2}{2E_k\left(E_k^2 - \tau_{2k}^2\right)\left(E_k^2 - \tau_{3k}^2\right)} \tanh\left(\frac{E_k}{2T}\right)\left[\varphi_k(E_k)\varphi_k(-E_k) - 16C_1\tau_+^2\Psi_k(E_k)\Psi_k(-E_k)\right],$$

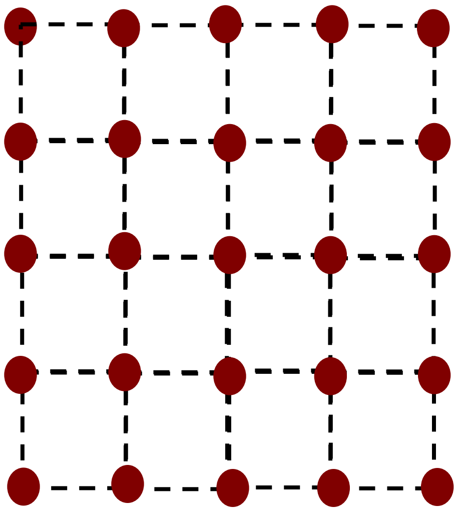
where: $\Psi_k(\omega) = (\omega - \varepsilon_p)(1 + \gamma_1(k)) - 2t\chi(k),$

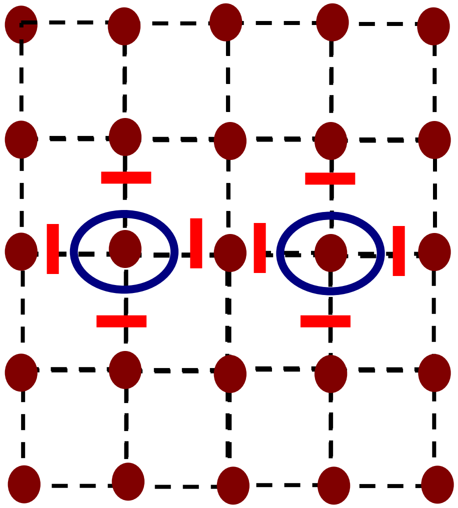
W h e n a m p l i t u

Then we get equation for the superconducting transition temperature T_c:

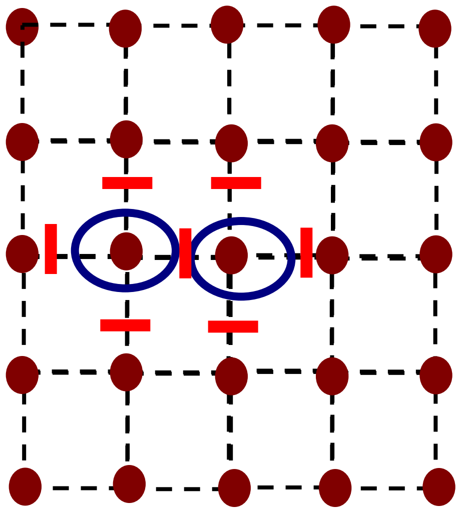
$$1 = \frac{I_1}{N}\sum_k \frac{(\cos k_x - \cos k_y)^2}{2\tau_{1k}\left(\tau_{1k}^2 - \tau_{2k}^2\right)\left(\tau_{1k}^2 - \tau_{3k}^2\right)} \tanh\left(\frac{\tau_{1k}}{2T}\right)\left[\varphi_k(\tau_{1k})\varphi_k(-\tau_{1k}) - 16C_1\tau_+^2\Psi_k(\tau_{1k})\Psi_k(-\tau_{1k})\right],$$

N.B. As the coupling constant we have the exchange interaction constant in the subsystem of localized spin moments.





Growth of the energy: 8I



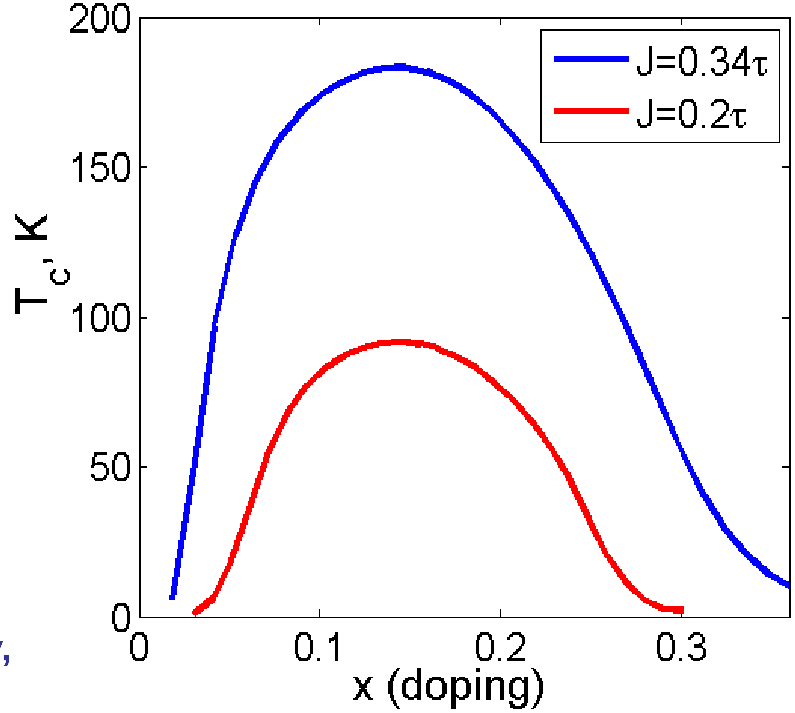
Growth of the energy: 7I

Effect of doping on the transition temperature to the superconducting phase

Equation for the chemical potential:

$$\frac{x}{4} = \frac{1}{N}\sum_k \frac{F_k(E_k) f(E_k/T) - F_k(-E_k) f(-E_k/T)}{2E_k\left(E_k^2 - \mathrm{T}_{2k}^2\right)\left(E_k^2 - \mathrm{T}_{3k}^2\right)},$$

Changes in the spin correlator C_j at doping have also been accounted.



The concentration dependence of the critical temperature for the d-wave superconducting phase at two values of the exchange integral.

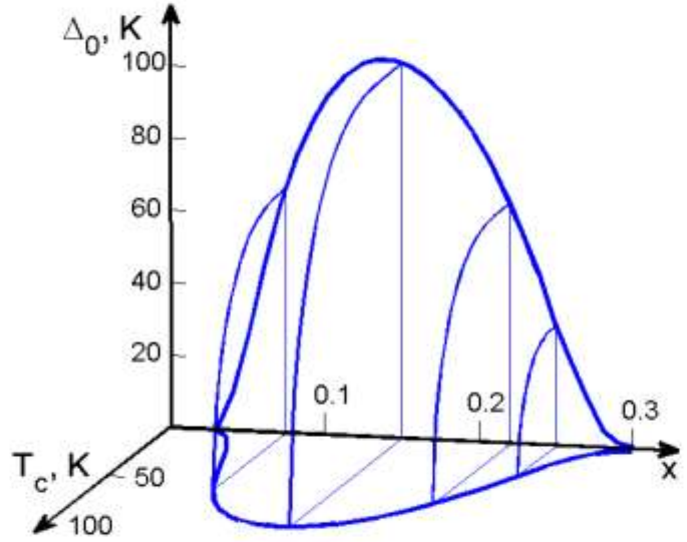
Other parameters of the model are:

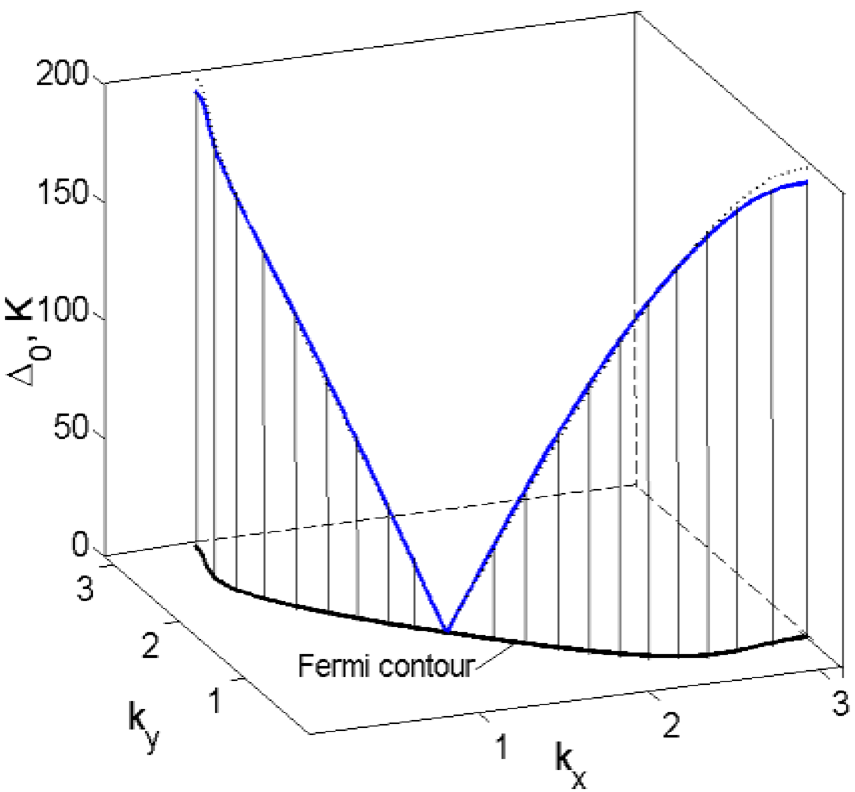
$$t = 0.1\ (eV),\ \ \tau = 0.47\ (eV),\ \eta = 0.52.$$

V.V Val'kov, D.M. Dzebisashvili, A.F. Barabanov, Phys. Lett. A (2015)

Effect of doping on the superconducting order parameter

Changes in the amplitude of superconducting order parameter and critical temperature at doping.





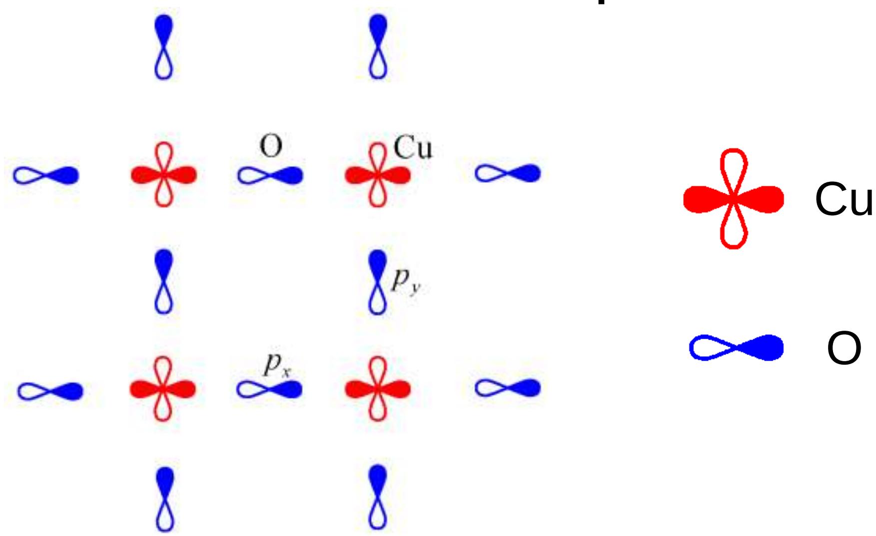
Dependence of the superconducting gap on the quasimomentum on the Fermi contour. Fermi contour is depicted by the solid line in the horizontal plane.
The calculation is performed at the

$$x = 0.125,\ I = 0.2\,\tau,\ T = 0,\ t = 0.1\ (eV),$$
$$\tau = 0.47\ (eV),\ \eta = 0.52.$$

V.V Val'kov, D.M. Dzebisashvili, A.F. Barabanov, Phys. Lett. A (2015)

Models for cuprate superconductors

Structure of the CuO2-plane



Three band p-d-model (Emery model)

$$H=\varepsilon_d\sum_f \hat{n}_f^d+\frac{\varepsilon_p}{2}\sum_{f\delta}\hat{n}^p_{f+\delta}+U_d\sum_f \hat{n}^d_{f\uparrow}\hat{n}^d_{f\downarrow}+\frac{U_p}{2}\sum_{f\delta}\hat{n}^p_{f+\delta,\uparrow}\hat{n}^p_{f+\delta,\downarrow}+$$

$$+\sum_{f\delta\sigma}t_{pd}(\delta)\left(d^\dagger_{f\sigma}p_{f+\delta,\sigma}+h.c.\right)+\frac{1}{2}\sum_{f\delta\Delta\sigma}t_{pp}(\Delta)p^\dagger_{f+\delta,\sigma}p_{f+\delta+\Delta,\sigma}+$$

$$+V_{pd}\sum_{f\delta}\hat{n}^d_f\hat{n}^p_{f+\delta}+V_{pp}\sum_f\hat{n}^p_{f+x/2}\hat{n}^p_{f+x/2+\Delta}$$

V.J. Emery, PRL 58, 2794 (1987)

C.M. Varma et al, Solid State Commun. 62, 681 (1987)

Multiband p-d-model

Yu.B. Gaididei, V.M. Loktev, Phys. Stat. Sol. B 147 (1988)
C. DiCastro, L.F. Feiner, M. Grilli, PRL (1991)
V. Gavrichkov, A. Borisov, S.G. Ovchinnikov, PRB 64 (2001)

Hubbard model

$$H=\sum_{fm\sigma}t_{fm}a^\dagger_{f\sigma}a_{m\sigma}+U\sum_f n_{f\uparrow}n_{f\downarrow}$$

J.C. Hubbard, Proc. R. Soc. London A 276, 238 (1963)

D.J. Scalapino et al, PRB (1987)

t-J- and t-J*-models

$$H_{t-J}=\sum_{f\sigma}(\varepsilon-\mu)X_f^{\sigma\sigma}+\sum_{fm\sigma}t_{fm}X_f^{\sigma 0}X_f^{0\sigma}$$

$$+\frac{1}{2}\sum_{fm\sigma}J_{fm}\left(X_f^{\sigma\bar{\sigma}}X_m^{\bar{\sigma}\sigma}-X_f^{\sigma\sigma}X_m^{\bar{\sigma}\bar{\sigma}}\right)+$$

$$+\sum_{\substack{fmg\sigma\\(f\neq g)}}\frac{t_{fm}t_{mg}}{U}\left(X_f^{\sigma 0}X_m^{\bar{\sigma}\sigma}X_g^{0\bar{\sigma}}-X_f^{\sigma 0}X_m^{\bar{\sigma}\bar{\sigma}}X_g^{0\sigma}\right)$$

P.W. Anderson, Science 235, 1196 (1987)

R.O. Zaitsev, FTT (1988)

N.M. Plakida et al, Physica C (1989)

A. Ramsak, P. Prelovsek, PRB (1989)

Yu.A. Izyumov, UFN (1991, 1995, 1997, 1999)

V.V. Val'kov, D.M. Dzebisashvili, T.A. Val'kova, S.G. Ovchinnikov, JETPL (2002)

S.G. Ovchinnikov, M.M. Korshunov, E.I. Shneider, JETP 136 (2009)

The spin-fermion model

In the SEC regime the low energy Hamiltonian of the p-d-model takes the form: $U_d > \Delta_{pd} >> t_{pd}$

$$\hat{H} = \hat{H}_0 + \hat{J} + \hat{V} + \hat{I},$$

$$\hat{H}_0 = \sum_{k\alpha}\Big(\xi_0(k_x)a^\dagger_{k\alpha}a_{k\alpha} + \xi_0(k_y)b^\dagger_{k\alpha}b_{k\alpha} + t_k\left(a^\dagger_{k\alpha}b_{k\alpha} + b^\dagger_{k\alpha}a_{k\alpha}\right)\Big),$$

$$\hat{J} = \frac{J}{N}\sum_{\substack{fkq\\ \alpha\beta}} e^{if(q-k)}u^\dagger_{k\alpha}\left(\vec{S}_f\vec{\sigma}_{\alpha\beta}\right)u_{q\beta}, \quad \hat{V} = V_1\sum_{f\Delta}\hat{n}_{f+x/2}\hat{n}_{f+x/2+\Delta}, \quad \hat{I} = \frac{I}{2}\sum_{\langle fm\rangle}\vec{S}_f\vec{S}_m.$$

A.F. Barabanov, L.A. Maksimov, G.V. Uimin, JETP Lett (1988)

E.B. Stechel, D.R. Jennison, PRB (1988)

J. Zaanen, A.M. Oles, PRB (1988)

V.J. Emery, G. Reiter, PRB (1988)

$$\xi_0\left(k_{x(y)}\right) = \varepsilon_p - \mu + \tau\left(1 + \cos k_{x(y)}\right),$$

$$t_k = (2\tau - 4t)\cos\frac{k_x}{2}\cos\frac{k_y}{2},$$

$$u_{k\beta} = \sin\frac{k_x}{2}a_{k\beta} + \sin\frac{k_y}{2}b_{k\beta},$$

$$\tau = \frac{t^2_{pd}}{\Delta_{pd}}\left(1 - \frac{\Delta_{pd}}{U_d - \Delta_{pd} - 2V_{pd}}\right),$$

$$J = \frac{4t^2_{pd}}{\Delta_{pd}}\left(1 + \frac{\Delta_{pd}}{U_d - \Delta_{pd} - 2V_{pd}}\right), \quad J = 3.4eV >> \tau \approx 0.1eV$$

Parameters of the spin-fermion model

$$t_{pd} = 1.3eV,\ \ \Delta_{pd} = 3.6eV,\ \ t = 0.1eV,$$
$$U_d = 10.5eV,\ \ U_p = 4eV,\ \ V_{pd} = 1.2eV,$$
$$V = 1 - 2eV.$$

$$\vec{\sigma} = (\sigma^x, \sigma^y, \sigma^z)$$

M.S. Hybertsen et al, PRB (1989)
M.H. Fischer, E.-A. Kim, PRB (2011)

$$I = \frac{4t^2_{pd}}{\left(\Delta_{pd} + V_{pd}\right)^2}\left(\frac{1}{U_d} + \frac{2}{2\Delta_{pd} + U_p}\right) \quad I = 0.136eV$$

Set of basis operators

It is necessary to account the strong coupling between copper and oxygen subsystems, because

$$J = 3.4 eV >> \tau \approx 0.1 eV$$

Set of basis operators

$$a_{k\uparrow}, \quad b_{k\uparrow}, \quad L_{k\uparrow} = \frac{1}{N}\sum_{fq\beta} e^{if(q-k)}\left(\vec{S}_f\vec{\sigma}_{\uparrow\beta}\right)u_{q\beta};$$

$$a^{\dagger}_{-k\downarrow}, \quad b^{\dagger}_{-k\downarrow}, \quad L^{\dagger}_{-k\downarrow}$$

$$u_{k\beta} = \sin\frac{k_x}{2}a_{k\beta} + \sin\frac{k_y}{2}b_{k\beta}$$

A.F. Barabanov, V.M. Berezovsky, E.Zasinas, L.A. Maksimov, JETP (1996)
V.V Val'kov, D.M. Dzebisashvili, A.F. Barabanov, Phys. Lett. A (2015)

The normal and anomalous Green's functions

$$G_{11} = \left\langle\left\langle a_{k\uparrow} \middle| a^{\dagger}_{k\uparrow}\right\rangle\right\rangle, \quad G_{21} = \left\langle\left\langle b_{k\uparrow} \middle| a^{\dagger}_{k\uparrow}\right\rangle\right\rangle, \quad G_{31} = \left\langle\left\langle L_{k\uparrow} \middle| a^{\dagger}_{k\uparrow}\right\rangle\right\rangle,$$

$$F_{11} = \left\langle\left\langle a^{\dagger}_{-k\downarrow} \middle| a^{\dagger}_{k\uparrow}\right\rangle\right\rangle, \quad F_{21} = \left\langle\left\langle b^{\dagger}_{-k\downarrow} \middle| a^{\dagger}_{k\uparrow}\right\rangle\right\rangle, \quad F_{31} = \left\langle\left\langle L^{\dagger}_{-k\downarrow} \middle| a^{\dagger}_{k\uparrow}\right\rangle\right\rangle.$$

The equations for normal and anomalous Green's functions with respect to the intersite Coulomb interaction *V₁*

The system of equations obtained on the basis of projection technique is

$$(\omega-\xi_x)G_{1j}=\delta_{1j}+t_kG_{2j}+J_xG_{3j}+\Delta_{1k}F_{2j},$$

$$(\omega-\xi_y)G_{2j}=\delta_{2j}+t_kG_{1j}+J_yG_{3j}+\Delta_{2k}F_{1j},$$

$$(\omega-\xi_3)G_{3j}=\delta_{3j}K_k+\left(J_xG_{1j}+J_yG_{2j}\right)K_k+\Delta_{3k}F_{3j},$$

$$(\omega+\xi_x)F_{1j}=\Delta^*_{2k}G_{2j}-t_kF_{2j}-J_xF_{3j},$$

$$(\omega+\xi_y)F_{2j}=\Delta^*_{1k}G_{1j}-t_kF_{1j}-J_yF_{3j},$$

$$(\omega+\xi_3)F_{3j}=\Delta^*_{3k}G_{3j}-\left(J_xF_{1j}+J_yF_{2j}\right)K_k.$$

$$\xi_{x(y)}=\xi_0\left(k_{x(y)}\right)+4n_pV_1,$$

$$J_{x(y)}=J\cos\frac{k_x}{2},\quad K_k=3/4+C_1\gamma_{1k},$$

$$\xi_3=\varepsilon_p-\mu-2t+5\tau/2-J+V_1n_p+$$
$$+\left[(\tau-2t)\left(C_1\gamma_{1k}+C_2\gamma_{2k}\right)+\right.$$
$$+\tau\left(C_1\gamma_{1k}+C_3\gamma_{3k}\right)/2+$$
$$\left.+JC_1(1-4\gamma_{1k})/4+IC_1(\gamma_{1k}-4)\right]K_k^{-1}.$$

$$\Delta_{1k}=-\frac{4V_1}{N}\sum_q\phi_{k-q}\langle a_{q\uparrow}b_{-q\downarrow}\rangle,\qquad \phi_k=\cos\frac{k_x}{2}\cos\frac{k_y}{2},$$

$$\Delta_{2k}=-\frac{4V_1}{N}\sum_q\phi_{k-q}\langle b_{q\uparrow}a_{-q\downarrow}\rangle,$$

$$\Delta_{3k}=\frac{1}{N}\sum_q\Big\{I_{k-q}\big[\langle L_{q\uparrow}L_{-q\downarrow}\rangle-C_{1x}\langle a_{q\uparrow}a_{-q\downarrow}\rangle-C_{1y}\langle b_{q\uparrow}b_{-q\downarrow}\rangle\big]+$$
$$+\left(\tilde{V}_k-C_1I_{k-q}\right)\phi_q\left(\langle a_{q\uparrow}b_{-q\downarrow}\rangle+\langle b_{q\uparrow}a_{-q\downarrow}\rangle\right)\Big\}K_q^{-1}.$$

$$C_{1x(1y)}=C_1\cos^2\frac{q_{x(y)}}{2},$$

$$I_k=4I\gamma_{1k}$$

$$\tilde{V}_k=V_1\left(3/4+2C_1\gamma_{1k}+C_2\gamma_{2k}\right)$$

The system of equations for the critical temperature with respect to the intersite Coulomb interaction V_1

$$\Delta^*_{1k} = \frac{4V_1}{N}\sum_{jq}\phi_{k-q} M^{(j)}_{21}(q)\Delta^*_{jq}, \qquad j=1,2,3$$

$$\Delta^*_{2k} = \frac{4V_1}{N}\sum_{jq}\phi_{k-q} M^{(j)}_{12}(q)\Delta^*_{jq}, \qquad \phi_k = \cos\frac{k_x}{2}\cos\frac{k_y}{2},$$

$$\Delta^*_{3k} = \frac{1}{N}\sum_{jq}\Big\{ I_{k-q}\left[C_{1x}M^{(j)}_{11}(q) + C_{1y}M^{(j)}_{22}(q) - M^{(j)}_{33}(q)\right] + (I_{k-q}C_1 - \tilde{V}_k)\phi_q\left[M^{(j)}_{12}(q) + M^{(j)}_{21}(q)\right]\Big\} K^{-1}_q \Delta^*_{jq},$$

$$C_{1x(1y)} = C_1 \cos^2\frac{q_{x(y)}}{2},$$

$$\tilde{V}_k = V_1\left(3/4 + 2C_1\gamma_{1k} + C_2\gamma_{2k}\right),$$

$$I_k = 4I\gamma_{1k}$$

Lattice invariants:

$$\gamma_{1k} = (\cos k_x + \cos k_y)/2,$$

$$\gamma_{2k} = \cos k_x \cos k_y,$$

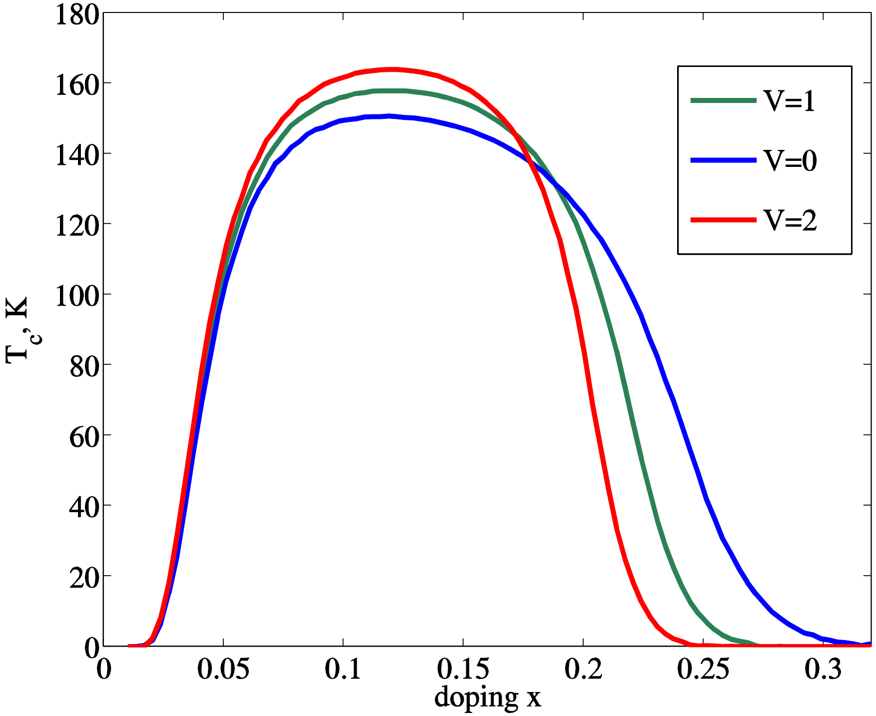
$$\gamma_{3k} = (\cos 2k_x + \cos 2k_y)/2$$

$$M^{(j)}_{nm}(q) = \frac{S^{(j)}_{nm}(q, E_{1q}) + S^{(j)}_{nm}(q, -E_{1q})}{4E_{1q}(E^2_{1q} - E^2_{2q})(E^2_{1q} - E^2_{3q})}\tanh\left(\frac{E_{1q}}{2T}\right).$$

For the d-wave superconducting phase, when $\Delta_{3k} = \Delta_0(\cos k_x - \cos k_y)$ it follows from the system that $\Delta_{1k} = 0, \quad \Delta_{2k} = 0$

From the third equation, it is seen that the contribution of the intersite Coulomb potential in the kernel of the equation vanishes.

Concentration dependence of the critical temperature for d-wave superconducting phase



Equation for the critical temperature:

$$1=\frac{I}{N}\sum_{q}\frac{(\cos q_x-\cos q_y)^2}{2E_{1q}}\Psi_q\tanh\left(\frac{E_{1q}}{2T_c}\right)$$

$$\Psi_q=\Big\{S_{33}^{(3)}\left(q,E_{1q}\right)-C_{1x}S_{11}^{(3)}\left(q,E_{1q}\right)-C_{1y}S_{22}^{(3)}\left(q,E_{1q}\right)$$

$$-C_1\phi_q\left(S_{12}^{(3)}\left(q,E_{1q}\right)+S_{21}^{(3)}\left(q,E_{1q}\right)\right)\Big\}\times$$

$$\times\left[K_q\left(E_{1q}^2-E_{2q}^2\right)\left(E_{1q}^2-E_{3q}^2\right)\right]^{-1}$$

Account for the intersite Coulomb interaction of holes leads only to a slight modification of Tc(x) due to weak renormalization of the holes energy by V. It is important that the intersite Coulomb interaction does not change the coupling constant.

V.V Val'kov, D.M. Dzebisashvili, M.M. Korovushkin, A.F. Barabanov, JETP Letters (2016)

What about the long-range Coulomb interaction V_2 ?

Hamiltonian of the spin-fermion model is

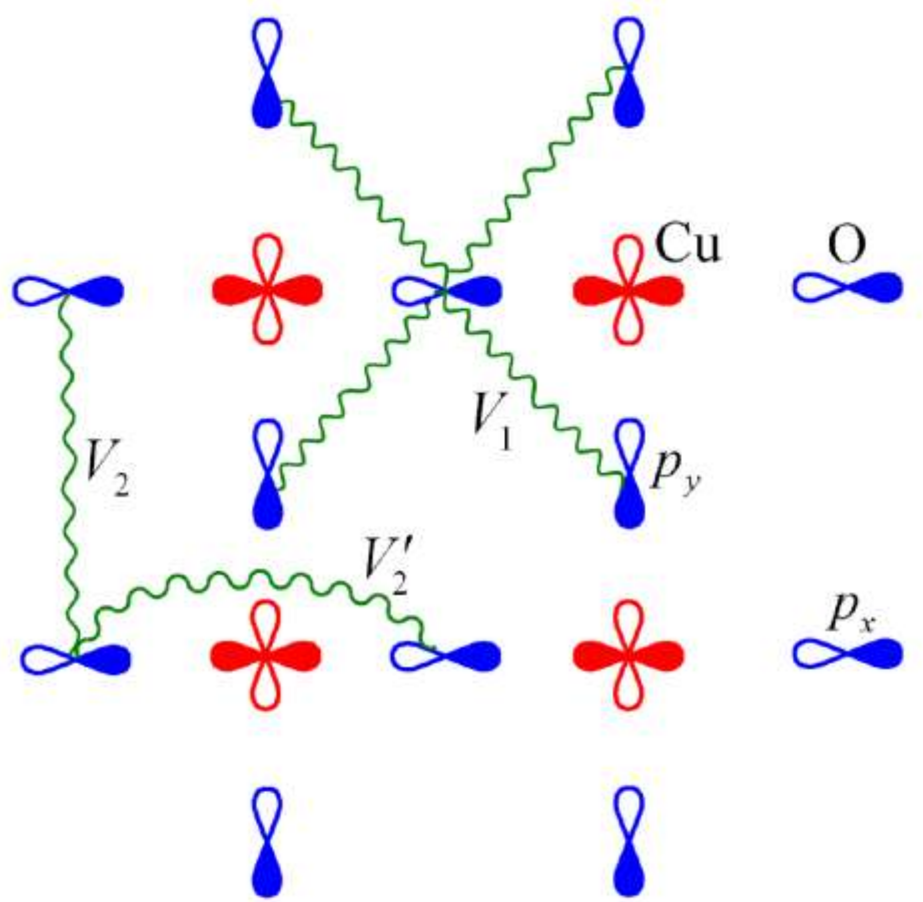
$$\hat{H} = \hat{H}_0 + \hat{J} + \hat{V} + \hat{I},$$

$$\hat{H}_0 = \sum_{k\alpha}\Big(\xi_0\left(k_x\right)a^\dagger_{k\alpha}a_{k\alpha} + \xi_0\left(k_y\right)b^\dagger_{k\alpha}b_{k\alpha} + $$
$$+ t_k\left(a^\dagger_{k\alpha}b_{k\alpha} + b^\dagger_{k\alpha}a_{k\alpha}\right)\Big),$$

$$\hat{J} = \frac{J}{N}\sum_{\substack{fkq\\ \alpha\beta}} e^{if(q-k)}u^\dagger_{k\alpha}\left(\vec{S}_f\vec{\sigma}_{\alpha\beta}\right)u_{q\beta},$$

$$\hat{I} = \frac{I}{2}\sum_{\langle fm\rangle}\vec{S}_f\vec{S}_m, \quad \hat{V} = \hat{V}_1 + \hat{V}_2,$$

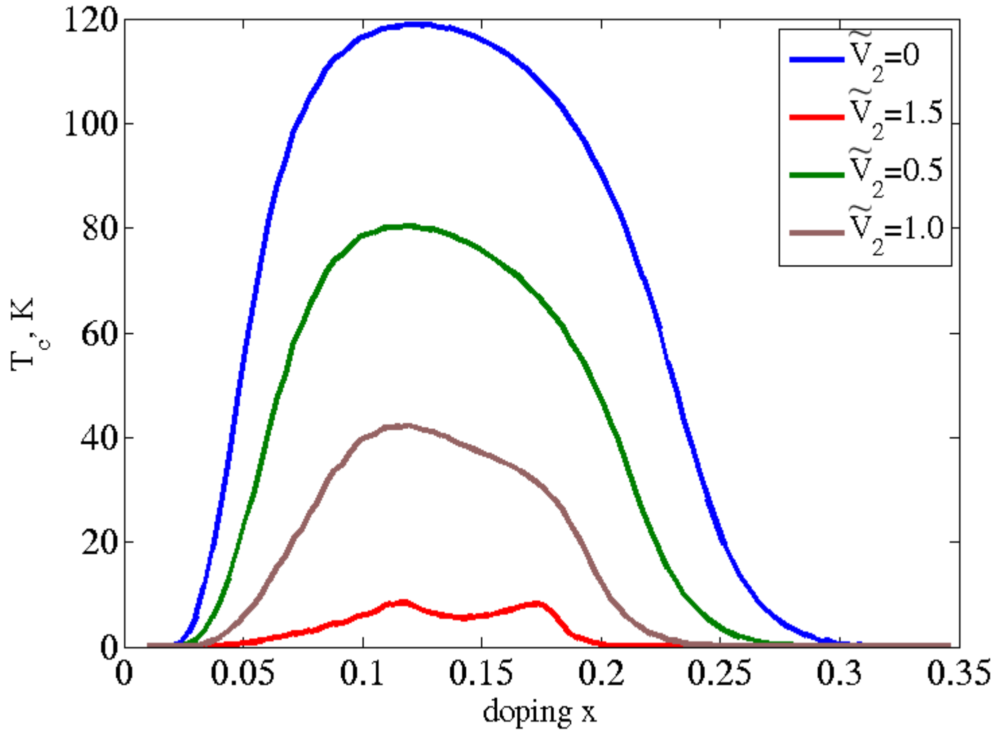
$$\hat{V} = V_2\sum_f \hat{n}_{f+x/2}\hat{n}_{f+x/2+y} + V_2\sum_f \hat{n}_{f+y/2}\hat{n}_{f+y/2+x} +$$
$$+ V_2'\sum_f \hat{n}_{f+x/2}\hat{n}_{f+x/2+x} + V_2'\sum_f \hat{n}_{f+y/2}\hat{n}_{f+y/2+y}.$$



Concentration dependence of the critical temperature for d-wave superconducting phase with respect to *V2*

$$\Delta_{1k}^* = \frac{4\tilde{V}_2}{N}\sum_{jq}\left(\cos\left(k_x - q_x\right) + \cos\left(k_y - q_y\right)\right) M_{11}^{(j)}(q)\Delta_{jq}^*, \qquad j = 1, 2,$$

$$\Delta_{2k}^* = \frac{1}{N}\sum_{jq}\Big\{ I_{k-q}\Big[C_{1x}M_{11}^{(j)}(q) + C_{1y}M_{22}^{(j)}(q) - M_{33}^{(j)}(q) + C_1\left(M_{12}^{(j)}(q) + M_{21}^{(j)}(q)\right)\Big] +$$
$$+2\tilde{V}_2\Big[\left(C_1\cos k_y - C_2\gamma_{2k}\right)\cos q_y + \left(C_1\cos k_x - C_2\gamma_{2k}\right)\cos q_x\Big] M_{11}^{(j)}(q)\Big\} K_q^{-1}\Delta_{jq}^*,$$



$$M_{nm}^{(j)}(q) = \frac{S_{nm}^{(j)}(q, E_{1q}) + S_{nm}^{(j)}(q, -E_{1q})}{4E_{1q}(E_{1q}^2 - E_{2q}^2)(E_{1q}^2 - E_{3q}^2)} \tanh\left(\frac{E_{1q}}{2T}\right).$$

$$\tilde{V}_2 = \frac{V_2 + V_2'}{2}$$

V.V Val'kov, D.M. Dzebisashvili, M.M. Korovushkin, A.F. Barabanov, submited to JMMM

Conclusions

1) **In the framework of spin-fermion model taking into account the strong coupling between the charge and spin degrees of freedom, and the actual lattice structure of the CuO_2-plane with two oxygen ions per unit cell, the band structure of Fermi excitations of the spin-polaron quasiparticles was calculated.**

2) **The spectrum was calculated at first using the variational method for a doped hole. It was shown that the lower polaron band splitting-off is entirely due to the third basis operator reflecting a strong correlation between the subsystem of localized spin moments of copper ions and subsystem of holes moving over oxygen ions. This proofs the spin-polaron nature of Fermi quasiparticles in the Emery model.**

3) **Then the spectrum of the ensemble of spin-polaron quasiparticles was considered in the framework of Zwanzig-Mori projection method and the same dispersion (as in variational method) equation was obtained. On the basis of numerical calculations it was shown that fine details of the Fermi surface evolution in $La_{2-x}Sr_xCuO_4$, observed in the normal phase in ARPES experiments at doping, are well reproduced, if basis of operators, used in finding of energy structure, includes the operator describing the strong coupling of spin and charge degrees of freedom.**

Conclusions

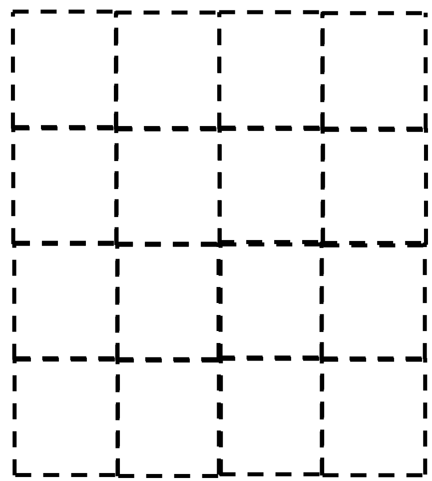
4) It was shown that mechanism ensuring the Cooper pairing of spin polarons is the exchange interaction, which transforms to an effective attraction between spin polarons due to the strong spin-charge coupling. In this regard, it should be emphasized the important role of the spin-flip processes in the formation of the Cooper instability.

5) The Coulomb interaction of two holes on the nearest sites does not contribute to the solution of the integral equations for the d-wave superconducting order parameter. As a result, the Coulomb repulsion of two holes on the nearest oxygen ions, does not suppress the Cooper pairing in the d-wave channel.

6) The Coulomb interaction of two holes on the next-nearest sites contributes to the solution of the integral equations for the d-wave pairing and causes its suppression, however superconductivity survives at reasonable values of V2.

7) In cuprate superconductors, neutralization of the intersite Coulomb repulsion for the dx2-y2-wave superconducting phase is caused by complicated unit cell and the specifics of the Fourier transform of the Coulomb potential, in contrast to conventional superconductors described by the BCS theory, where the Coulomb potential is renormalized due to the electron-phonon interaction.

Thank you for attention!



$$\langle X_f^{0\bar{\sigma}} X_f^{0\sigma} \rangle = \frac{T}{N} \sum_{\vec{k},\omega_m} \exp(i\omega_m \delta) \left\langle X_{-\vec{k}\bar{\sigma}} X_{\vec{k}\sigma} \right\rangle_{\omega_m} = 0, \qquad \delta \to +0,$$

$$\left\langle X_{-\vec{k}\bar{\sigma}} X_{\vec{k}\sigma} \right\rangle_{\omega_m} = \frac{\Sigma_{0\sigma,\bar{\sigma}0}(k) P_{\bar{\sigma}0,\bar{\sigma}0}(k) + \left[i\omega_m + \varepsilon - \mu - \Sigma_{\bar{\sigma}0,\bar{\sigma}0}(k) \right] P_{0\sigma,\bar{\sigma}0}(k)}{\det(k, i\omega_m)}$$

$$\det(k,i\omega_m) = \left\{ i\omega_m + \varepsilon - \mu + t_k P_{\bar{\sigma}0,\bar{\sigma}0}(k,i\omega_m) - \Sigma_{\bar{\sigma}0,\bar{\sigma}0}(k,i\omega_m) \right\} \times$$
$$\times \left\{ i\omega_m - \varepsilon + \mu - t_k P_{0\sigma,0\sigma}(k,i\omega_m) - \Sigma_{0\sigma,0\sigma}(k,i\omega_m) \right\} -$$
$$- \left\{ \Sigma_{0\sigma,\bar{\sigma}0}(k,i\omega_m) - t_k P_{0\sigma,\bar{\sigma}}(k,i\omega_m) \right\} \left\{ \Sigma_{\bar{\sigma}0,0\sigma}(k,i\omega_m) + t_k P_{\bar{\sigma}0,0\sigma}(k,i\omega_m) \right\}$$