Bogoliubov Laboratory of Theoretical Physics

ANTIFERROMAGNETIC EXCHANGE AND SPIN-FLUCTUATION PAIRING IN CUPRATES

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CORPES, Dresden, 26.05.2005

Publications and collaborators:

- *N.M. Plakida,* L. Anton, S. Adam, and Gh. Adam,

  Exchange and Spin-Fluctuation Mechanisms of Ssuperconductivity in Cuprates. JETP **97**, 331 (2003).

- *N.M. Plakida* , Antiferromagnetic exchange mechanism of superconductivity in cuprates. JETP Letters **74**, 36 (2001)

- *N.M. Plakida,* V.S. Oudovenko,

  Electron spectrum and superconductivity in the **t-J** model at moderate doping.

  Phys. Rev. B **59**, 11949 (1999)

- S. Krivenko, A.Avella, F. Mancini, *N.M. Plakida,*

  SCBA within composite operator method for the Hubbard model

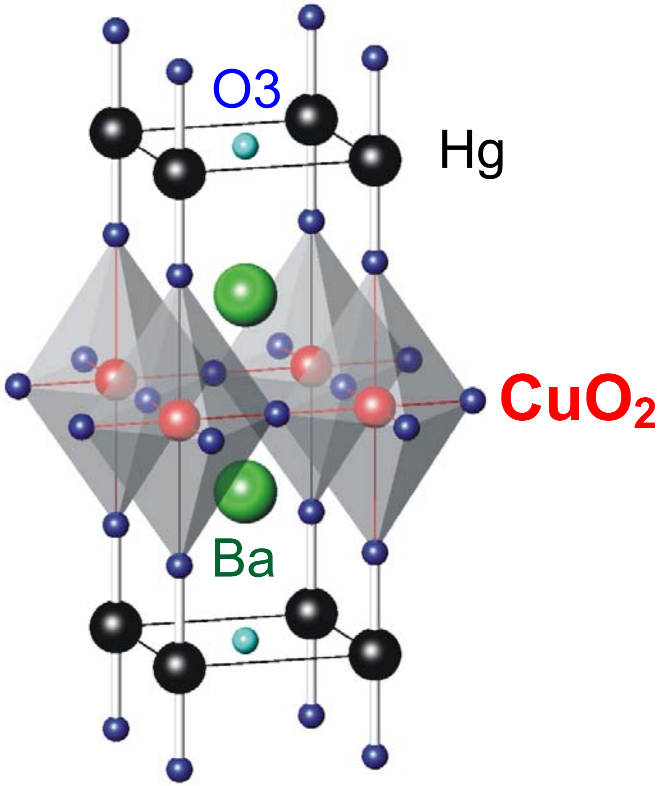
  Physica B, *in press* (2005)

Outline

Two mechanisms of AFM pairing

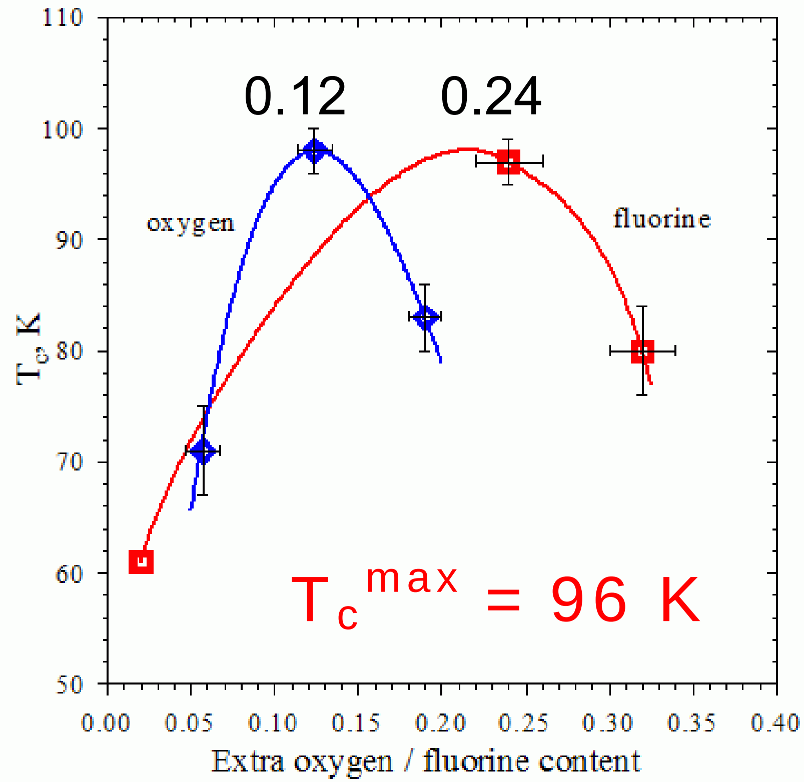
Effective p-d Hubbard model

- AFM exchange pairing in MFA
- Self-energy corrections in SCBA
- Results for T_c and SC gaps
- T_c (a) and isotope effect
- Comparison with t-J model



Structure of Hg-1201 compound ($HgBa_2CuO_{4+\delta}$)

After A.M. Balagurov et al.



Tc as a function of doping (oxygen or fluorine)

Abakumov et al. Phys.Rev.Lett. (1998)

WHY ARE COPPER–OXIDES THE ONLY HIGH–T_c SUPERCONDUCTORS with T_c > 100 K?

Cu $^{2+}$ in $3d^9$ state has the lowest 3d level in transition metals

with strong Coulomb correlations $U_d > \Delta_{pd} = \varepsilon_p - \varepsilon_d$.

They are **CHARGE-TRANSFER INSULATORS**

with **HUGE** super-exchange interaction $J \sim 1500$ K —>

- AFM long–range order with high T_N = 300 – 500 K
- Strong coupling of doped holes (electrons) with spins
- Pseudogap due to AFM short – range order
- **High-T_c superconductivity ?**

EFFECTIVE HUBBARD p-d MODEL

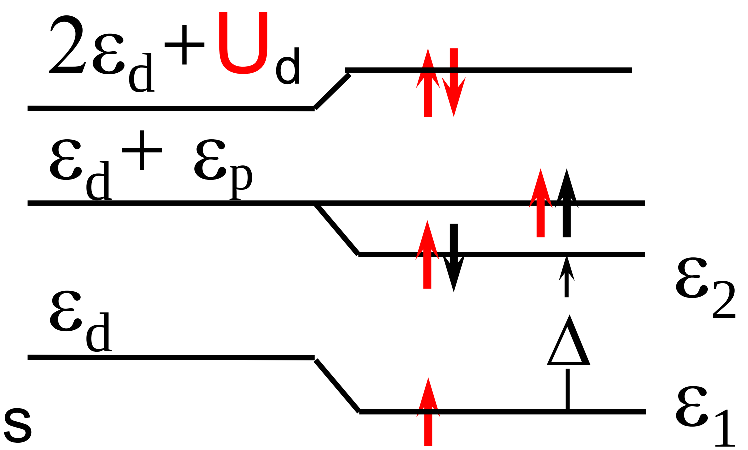
Model for CuO_2 layer:

Cu-3d (ε_d) and

O-2p (ε_p) states

$\Delta = \varepsilon_p - \varepsilon_d \approx 2\, t_{pd} \sim 3$ eV

In terms of O-2p Wannier states



$$H = \sum_{i\sigma} \{\varepsilon_d\, n^d_{i\sigma} + \varepsilon_p\, n^p_{i\sigma} + H_i(U_d, U_p, V_{pd}, t_{pp})\}$$

$$+ \sum_{i,j,\sigma} V_{ij}\, (d^{+}_{i\sigma} p_{j\sigma} + H.c.) = \sum_i H_i^{(0)} + H_{int}(i \neq j)$$

where $V_{ij} = 2t_{pd}\nu_{ij}$, $V_{ii} \simeq 2t_{pd} \simeq \Delta \gg |V_{j\neq i}|$

Cell-cluster perturbation theory and Hubbard operators

Exact diagonalization of the unit cell Hamiltonian $H_i^{(0)}$ gives new eigenstates:

$E_1 = \varepsilon_d - \mu$ → one hole d - like state: $| \sigma >$

$E_2 = 2 E_1 + \Delta$ → two hole (p - d) singlet state: $| \uparrow\downarrow >$

We introduce the Hubbard operators for these states:

$X_i^{\alpha\beta} = | i\alpha > < i\beta |$ with $| \alpha > = | 0 >, \; | \sigma >, \; | \uparrow\downarrow >$

Hubbard operators rigorously obey the constraint:

$$X_i^{00} + X_i^{\uparrow\uparrow} + X_i^{\downarrow\downarrow} + X_i^{22} = 1$$

— only one quantum state can be occupied at any site *i*.

In terms of the projected Fermi operators:

$X_i^{0\sigma} \to c_{i\sigma}(1 - n_{i-\sigma})$, $\quad X_i^{\sigma 2} \to c_{i-\sigma}\, n_{i\sigma}$

Commutation relations: $[X_i^{\alpha\beta}, X_i^{\gamma\delta}]_{\pm} = \delta_{\beta\gamma} X_i^{\alpha\delta} \pm \delta_{\delta\alpha} X_i^{\gamma\beta}$

The two-subband effective Hubbard model reads:

$$\begin{aligned} H \;=\; & E_1 \sum_{i,\sigma} X_i^{\sigma\sigma} + E_2 \sum_{i} X_i^{22} + \sum_{i\neq j,\sigma} \{\, t_{ij}^{11} X_i^{\sigma 0} X_j^{0\sigma} + \\ + \; & t_{ij}^{22} X_i^{2\sigma} X_j^{\sigma 2} + \sigma\, t_{ij}^{12} (X_i^{2\bar\sigma} X_j^{0\sigma} + X_j^{\sigma 0} X_i^{\bar\sigma 2}) \,\} \end{aligned}$$

where $\bar\sigma = -\sigma = \pm 1$ and hopping parameters

$$t_{ij}^{\alpha\beta} = \Gamma_{\alpha\beta}\, \nu_{ij}\, 2\, t_{pd} \simeq 0.1\, t_{pd} \ll \Delta$$

Kinematic interaction for the Hubbard operators:

$$\begin{aligned} Z_i^{\sigma 2} \;=\; & [X_i^{\sigma 2}, H] = (E_1 + \Delta) X_i^{\sigma 2} - \sum_{m} X_i^{02} \left(t_{im}^{11} X_m^{\sigma 0} + \sigma\, t_{im}^{21} X_m^{2\bar\sigma} \right) \\ + \; & \sum_{m,\sigma'} \left(t_{im}^{22}\, B_{i\sigma\sigma'}^{22}\, X_m^{\sigma' 2} - \sigma t_{im}^{21}\, B_{i\sigma\sigma'}^{21}\, X_m^{0\bar\sigma'} \right), \end{aligned}$$

where Bose-like operators are: $B_{i\sigma\sigma'}^{22(21)} =$

$$(X_i^{22} + X_i^{\sigma\sigma}) \delta_{\sigma'\sigma} \pm X_i^{\sigma\bar\sigma}\, \delta_{\sigma'\bar\sigma} = (N_i/2 + S_i^z) \delta_{\sigma'\sigma} \pm S_i^{\sigma} \delta_{\sigma'\bar\sigma}$$

Dyson equation for GF in the Hubbard model

We introduce the (4x4) matrix Green Functions:

$$\tilde{G}_{ij\sigma}(t-t') = \langle\langle \hat{X}_{i\sigma}(t) \mid \hat{X}^{\dagger}_{j\sigma}(t') \rangle\rangle$$

for Nambu operators: $\hat{X}^{\dagger}_{i\sigma} = (X_i^{2\sigma}\ X_i^{\bar{\sigma}0}\ X_i^{\bar{\sigma}2}\ X_i^{0\sigma})$

$$\tilde{G}_{ij\sigma}(\omega) = \begin{pmatrix} \hat{G}_{ij\sigma}(\omega) & \hat{F}_{ij\sigma}(\omega) \\ \hat{F}^{\dagger}_{ji\sigma}(\omega) & -\hat{G}_{ji\bar{\sigma}}(-\omega) \end{pmatrix}$$

where $\hat{G}_{ij\sigma}(\omega)$– normal and $\hat{F}_{ij\sigma}(\omega)$– anomalous (2×2) matrix GF for two Hubbard subbands.

Equations of motion for the matrix GF are solved within the Mori-type projection technique:

$$\omega \tilde{G}_{ij\sigma}(\omega) = \delta_{i,j}\,\tilde{\chi} + \langle\langle [\hat{X}_{i\sigma}, H] \mid \hat{X}^{\dagger}_{j\sigma}\rangle\rangle_{\omega}, \qquad \tilde{\chi} = \langle \{\hat{X}_{i\sigma}, \hat{X}^{\dagger}_{i\sigma}\}\rangle$$

$$\text{Projection} \;\; \rightarrow \;\; [\hat{X}_{i\sigma}, H] = \sum_{m} \tilde{E}_{im\sigma}\hat{X}_{m\sigma} + \hat{Z}^{(ir)}_{i\sigma}, \;\; \langle \{\hat{Z}^{(ir)}_{i\sigma}, \hat{X}^{\dagger}_{j\sigma}\}\rangle = 0,$$

Frequency matrix: $\tilde{E}_{ij\sigma} = \langle \{[\hat{X}_{i\sigma}, H], \hat{X}^{\dagger}_{j\sigma}\}\rangle\, \tilde{\chi}^{-1}$

The Dyson equation reads:

$$\left(\tilde{G}_{\sigma}(\mathbf{q}, \omega)\right)^{-1} = \left\{\omega \tilde{\tau}_0 - \tilde{E}_{\sigma}(\mathbf{q}) - \tilde{\Sigma}_{\sigma}(\mathbf{q}, \omega)\right\} \tilde{\chi}^{-1}$$

with the self-energy as the multi-particle GF:

$$\tilde{\Sigma}_{\sigma}(\mathbf{q}, \omega) = \tilde{\chi}^{-1}\langle\langle \hat{Z}^{(ir)}_{\mathbf{q}\sigma} \mid \hat{Z}^{(ir)\dagger}_{\mathbf{q}\sigma}\rangle\rangle^{(prop)}_{\omega}$$

Mean-Field approximation: zero order GF

$$\tilde{G}^{0}_{\sigma}(\mathbf{q},\omega) = (\omega\tilde{I} - \tilde{E}_{\sigma}(\mathbf{q}))^{-1}\tilde{\chi}$$

where frequency matrix: $\tilde{E}_{ij\sigma} = \begin{pmatrix} \hat{\omega}_{ij\sigma} & \hat{\Delta}_{ij\sigma} \\ (\hat{\Delta}^{*}_{ji\sigma}) & \hat{\omega}_{ji-\sigma} \end{pmatrix} \tilde{\chi}^{-1}$

with $\hat{\omega}_{ij}$ – frequency matrix of the normal state

QP spectrum: $\Omega_2(\mathbf{q})$ for *UHD* and $\Omega_1(\mathbf{q})$ — *LHB*

$\hat{\Delta}_{ij\sigma}$ – matrix of anomalous correlation functions: e.g.,

$\Delta^{22}_{ij\sigma} = -\sigma\, t^{12}_{ij} \langle X^{02}_{i} N_{j} \rangle$ – SC gap for singlets (*UHB*)

Normal state MFA GF: one-hole $\Omega_D(\mathbf{q})$ and two-hole $\Omega_\psi(\mathbf{q})$ spectra

$$\hat{G}^0_\sigma(\mathbf{q},\omega) = \begin{Bmatrix} [\omega - \omega_D(\mathbf{q})]\chi_\psi & -W_\sigma^{\psi D}\chi_D \\ -W_\sigma^{D\psi}\chi_\psi & [\omega - \omega_\psi(\mathbf{q})]\chi_D \end{Bmatrix} \cdot \{[\omega - \Omega_\psi(\mathbf{q})][\omega - \Omega_D(\mathbf{q})]\}^{-1} ,$$

Spectral weights:

$$\chi_\psi = 1 - \chi_D = n/2$$

$$\Omega_{\psi,D}(\mathbf{q}) = \frac{1}{2}[\omega_\psi(\mathbf{q}) + \omega_D(\mathbf{q})] \pm \frac{1}{2}\{[\omega_\psi(\mathbf{q}) - \omega_D(\mathbf{q})]^2 + 4W_\sigma^{\psi D}W_\sigma^{D\psi}\}^{1/2} .$$

$$\omega_\psi(\mathbf{q}) = E_\psi - E_D - \mu + \Delta_\sigma^{\psi\psi} + V_\sigma^{\psi\psi}(\mathbf{q}),$$
$$\omega_D(\mathbf{q}) = E_D - \mu + \Delta_\sigma^{DD} + V_\sigma^{DD}(\mathbf{q}),$$

Hybridization:

$$W_\sigma^{\psi D} = \Delta_\sigma^{\psi D} + V_\sigma^{\psi D}(\mathbf{q})$$

Dispersion in n.n. $\gamma_1(\mathbf{q})$ and n.n.n. $\gamma_2(\mathbf{q})$ approximation:

$$V_\sigma^{\psi\psi}(q) = tK_{\psi\psi}\chi_\psi \sum_i \gamma_i(\mathbf{q})(1 + \chi_s^{(i)}/\chi_\psi^2)$$

where $1/\chi_\psi^2 = 4 / n^2$

Spin-correlation functions:

$\chi_s^{(1)} = \langle \mathbf{S}_i\mathbf{S}_{i\pm a_{x/y}} \rangle$ **< 0,** $\chi_s^{(2)} = \langle \mathbf{S}_i\mathbf{S}_{i\pm a_x \pm a_y} \rangle$ **> 0,** Spin-correlation functions gives a strong renormalization for spectra

$$\langle \mathbf{S}_0 \mathbf{S}_j \rangle = \frac{1}{N} \sum_q \chi_q e^{i\mathbf{q}\cdot\mathbf{j}} , \qquad \chi_q = \frac{C(\xi)}{1 + \xi^2[1 + \frac{1}{2}(\cos q_x + \cos q_y)]} .$$

Normalization condition $\langle \mathbf{S}_i \mathbf{S}_i \rangle = 3/4$ defines $C(\xi)$ = χ_q at q = (π, π)

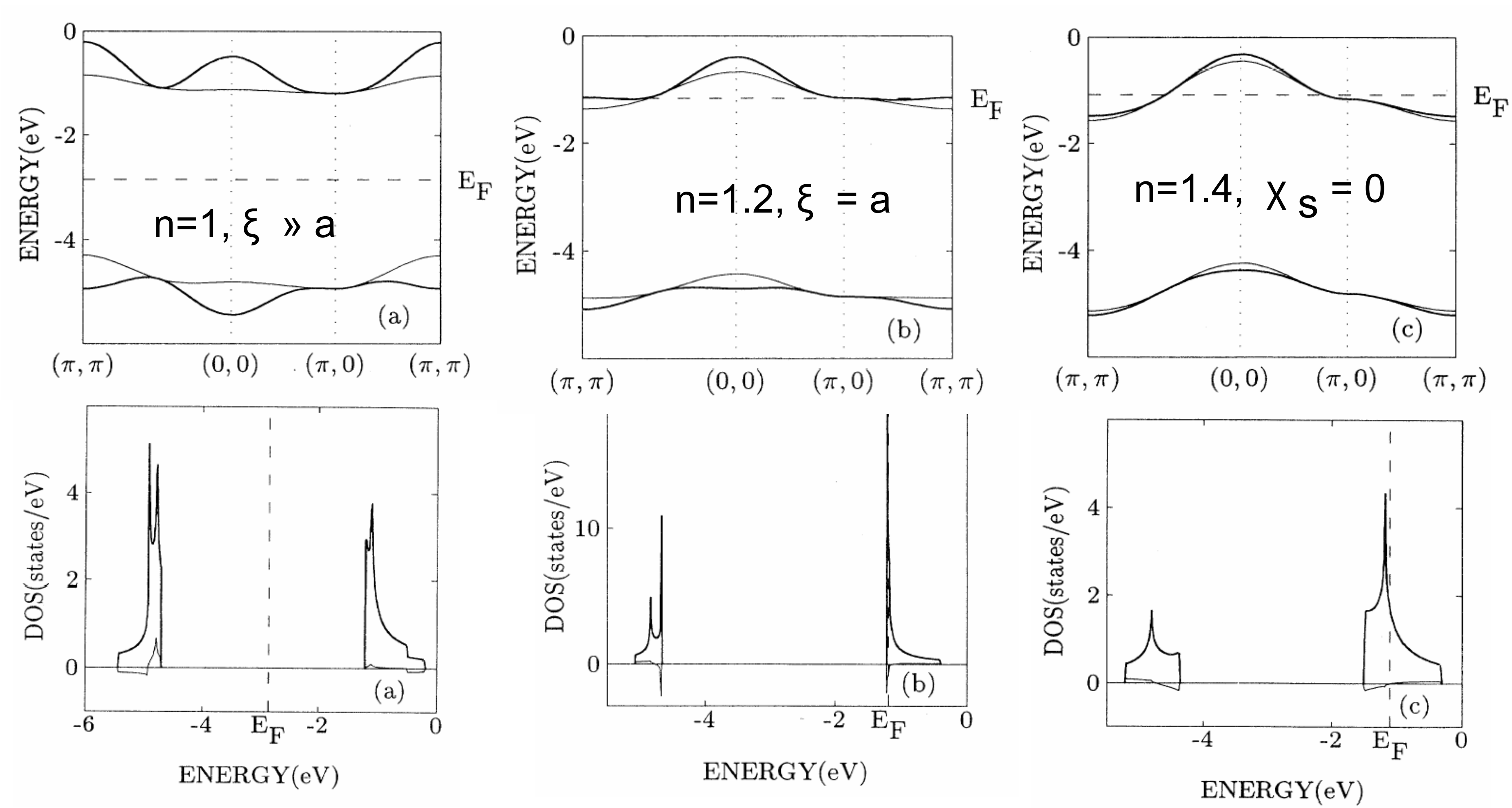
for a given AF correlation length ξ — the fitting parameter

n = 1 ξ » *a:* $\chi_s^{(1)}$ = - 0.336, $\chi_s^{(2)}$ = 0.202,

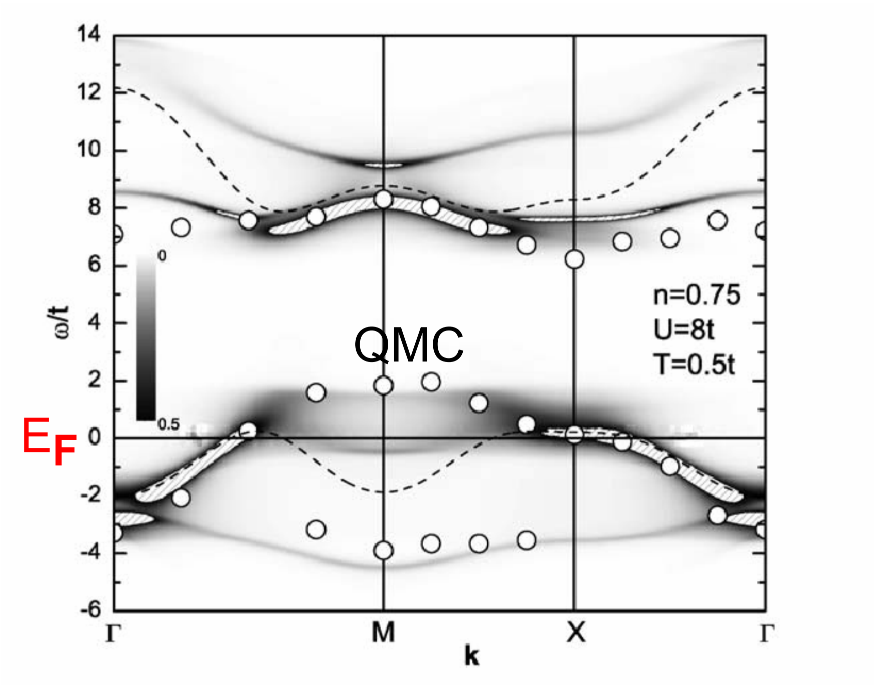
n = 1.2 ξ = *a:* $\chi_s^{(1)}$ = - 0.10, $\chi_s^{(2)}$ = 0.03,

n = 1.4 $\chi_s^{(1)}$ = $\chi_s^{(2)}$ = 0, — no AF corelations

2-pole approximation for the effective Hubbard model: *spectra* and *DOS*

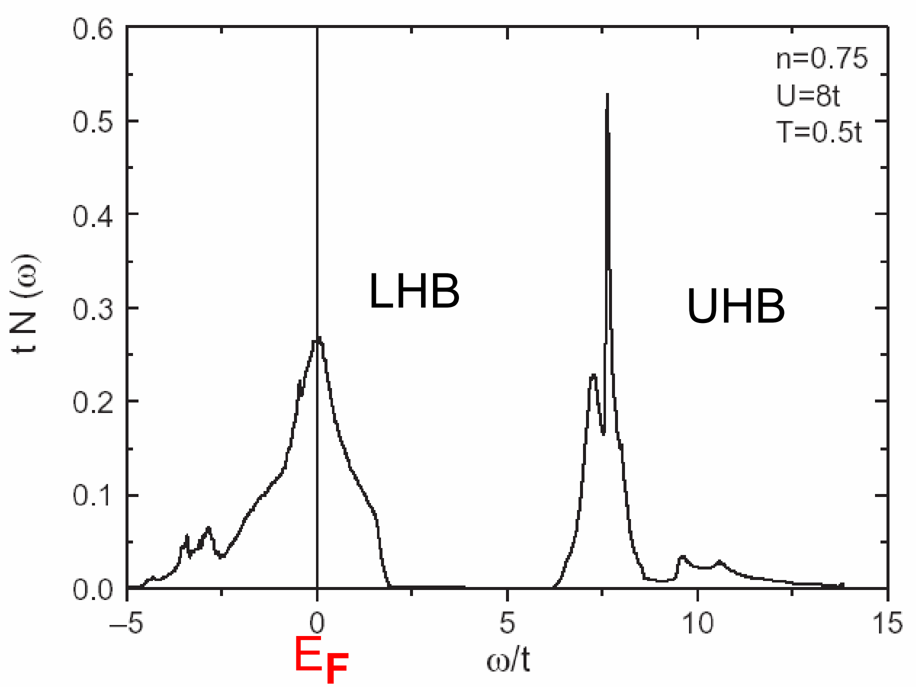


Self-energy corrections to the 2-pole approximation in the SCBA for the Hubbard model



Spectral density A(**k**,ω)

U = 8 t, n = 0.75, T = 0.5 t



Density of states A(ω)

Krivenko et al. Physica B (2005)

Mean-Field approximation for the gap function

Frequency matrix:

$$\tilde{E}_{ij\sigma} = \begin{pmatrix} \hat{\omega}_{ij\sigma} & \hat{\Delta}_{ij\sigma} \\ (\hat{\Delta}^{*}_{ji\sigma}) & \hat{\omega}_{ji-\sigma} \end{pmatrix} \tilde{\chi}^{-1}$$

where $\hat{\Delta}_{ij\sigma}$ – matrix of anomalous correlation functions

$$\Delta^{22}_{ij\sigma} = -\sigma\, t^{12}_{ij} \langle X^{02}_{i} N_j \rangle$$

– anomalous correlation function

– SC gap for singlets in *UHB*

→ PAIRING at ONE lattice site but in TWO subbands

$$\langle X^{02}_{i} N_j \rangle = \langle X^{0\downarrow}_{i} X^{\downarrow 2}_{i} N_j \rangle = \langle c_{i\downarrow} c_{i\uparrow} N_j \rangle$$

Equation for the pair correlation Green function $\langle\langle X_i^{02}(t) \mid N_j(t')\rangle\rangle$ gives:

$$\langle X_i^{02} N_j \rangle = \int_{-\infty}^{+\infty} \frac{d\omega}{1 - \exp(-\omega/T)} \sum_{m,\sigma} \sigma\, t_{im}^{12}$$

$$\{-\frac{1}{\pi} \mathrm{Im} \frac{1}{\omega - E_2} [\langle\langle X_i^{0\bar{\sigma}} X_m^{0\sigma} | N_j \rangle\rangle_\omega - \langle\langle X_i^{\sigma 2} X_m^{\bar{\sigma} 2} | N_j \rangle\rangle_\omega]\}$$

For the singlet subband (*UHB*) : $\mu \approx \Delta$ and $E_2 \approx E_1 \approx -\Delta$:

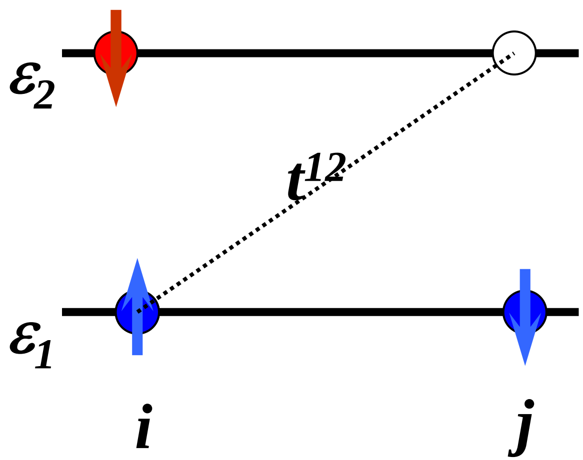
$$= -\frac{1}{\Delta} \sum_{m,\sigma} \sigma t_{im}^{12} \langle X_i^{\sigma 2} X_m^{\bar{\sigma} 2} N_j \rangle |_{m=j} \simeq -(4 t_{ij}^{12}/\Delta) \sigma \, \langle X_i^{\sigma 2} X_j^{\bar{\sigma} 2} \rangle$$

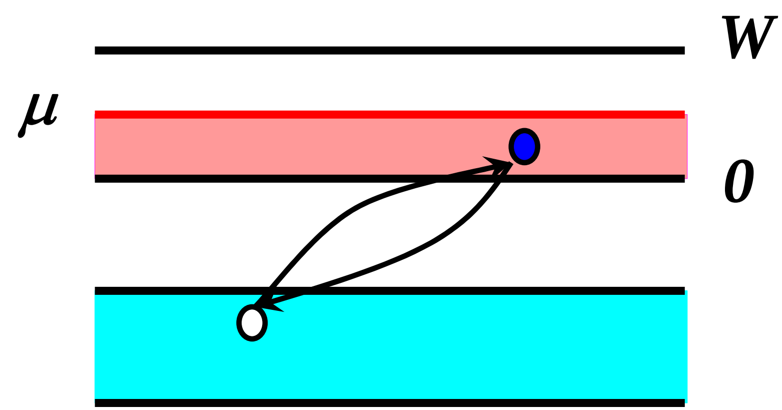
Gap function for the singlet subband in MFA :

$$\Delta_{ij\sigma}^{22} = J_{ij} \, \langle X_i^{\sigma 2} X_j^{\bar{\sigma} 2} \rangle, \qquad J_{ij} = 4\, (t_{ij}^{12})^2 / \Delta$$

is equvalent to the MFA in the t-J model

AFM exchange pairing





All electrons (holes) are paired in the conduction band.
Estimate in WCA gives for T_c^{ex} :

$$T_c^{ex} \simeq \sqrt{\mu(W-\mu)}\, \exp(-1/\lambda_J) \simeq (30 - 150)\,\mathrm{K}$$

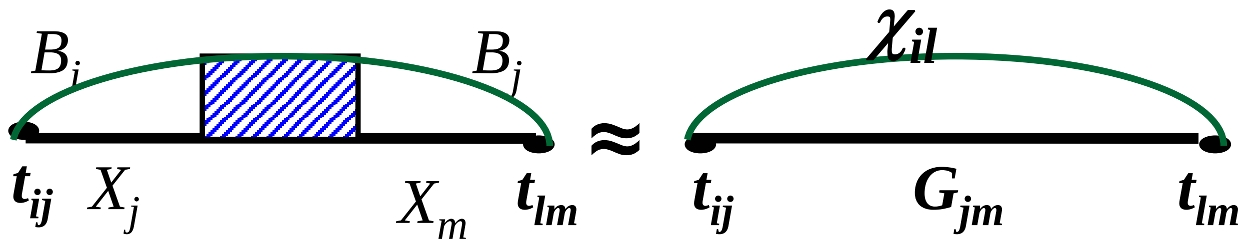
$$\text{for} \;\; \mu = W/2 \simeq 0.35 \;\text{eV}, \qquad \lambda_J = J N_\delta \simeq 0.2 - 0.3$$

Self-energy in the Hubbard model

$$\tilde{\Sigma}_\sigma(\mathbf{q},\omega) = \tilde{\chi}^{-1} \langle\langle \hat{Z}_\sigma^{(ir)} \mid \hat{Z}_\sigma^{(ir)\dagger} \rangle\rangle_{\mathbf{q},\omega}^{(prop)} ,$$ where

$$\left(Z_i^{\sigma 2}\right)^{ir} = \sum_{m,\sigma} \left(t_{im}^{22}\, \delta B_{i\sigma\sigma'}^{22} X_m^{\sigma' 2} - \sigma t_{im}^{21}\, \delta B_{i\sigma\sigma'}^{21} X_m^{0\bar{\sigma}'} \right)$$

SCBA:



$$\langle B_{1'}(t) X_1(t) \mid B_{2'} X_2 \rangle \simeq \langle X_1(t) X_2 \rangle \, \langle B_{1'}(t) B_{2'} \rangle_{(1' \neq 1)}$$

Self-energy matrix:

$$\tilde{\Sigma}_{ij\sigma}(\omega) = (\tilde{\chi})^{-1} \begin{pmatrix} \hat{M}_{ij\sigma}(\omega) & \hat{\Phi}_{ij\sigma}(\omega) \\ \hat{\Phi}_{ji\sigma}^{\dagger}(\omega) & -\hat{M}_{ji\bar{\sigma}}(-\omega) \end{pmatrix}$$

Gap equation for the singlet (p-d) subband:

$$\Phi_{\sigma}^{22}(\mathbf{q},\omega) = \frac{1}{N}\sum_{\mathbf{k}}\int_{-\infty}^{+\infty} d\omega_1 K(\omega,\omega_1|\mathbf{k},\mathbf{q}-\mathbf{k})$$

$$\times\{-\frac{1}{\pi}\,\mathrm{Im}\,[\,\Gamma_{22}^{2}\,F_{\sigma}^{22}(\mathbf{k},\omega_1) - \Gamma_{12}^{2}\,F_{\sigma}^{11}(\mathbf{k},\omega_1)]\,\}$$

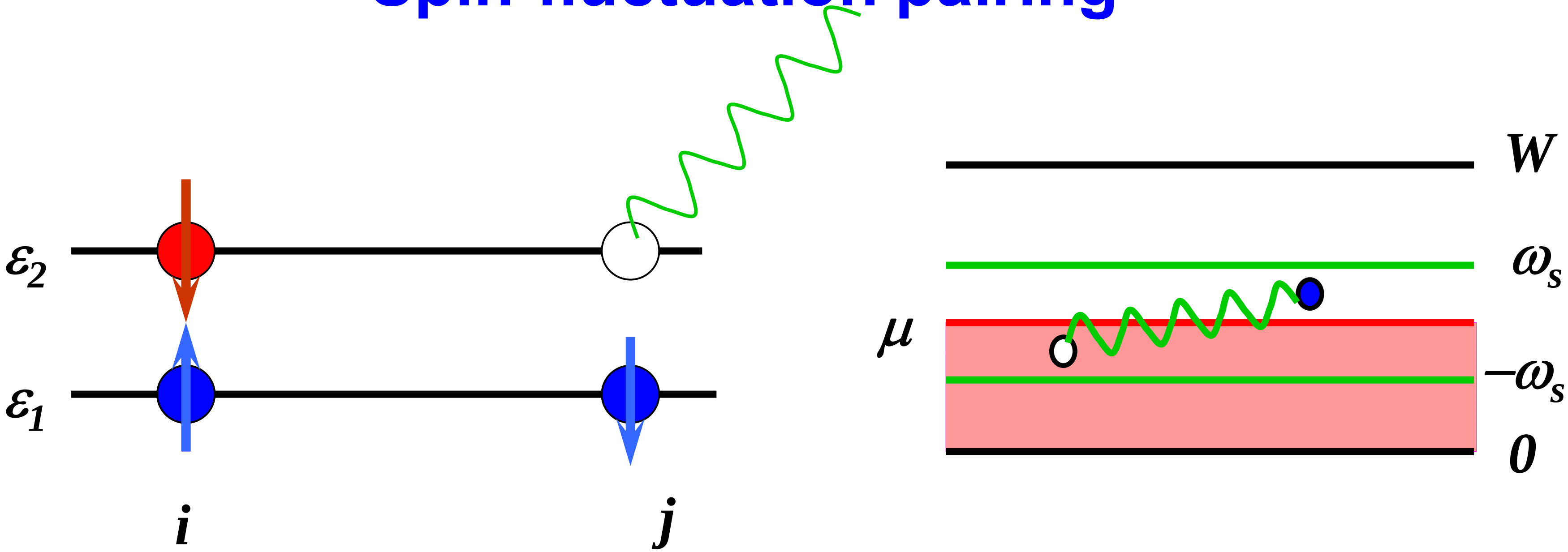
where the kernel of the integral equation in SCBA

$$K(\omega,\omega_1|\mathbf{k},\mathbf{q}) = \frac{1}{2\pi}\int_{-\infty}^{+\infty}\frac{d\omega_2}{(\omega-\omega_1-\omega_2)}(\tanh\frac{\omega_1}{2T} + \coth\frac{\omega_2}{2T})$$

$$\times|t(\mathbf{k})|^2\,\mathrm{Im}\,[\langle\langle S_q \mid S_{-q}\rangle\rangle - \frac{1}{4}\langle\langle N_q \mid N_q^{+}\rangle\rangle]_{\omega_2+i\delta}$$

defines pairing mediated by spin and charge fluctuations.

Spin-fluctuation pairing



Estimate in WCA gives for T_c^{sf} :

$$T_c^{sf} \simeq \omega_s \exp\left(-1/V_{sf}\right) \simeq 10 - 50 \text{ K}$$

for $\omega_s \simeq 0.12$ eV, $\quad V_{sf} = \lambda_s N_F \simeq 0.2 - 0.3$

Equation for the gap and T_c in WCA

$$\Delta(\mathbf{q}) = \frac{1}{N}\sum_{\mathbf{k}} \frac{\Delta(\mathbf{k})}{2\mathsf{E}(\mathbf{k})} \tanh\frac{\mathsf{E}(\mathbf{k})}{2\mathsf{T}} \left[\mathsf{J}(\mathbf{k}-\mathbf{q}) - \lambda_s(\mathbf{k},\mathbf{k}-\mathbf{q}) \right]$$

$$\mathsf{E}(\mathbf{k}) = \{\varepsilon^2(\mathbf{k}) + |\Delta(\mathbf{k})|^2\}^{1/2},$$

$$\lambda_s(\mathbf{k},\mathbf{k}-\mathbf{q}) = t_{\mathrm{eff}}^2\, \gamma(\mathbf{k})^2\, \chi_s(\mathbf{k}-\mathbf{q}),$$

$$t_{\mathrm{eff}} \simeq 0.14 t_{pd}, \qquad \gamma(\mathbf{q}) = (1/2)(\cos q_x + \cos q_y)$$

$$\chi_s(\mathbf{q}) = \frac{1}{\omega_s}\langle \mathbf{S}_{\mathbf{q}}\mathbf{S}_{-\mathbf{q}}\rangle = \frac{\chi_0(\xi)}{1+\xi^2(1+\gamma(\mathbf{q}))},$$

Normalization condition: $\frac{1}{N}\sum_{\mathbf{q}}\langle \mathbf{S}_{\mathbf{q}}\mathbf{S}_{-\mathbf{q}}\rangle = \frac{3}{4}(1-\delta)$

where ξ — short-range AFM correlation length,

$\omega_s \approx J$ — cut-off spin-fluctuation energy.

Estimate for T_c in the weak coupling approximation

$$1 \simeq J \int_{-\mu}^{W-\mu} \frac{d\epsilon}{2\epsilon} \tanh \frac{\epsilon}{2T_c} N_d(\epsilon) + \lambda_s \int_{-\omega_s}^{\omega_s} \frac{d\epsilon}{2\epsilon} \tanh \frac{\epsilon}{2T_c} N_{sf}(\epsilon)$$

$$T_c \simeq \omega_s \exp(-\frac{1}{\tilde{V}_s}), \qquad \tilde{V}_s = V_{sf} + \frac{V_{ex}}{1 - V_{ex} \ln(\mu/\omega_s)},$$

$$V_{ex} \simeq J N_d(0), \qquad V_{sf} \simeq \lambda_s N_{sf}(0), \; \lambda_s = t_{eff}^2/\omega_s$$

Effective spin-fluctuation pairing constant V_s enhanced by exchange

$$T_c \simeq \omega_s \exp(-1/\tilde{V}_s) \simeq (150 - 350)\,K$$

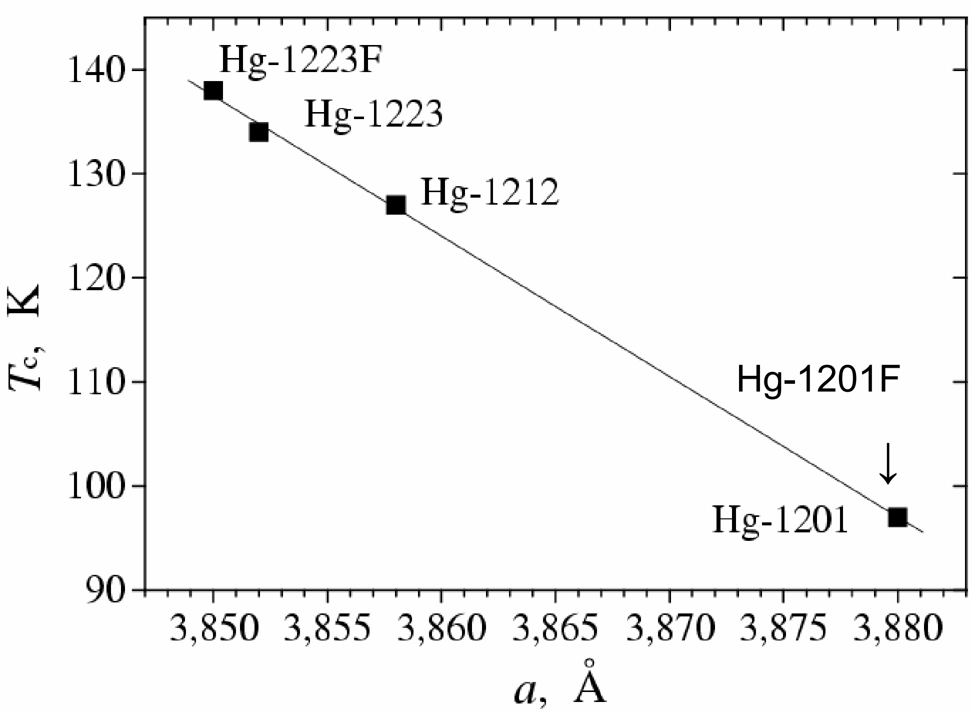
for $V_{sf} \simeq V_{ex} = 0.2 - 0.3$ and

$$\tilde{V}_s = V_{sf} + \frac{V_{ex}}{1 - V_{ex} \ln(\mu/\omega_s)} \simeq 0.45 - 0.72$$

T_c (a) and pressure dependence

For mercury compounds, Hg-12(n-1)n, experiments show $dT_c / da \approx -1.35 \cdot 10^{3}$ (K /Å), or $d \ln T_c / d \ln a \approx -50$

*[Lokshin et al. PRB **63** (2000) 64511]*



For exchange pairing

$T_c \approx E_F \exp(-1/V_{ex})$,
$V_{ex} = J\, N(0)$, we get:

$d \ln T_c / d \ln a$
$= (d \ln T_c / d \ln J)$
$\times (d \ln J / d \ln a)$
$\approx -14\,(1/V_{ex}) \approx -50$,

where $V_{ex} \approx 0.3$ and
$J \approx t_{pd}^4 \sim 1/a^{14}$

For conventional, electron-phonon superconductors, $d\,Tc / d\,P < 0$, e.g., for MgB_2, $d\,Tc / d\,P \approx -1.1$ K/GPa, while for cuprates superconductors, $d\,Tc / d\,P > 0$

Isotope shift: $^{16}O \rightarrow {}^{18}O$

Isotope shift of $T_N = 310K$ for La_2CuO_4, $\Delta T_N \approx -1.8$ K

*[G.Zhao et al., PRB **50** (1994) 4112]*

and $\alpha_N = - d\ln T_N / d\ln M \approx -(d\ln J / d\ln M) \approx 0.05$

Isotope shift of T_c : $\alpha_c = - d\ln T_c / d\ln M =$

$= -(d\ln T_c / d\ln J)(d\ln J / d\ln M) \approx (1/V_{ex})\,\alpha_N \approx 0.16$

Equation for the gap and T_c in WCA

$$\Delta(\mathbf{q}) = \frac{1}{N}\sum_{\mathbf{k}} \frac{\Delta(\mathbf{k})}{2\mathsf{E}(\mathbf{k})} \tanh\frac{\mathsf{E}(\mathbf{k})}{2\mathsf{T}} \left[\, \mathsf{J}(\mathbf{k}-\mathbf{q}) - \lambda_s(\mathbf{k},\mathbf{k}-\mathbf{q})\right]$$

$$\mathsf{E}(\mathbf{k}) = \{\varepsilon^2(\mathbf{k}) + |\Delta(\mathbf{k})|^2\}^{1/2},$$

$$\lambda_s(\mathbf{k},\mathbf{k}-\mathbf{q}) = t_{eff}^2\, \gamma(\mathbf{k})^2\, \chi_s(\mathbf{k}-\mathbf{q}),$$

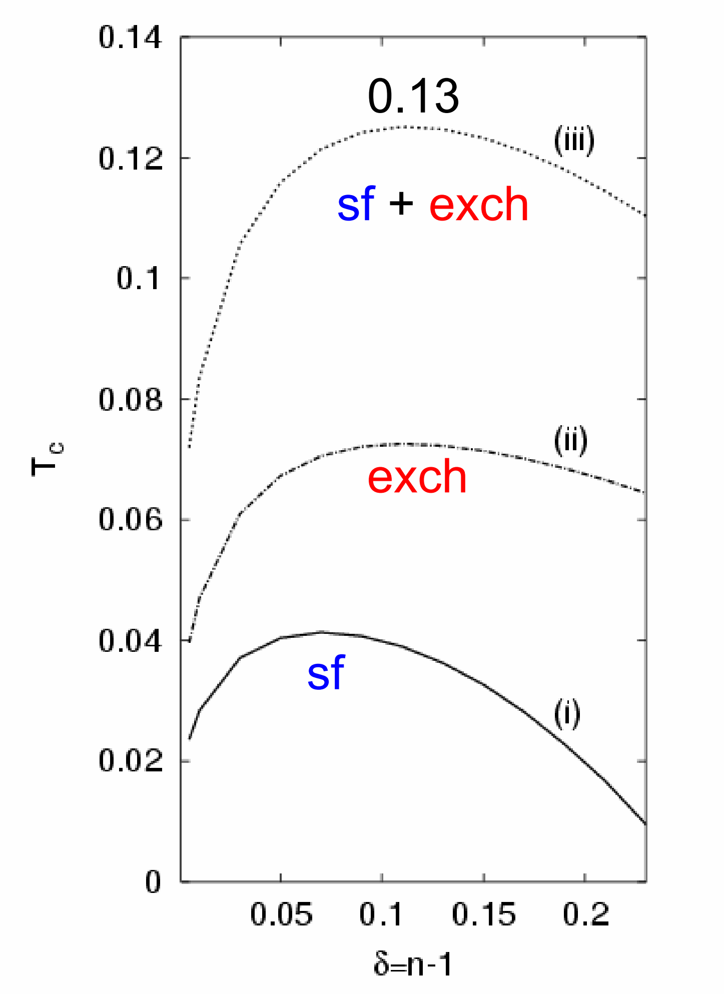
$$t_{eff} \simeq 0.14 t_{pd}, \qquad \gamma(\mathbf{q}) = (1/2)(\cos q_x + \cos q_y)$$

$$\chi_s(\mathbf{q}) = \frac{1}{\omega_s}\langle \mathbf{S_q S_{-q}}\rangle = \frac{\chi_0(\xi)}{1+\xi^2\,(1+\gamma(\mathbf{q}))},$$

Normalization condition: $\frac{1}{N}\sum_{\mathbf{q}}\langle \mathbf{S_q S_{-q}}\rangle = \frac{3}{4}(1-\delta)$

where ξ — short-range AFM correlation length,
$\omega_s \approx J$ — cut-off spin-fluctuation energy.

NUMERICAL RESULTS



Parameters:

$\Delta_{pd} / t_{pd} = 2$, $\omega_s / t_{pd} = 0.1$,

$\xi = 3$, $J = 0.4\ t_{eff}$,

$\mathbf{t_{eff}} \approx 0.14\ t_{pd} \approx$ **0.2 eV**,

$t_{pd} = 1.5$ eV

Fig.1. Tc (in t_{eff} units):

(i)~spin-fluctuation pairing,

(ii)~AFM exchange pairing ,

(iii)~both contributions

Unconventional d-wave pairing:

$\Delta(k_x, k_y) \sim \Delta\,(\cos k_x - \cos k_y)$

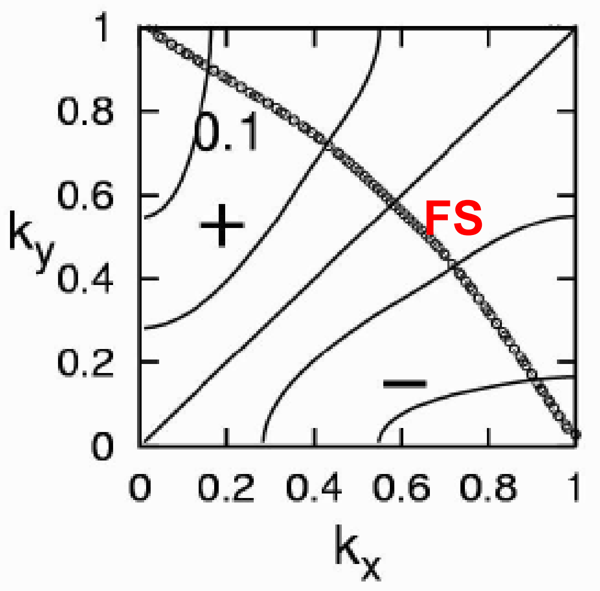


Fig. 2. $\Delta(k_x, k_y)$
$(0 < k_x, \; k_y < \pi)$
at optimal doping $\delta \approx 0.13$

Large Fermi surface (FS)

Comparison with the t-J model

The Hamiltonian of the t-J model in *X*- operators reads:

$$H_{t-J} = -\sum_{i\neq j,\sigma} t_{ij} X_i^{\sigma 0} X_j^{0\sigma} - \mu \sum_{i\sigma} X_i^{\sigma\sigma}$$

$$+ \frac{1}{2} \sum_{i\neq j,\sigma} J_{ij} \left(X_i^{\sigma\bar{\sigma}} X_j^{\bar{\sigma}\sigma} - X_i^{\sigma\sigma} X_j^{\bar{\sigma}\bar{\sigma}} \right)$$

Interband hopping determines the exchange interaction:

$J_{ij} = 4\, (t_{ij})^2 / \Delta$

Matrix Green function for the X-operators: $\Psi_{i\sigma}^{+} = (X_i^{\sigma 0}\ X_i^{0\bar{\sigma}})$

$$\hat{G}_{ij,\sigma}(t-t') = \langle\langle \Psi_{i\sigma}(t) | \Psi_{j\sigma}^{+}(t') \rangle\rangle,$$

$$\hat{G}_{ij\sigma}(\omega) = Q \begin{pmatrix} G_{ij\sigma}^{11}(\omega) & G_{ij\sigma}^{12}(\omega) \\ G_{ij\sigma}^{21}(\omega) & G_{ij\sigma}^{22}(\omega) \end{pmatrix}$$

where $Q = 1 - n/2$

Self-consistent system of equation in SCBA

$$\Sigma_{\sigma}^{11(12)}(\mathbf{k},\omega) = \frac{1}{N}\sum_{q} g^2(\mathbf{q},\mathbf{k}-\mathbf{q}) \iint_{-\infty}^{+\infty} \frac{dz d\Omega}{\omega - z - \Omega} \frac{1}{2}\left(\tanh\frac{z}{2T} + \coth\frac{\Omega}{2T}\right) \times A_{\sigma}^{11(12)}(\mathbf{q},z)\,;[-(1/\pi)\mathrm{Im}D^{\pm}(\mathbf{k}-\mathbf{q},\Omega+i\delta)]\,,$$

where the interaction $g(\mathbf{q},\mathbf{k}-\mathbf{q}) = t(\mathbf{q}) - \frac{1}{2}J(\mathbf{k}-\mathbf{q})$

is determined by spin- charge- fluctuations

$$D^{\pm}(\mathbf{q},\Omega) = \langle\langle \mathbf{S}(\mathbf{q}) \mid \mathbf{S}(-\mathbf{q})\rangle\rangle_{\Omega} \pm \frac{1}{4}\langle\langle n(\mathbf{q}) \mid n(-\mathbf{q})\rangle\rangle_{\Omega}$$

Spectral functions for the normal and anomalous GF:

$$A_{\sigma}^{11(12)}(\mathbf{q},z) = -\frac{1}{\pi}\mathrm{Im}G_{\sigma}^{11(12)}(\mathbf{q},z+i\delta).$$

Numerical solution of the linearized gap equation

$$\Phi_\sigma(\mathbf{k}, i\omega_n) = \frac{T}{N}\sum_{\mathbf{q}}\sum_{m}\{J(\mathbf{k}-\mathbf{q}) + \lambda_{12}(\mathbf{q}, \mathbf{k}-\mathbf{q} \mid i\omega_n - i\omega_m)\} \times G^{11}_\sigma(\mathbf{q}, i\omega_m) G^{11}_{\bar\sigma}(\mathbf{q}, -i\omega_m)\Phi_\sigma(\mathbf{q}, i\omega_m).$$

Interaction: $\lambda_{12}(\mathbf{q}, \mathbf{k}-\mathbf{q} \mid i\omega_\nu) = g^2(\mathbf{q}, \mathbf{k}-\mathbf{q}) D^{-}(\mathbf{k}-\mathbf{q}, i\omega_\nu)$

Model spin susceptibility with parameters:

$$\chi''_s(q,\omega) = -\frac{1}{\pi}\mathrm{Im}\langle\langle \mathbf{S}_q | \mathbf{S}_{-q}\rangle\rangle_{\omega+i\delta} = \chi_s(q)\chi''_s(\omega)$$

AF cor.length ξ and $\omega_s \sim J$

$$= \frac{\chi_0}{1+\xi^2[1+\gamma(q)]}\tanh\frac{\omega}{2T}\frac{1}{1+(\omega/\omega_s)^2}$$

Numerical results

1. Spectral functions A(k, ω)

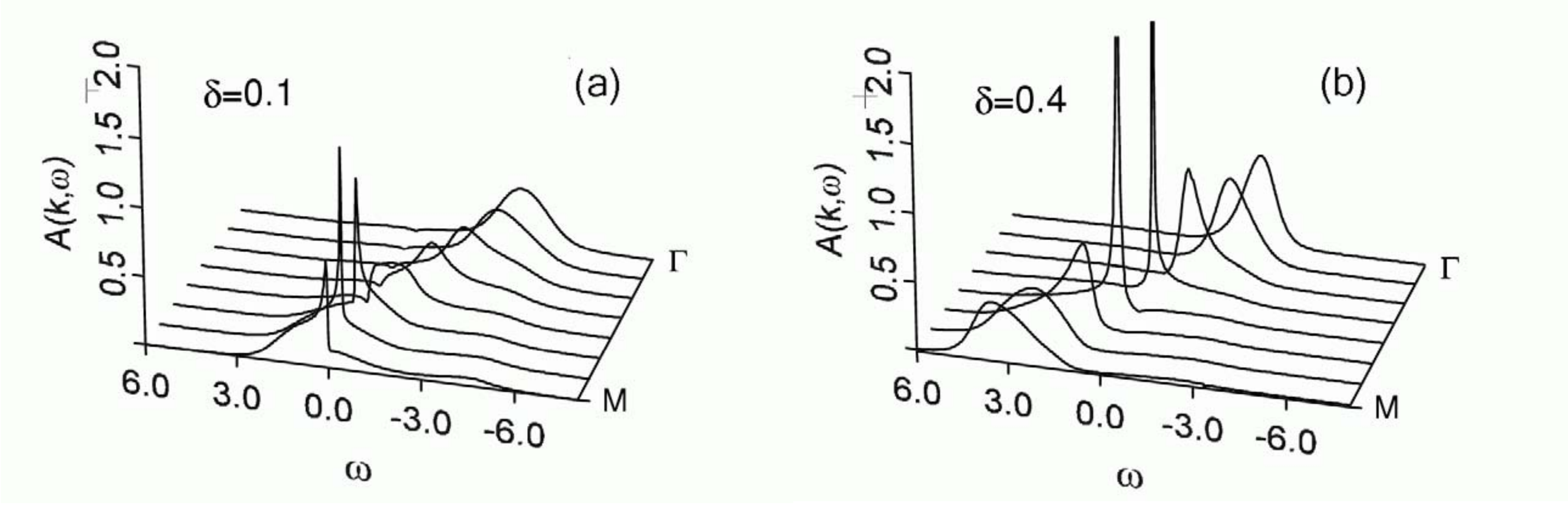


Fig.1. Spectral function for the t-J model in the symmemtry direction Γ(0,0) → M(π,π) at doping: (a) δ = 0.1 (ξ=3) , (b) δ = 0.4 (ξ=1).

2. Self-energy, Im Σ(k, ω)

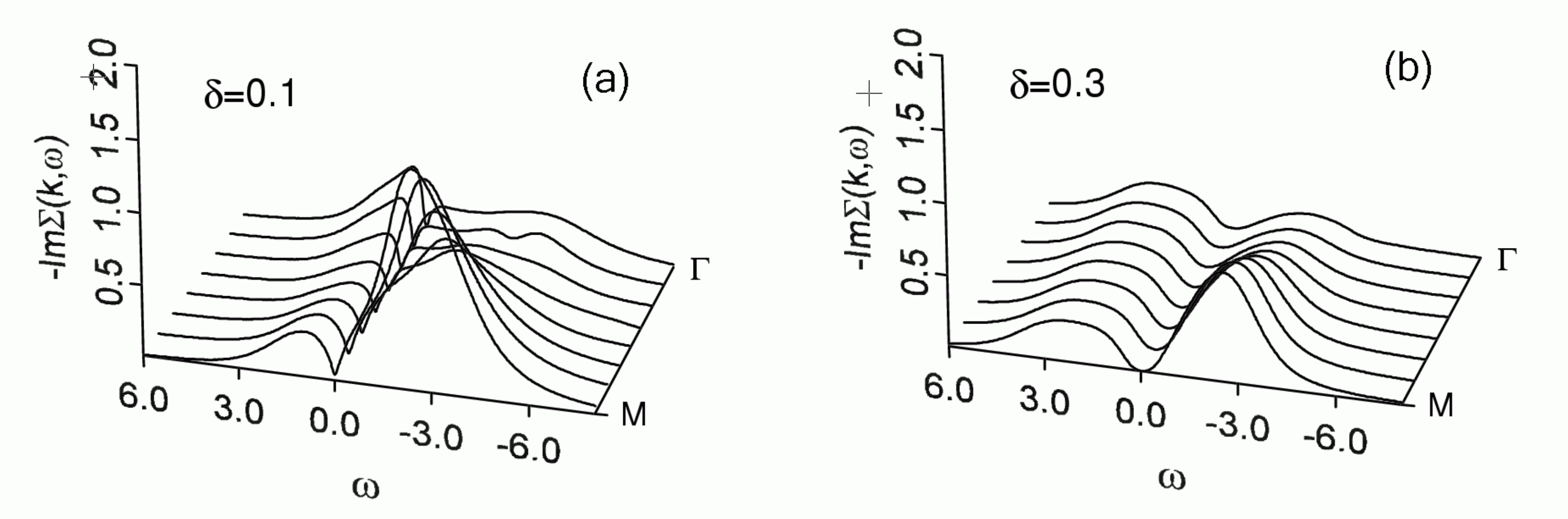
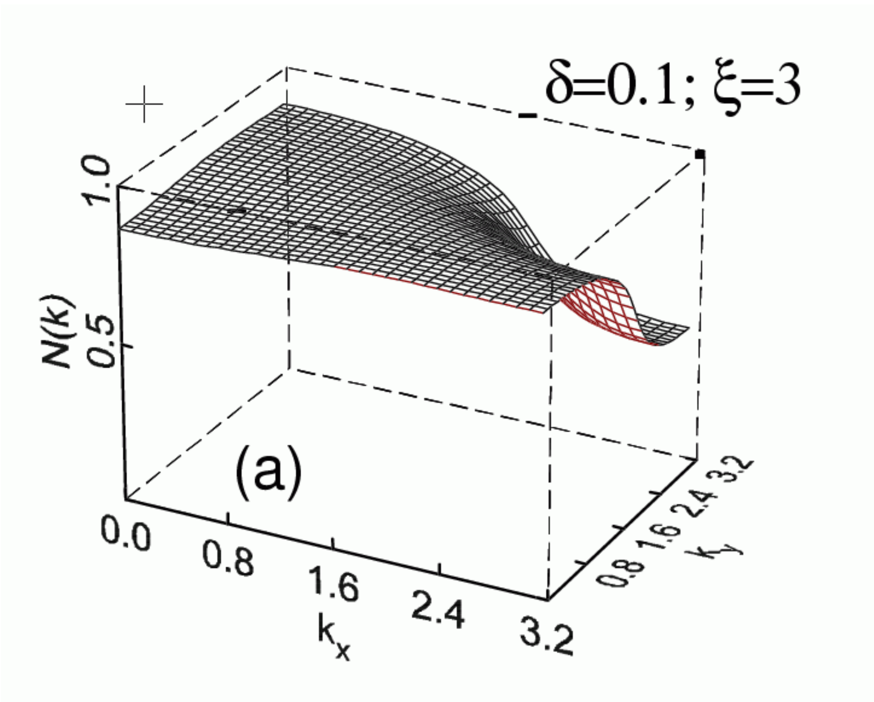


Fig.2. Self-energy for the t-J model in the symemtry direction

Γ(0,0) → M(π,π) at doping δ = 0.1 (a) and δ = 0.4 (b) .

3. Electron occupation numbers N(k) = n(k)/2



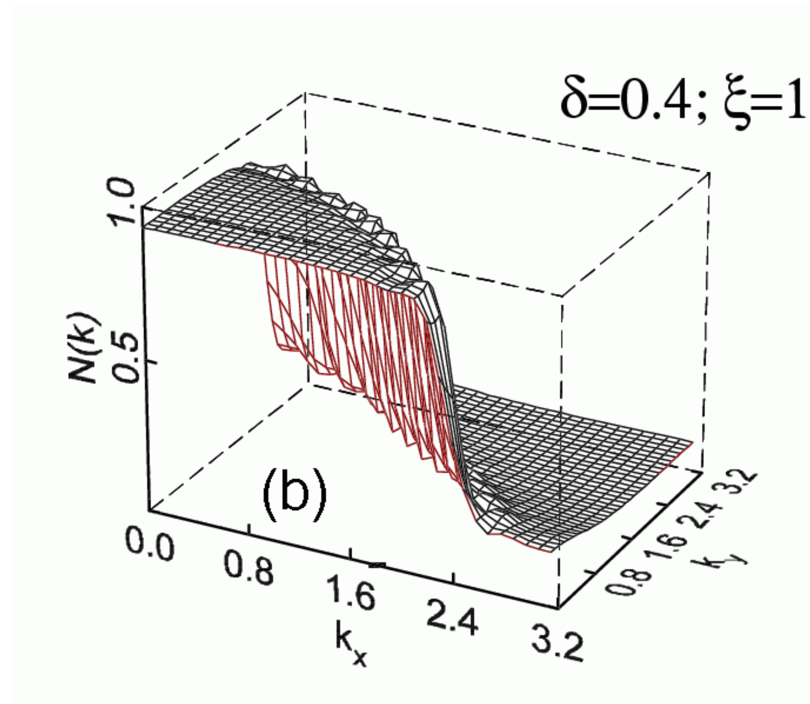


Fig.3. Electron occupation numbers for the t-J model in the quarter of BZ, ($0 < k_x, k_y < \pi$) at doping $\delta = 0.1$ (a) and $\delta = 0.4$ (b) .

4. Fermi surface and the gap function $\Phi(k_x, k_y)$

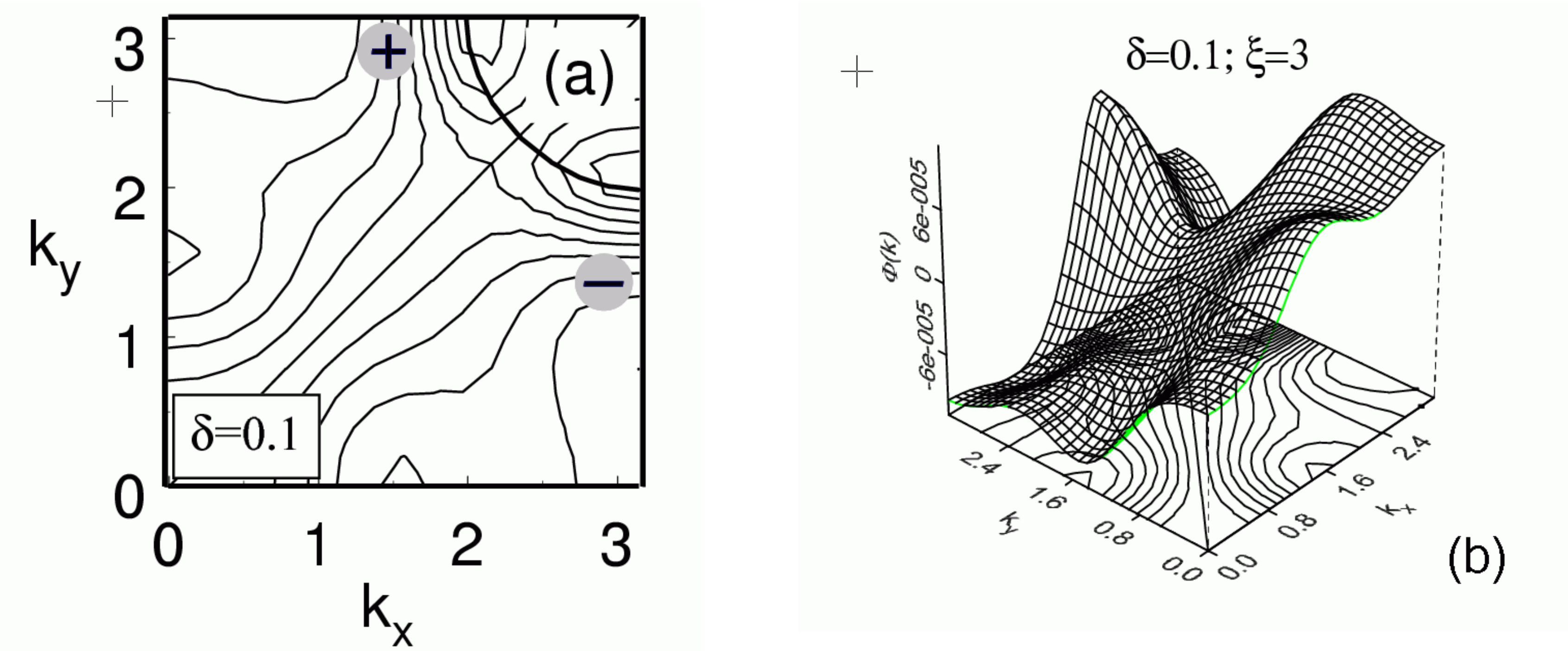


Fig.4. Fermi surface (a) and the gap $\Phi(k_x, k_y)$ (b) for the t-J model in the quarter of BZ ($0 < k_x, k_y < \pi$) at doping $\delta = 0.1$.

CONCLUSIONS

- Superconducting d-wave pairing with high-T_c mediated by the AFM superexchange and spin-fluctuations is proved for the p-d Hubbard model.
- Retardation effects for AFM exchange are suppressed:

  $\Delta_{pd} >> W$, that results in pairing of all electrons (holes) with high $T_c \sim E_F \approx W/2$.
- $T_c(a)$ and oxygen isotope shift are explained.
- The results corresponds to numerical solution to the t-J model in (q, ω) space in strong coupling limit.