I. INTRODUCTION

The key issue to understand the nature of high-temperature superconductivity in the cuprates is the evolution of the electronic structure from an antiferromagnetic insulator to a superconductor with hole doping. The appearance of the in-gap states above the top of the valence band in slightly doped cuprates has been found experimentally [1-4]. In the metallic underdoped regime the ARPES measurements [5] reveal the concentration of spin fluctuations at all temperatures that are present in the antiferromagnetic state as hole doping does – even without doping the spin excitations. Moreover the concentration of spin fluctuations $n_{sf}$ increases with temperature, and we expect the growth of the in-gap spectral weight $\sim n_{sf}$.

This state can be detected by the ARPES measurement as a weak satellite at the low energy shoulder of the main peak. The local excitation energy $E$ is $\sim 0.25$eV, and we expect the growth of the in-gap spectral weight $\sim n_{sf}$.

II. GTB METHOD RESULTS

A dispersion equation of the GTB method for the quasiparticle band structure of the CuO$_2$ layer looks like

$$\left( E - \Omega_m \right) \delta_{mn} - 2F^A (m) \sum_{\lambda \lambda'} \gamma_{\lambda \sigma} (m) T^{AB}_{\lambda \lambda'} \left( \vec{k} \right) \gamma_{\lambda' \sigma} (n) \right] = 0 \quad (1)$$

Here $m$ is a quasiparticle band indexes given by a pair $(p,q)$ of the initial and final multielectron configurations $E_p(n+1)$ and $E_q(n)$, $\Omega_m = E_p(n+1) - E_q(n)$ is a local excitation energy. The local excitation $\langle \sigma | q \rangle \rightarrow | p \rangle$ is described by the Hubbard operator $X^{pq} = | p \rangle \langle q |$, a filling factor $F(m) = \langle X^{pp} \rangle + \langle X^{pp} \rangle$. Two magnetic sublattices are denoted by indexes $A$ and $B$, and $\sigma$ is a spin projection. The interatomic hopping is $T_{\lambda \lambda'}$, where the single hole basis set $\lambda$ includes 5 orbitals: copper $d(x^2 - y^2)$, $d(3z^2 - r^2)$, in-plane oxygen $p(x)$, $p(y)$ and apical oxygen $p(z)$, $\gamma_{\lambda \sigma} (m)$ is a parameter of a single hole annihilation operator in term of the Hubbard operators

$$a_{\lambda \sigma} = \sum_m \gamma_{\lambda \sigma} (m) X^m \quad (2)$$

The local multielectron energies and parameters $\gamma_{\lambda \sigma} (m)$ are obtained after the exact diagonalization of the multiband $p - d$ model Hamiltonian for the unit cell. In our case the unit cell is CuO$_2$ cluster for La$_2$CuO$_4$ and CuO$_4$Cl$_2$ for Sr$_2$CuO$_2$Cl$_2$. The similar equation has been known long ago for the nondegenerate Hubbard model as the Hubbard I solution and has been used recently to study magnetic properties of transition metals [14, 15].

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The essential for undoped cuprates multielectron configurations are $d^{10}p^6$ (vacuum state $|0\rangle$ in a hole representation), single-hole configurations $d^9p^6$, $d^{10}p^5$, and two-hole configurations $d^8p^5$, $d^9p^5$, $d^{10}p^4$, $d^{10}p^5p^5$. The minimal energy in the single-hole sector of the Hilbert space has the $b_{1g}$ molecular orbital, and in the two-hole sector the $A_{1g}$ singlet that besides Zhang-Rice singlet contains several more local singlets. A staggered magnetic field split $b_{1g}$ levels by spin:

$$\varepsilon_{A\sigma} = \varepsilon_1 - \sigma h, \quad \varepsilon_{B\sigma} = \varepsilon_1 + \sigma h. \quad (3)$$

The top of the valence band is given by the quasiparticles with $m = 1$: $X_A^+ = |b_{1g}\uparrow\rangle \langle 1A_{1g}|$ and $X_B^+ = |b_{1g}\downarrow\rangle \langle 1A_{1g}|$, as usually there is spin degeneracy of the band in the antiferromagnetic state. The occupation number $n_p \equiv \langle X^{pp}\rangle$ are calculated self-consistently via the chemical potential equation. In the mean-field Hubbard I approximation the solution of this equation for the hole-doped cuprates with hole concentration $n_h = 1 + x$ is given by

$$n_{1\uparrow} \equiv n_{A1}(b_{1g}) = 1 - x, n_{1\downarrow} = 0, n_2 \equiv n(1A_{1g}) = x. \quad (4)$$

For the band $m = 1$ we get $F_{A1}(1) = 1$ while for the band $m = 2$ with $X_A^+ = |b_{1g}\downarrow\rangle \langle 1A_{1g}|$ the filling factor is $F_{A1}(2) = x$. The quasiparticle spectral weight is proportional to the filling factor, thus it is the band $m = 2$ that forms the in-gap state. In the limit $x \to 0$ its spectral weight is zero, when $x \neq 0$ this band acquires both dispersion and nonzero spectral weight. The corresponding concentration dependent bands structure has been obtained for $La_{2-x}Sr_xCuO_4$ in [13] and the chemical potential $\mu(x)$ dependence, the Fermi surface evolution with doping have been studied in [16].

To go beyond the mean-field Hubbard I approximation one has to calculate single-loop diagrams for the self-energy [17]. In the ferromagnetic or antiferromagnetic state the most important contribution is given by loops with spin-wave excitations [18] (a spin-polaron effect). According to [18], the main effect of the spin excitations is given by the spin-wave renormalization of the multielectron configuration’s occupation numbers, so instead of (4) one gets

$$n_{1\uparrow} = (1 - x)(1 - n_{sf}), n_{1\downarrow} = (1 - x)n_{sf}, n_2 = x, \quad (5)$$

where $n_{sf}$ is the occupation of the spin-minority level and it determines the spin-fluctuation decrease of the sublattice magnetization

$$\langle S^z_A \rangle = (1 - x)(1/2 - n_{sf}). \quad (6)$$

Concentration of the spin fluctuations is equal to $2n_{sf}$.

Thus the filling factors for the valence band $F(1) = 1 - n_{sf}$, and for the in-gap states $F(2) = x + n_{sf}$. It means that the spin-polaron effect results in the nonzero spectral weight of the in-gap states even for undoped cuprates $La_2CuO_4$ and $Sr_2CuO_2Cl_2$. The quasiparticle band structure and the spectral function for the undoped $La_2CuO_4$ with $n_{sf} = 0.1$ are given in the Fig. 1. Here the lowest band is formed by hole hopping via 2-hole triplet $^3B_{1g}$ state – this aspect was discussed in [13, 19]. The next band ($m = 1$) is the top of the valence band without spin fluctuations with a maximum at $k = (\pi/2, \pi/2)$. The upper band ($m = 2$) formed by the dispersion of the in-gap states. Despite of its width each state has a low spectral weight as seen in the Fig. 1b and the total number of states in this in-gap band (without doping) is equal to $n_{sf}$. The appearance of such non-Fermi liquid states is the direct effect of strong electron correlations. The maximal spectral weight of the in-gap state is near $(\pi, 0)$ point of the Brillouin zone (BZ). At the $(\pi/2, \pi/2)$ point the two bands are degenerate, and we cannot separate the contribution of the in-gap band to the spectral function $A_k(E)$. 

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**FIG. 1:** The quasiparticle band structure (a) and the spectral function (b) of the undoped $La_2CuO_4$ with a spin-fluctuations $n_{sf} = 0.2$ calculated by the GTB method. The Fermi level is above all bands shown here.
III. \( t - t' - J \) MODEL TREATMENT

To clarify the properties of the in-gap band we study the spin-polaron effect in the \( t - t' - J \) model, which is an effective low energy model for the multiband \( p - d \) model [20], with the Hamiltonian:

\[
H_{t-J} = (\varepsilon_1 - \mu) \sum_{\sigma, \gamma} X_j^{\sigma\gamma} + \sum_{\langle f, g \rangle} t_{fg} X_f^{\sigma\sigma} X_g^{\sigma}\nonumber
\]

\[
+ \sum_{\langle f, g \rangle} J_{fg} \left( S_f S_g - \frac{1}{4} n_f n_g \right),
\]

where \( S_f \) are spin operators and \( n_f \) is number of particle operator, \( t_{fg} \) and \( J_{fg} \) are the hopping and exchange integrals correspondingly. In the Hubbard I approximation it is easy to obtain in the undoped case the following intra-sublattice and intersublattice Green functions \( f \in A, g \in B \):

\[
\langle \langle X_f^{\sigma\sigma} | X_f^{\sigma\sigma} \rangle \rangle_E = \frac{2}{N} \sum_k G_{k\sigma}(E) e^{i \delta_k(f-g)},
\]

\[
\langle \langle X_f^{\sigma\sigma} | X_f^{\sigma\sigma} \rangle \rangle_E = \frac{2}{N} \sum_k G_{k\sigma}(E) e^{i \delta_k(f-g)}.
\]

Matrix Grin function in momentum space could be written as:

\[
\hat{G}_{k\sigma} = \left( \begin{array}{cc} G_{k\sigma}^{AA} & G_{k\sigma}^{AB} \\ G_{k\sigma}^{BA} & G_{k\sigma}^{BB} \end{array} \right) = \frac{1}{D} \left( \begin{array}{cc} n_{A\sigma}(E e^{i \delta_{k\sigma}}) & n_{A\sigma} n_{B\sigma} t_{B\sigma}^{B} \\ n_{A\sigma} n_{B\sigma} t_{B\sigma}^{A} & n_{B\sigma}(E e^{i \delta_{k\sigma}}) \end{array} \right),
\]

where \( D = (E - E_{k\sigma}^+)(E - E_{k\sigma}^-) \), \( \delta_{k\sigma} = (\varepsilon_1 - \mu) - (J_0^B - t_{B\sigma}^A) n_{A\sigma} - J_0^A n_{B\sigma} \), with \( \alpha = A, B \).

Here \( t_{B\sigma}^B \), and \( t_{B\sigma}^A \) \((J_0^B \) and \( J_0^A \)) are the hopping exchanges \( (E - E_{k\sigma}^+) \) in momentum space between different and the same sublattices correspondingly. In simple case of next-nearest-neighbors approximation we have

\[
t_{B\sigma}^B = 2t_0 (\cos k_x + \cos k_y), \quad t_{B\sigma}^A = 4t' \cos k_x \cos k_y,
\]

\[
J_0^B = 4J, \quad J_0^A = 4J',
\]

with primed values corresponding to next-nearest hoppings and exchanges. The occupation factors of one particle state with different spin projections are denoted by \( n_{A\sigma} \) and \( n_{B\sigma} \). In the mean field Hubbard I approximation \( n_{A\pi} = (1 - n_{sf}) \) and \( n_{A\downarrow} = 0 \) at \( T = 0 \). Using the same arguments as in the Section 10 we go beyond the Hubbard I approximation by renormalization the occupation numbers with spin fluctuations. It results in the undoped \( \text{La}_2\text{Cu}_4\text{O}_4 \) in

\[
n_{A\pi} = (1 - n_{sf}), n_{A\downarrow} = n_{sf}, n_{B\sigma} = n_{A\sigma}.
\]

The condition \( D = 0 \) gives two branches of quasiparticle spectrum:

\[
E_{k\uparrow}^+ = \varepsilon_1 - \mu + \frac{1}{2} \left[ t_{B\sigma}^A - J_0^B - J_0^A \pm \sqrt{\beta_k} \right].
\]

where

\[
\beta_k = (t_{B\sigma}^A - J_0^B - J_0^A)^2 (1 - 2n_{sf})^2 + 4(t_{B\sigma}^B)^2 (1 - n_{sf}) n_{sf}.
\]

If we set concentration of the magnons to zero we immediately get one dispersionless state and one dispersive state with dispersion governed by hoppings between different sublattices:

\[
E_{k\uparrow}^+ |_{n_{sf}=0} = \varepsilon_1 - \mu - J_0^A, E_{k\uparrow}^- |_{n_{sf}=0} = \varepsilon_1 - \mu + t_{B\sigma}^A - J_0^B.
\]

If the values of inter-sublattice hoppings and exchange are small then the difference between two energy levels is of order \( J \):

\[
\Delta E |_{n_{sf}=0} = \left( E_{k\uparrow}^+ - E_{k\uparrow}^- \right) |_{n_{sf}=0} \approx 4J.
\]

In Fig. 2 the quasiparticle dispersions corresponding to equations (10) and (11) are shown. Parameters were taken from effective low-energy model [20] of multiband \( p - d \) model and equal to: \( t = -0.587, t'/t = -0.085, J/t = 0.392, J'/t = 0.0037 \). The value \( n_{sf} \) is calculated in the effective quasi-two-dimensional Heisenberg antiferromagnetic model, \( n_{sf} = 0.2 \) for typical in \( \text{La}_2\text{Cu}_4\text{O}_4 \) ratio \( 10^{-5} \) of the interplane and intraplane exchange parameters [21].

The distance between two spectrum branches for non-zero concentration of the magnons is less then distance (12) for \( n_{sf} = 0 \) by factor proportional to \( (1 - 2n_{sf}) = 2 (\delta^2) \).

The lower quasiparticle branch for \( n_{sf} = 0.2 \) (but not for \( n_{sf} = 0! \)) clearly resembles the magnon dispersion obtained in self-consistent Born approximation [22] and GTB method [13]. This proves that two different approaches to treat spin fluctuations lead to the similar results.

Introducing energy difference \( \Delta E_k = E_{k\uparrow}^+ - E_{k\downarrow}^- \) we can write down spectral functions \( A_{k\sigma} (E) = -\frac{i}{\pi} \text{Im} \left[ S_p \hat{G}_{k\sigma} \right] \) in the form:

\[
A_{k\uparrow} (E) = u_k^2 \delta (E - E_{k\uparrow}^+) + v_k^2 \delta (E - E_{k\downarrow}^-),
\]

\[
A_{k\downarrow} (E) = u_k^2 \delta (E - E_{k\uparrow}^-) + u_k^2 \delta (E - E_{k\downarrow}^-),
\]

where

\[
u_k^2 = \frac{1}{2} (1 - 2n_{sf})^2 \left( \frac{J_0^B - J_0^A - t_{B\sigma}^A}{2\Delta E_k} \right), \quad v_k^2 = 1 - u_k^2.
\]

Obviously, for \( n_{sf} = 0 \) the value \( u_k^2 = 0, v_k^2 = 1 \) and there will be the non-zero spectral function \( A_{k\uparrow} (E) = \delta (E - E_{k\uparrow}^+) \) corresponding to only one dispersive state (11). In Fig. 2, the spectral functions versus energy for different symmetric points in momentum space are shown. Comparison of spectral intensities in case of presence and absence of \( n_{sf} \) (solid and dash-dotted lines) indicates that the second satellite peak appears above the main peak in \( (\pi/2, \pi/2) \) and \( (\pi, 0) \) points. It is the
satellite peak that represents the in-gap state. In the
\((\pi/2, \pi/2)\) point the distance between two peaks is pro-
portional to \(J\) (see equation (12)) but at \((\pi, 0)\) point
the distance is proportional to \(|J + t'\|\) (or, generally,
\(|J_B - t_A^B|\)) and will also take place even at zero \(J\).
The last statement emphasizes importance of next-nearest-
neighbor hoppings \(t'\) at low doping. Indeed, if one con-
sider \(t - J\) model with only nearest-neighbor hoppings
then the doped hole will not even be able to move with-
out spin fluctuations \((n_{sf} = 0\), see equation (11)) and
at low \(n_{sf}\) the dispersion will be governed by \((t_A^A - J_B^B)\)
term in equation (10) but not by nearest neighbor hop-
ning \(t_B^B\).

Now we will discuss the higher-order corrections to pre-
vious results. Two main effects are expected: i) quasi-
particle decay and ii) renormalization of the real part of
the self-energy. The main change with introduction of fi-
nite quasiparticle lifetime will be broadening of spectral
peaks. This effect indirectly presented in Fig. 2, where
the delta function peaks in spectral function are arti-
ficially broadened by the Lorentzian. To analyze renor-
malization of the real part of self-energy we will use more
rigorous approximation – generalized Hartree-Fock ap-
proximation [23]. In this approximation the equation
of motion for operator \(X_f^{\sigma}\) is renormalized by two-sites
static correlation functions:

\[
i \frac{d}{dt} X_f^{\sigma} = [(\varepsilon_1 - \mu) + M_{f\sigma} X_f^{\sigma}] + \sum_g \tau_{fg,\sigma} X_g^{\bar{\sigma}},
\]

where \(M_{f\sigma}\) and \(\tau_{fg,\sigma}\) are the renormalized chemical po-
tential (exchange integral) and hopping integrals corre-
spondingly:

\[
M_{f\sigma} = \sum_g t_{fg} \langle X_f^{\bar{\sigma}} X_g^{\sigma} \rangle
- \sum_g J_{fg} \left( \langle X_f^{\sigma} X_g^{\bar{\sigma}} \rangle - \langle X_f^{\bar{\sigma}} X_g^{\sigma} \rangle \right),
\]

\[
\tau_{fg,\sigma} = t_{fg} \left( \langle X_f^{\sigma} X_g^{\bar{\sigma}} \rangle + \langle X_f^{\bar{\sigma}} X_g^{\sigma} \rangle - \langle X_f^{\bar{\sigma}} X_g^{\bar{\sigma}} \rangle \right) + J_{fg} \langle X_f^{\bar{\sigma}} X_g^{\sigma} \rangle.
\]

It is clear that the equation (15) has the same lin-
erized form as in Hubbard I approximation but with renor-
malized chemical potential and hopping integrals. It
means the qualitative results of Hubbard I considera-
tion will be the same but quantitatively they may change.
Namely, due to renormalization of the exchange integ-
ral the distance between the in-gap and main spectral
peaks will be shorter then expected from (12) and the
underlying physics of the in-gap state will be unchanged and its
dispersion will be governed by spin fluctuations.

\[\]

IV. CONCLUSION

It is clear from the spectral function both in the Fig. 1b
and Fig. 2b that there is a pseudogap between the in-
gap band and the valence band, for the undoped cuprate
both bands are occupied and the chemical potential lies
above the in-gap band. With doping \(\mu(x)\) is pinned to the
in-gap state [16] up to optimal doping. The pseudogap
is \(k\)-dependent. In the \((\pi/2, \pi/2)\) point of the BZ
the value of the gap is \(\Delta E(\pi/2, \pi/2) \sim J (1 - 2n_{sf})\), while in
the \((\pi, 0)\) point \(\Delta E(\pi, 0) \sim |J + t'| (1 - 2n_{sf})\). We can
compare results of the \(p-d\) model and the \(t-J\) model in
our solution only in the limit \(U \to \infty\) \((J \to 0)\), then we
get \(\Delta E(\pi/2, \pi/2) \to 0\) and \(\Delta E(\pi, 0) \to |t'| (1 - 2n_{sf})\)
that corresponds to the Fig. 1. At \(J \neq 0\) there is the
additional contribution to the pseudogap, and we may
expect the in-gap satellite both in \((\pi/2, \pi/2)\) and \((\pi, 0)\)
points of the BZ.

In conclusion, we have shown that the spin-polaron
effect results in the formation of the in-gap band above
the top of the valence band even in the undoped cuprates.
The spectral function of the in-gap states has a form of
small low energy satellite that can be detected by ARPES
measurements. The most interesting to the ARPES stud-
ies are \((\pi, 0)\) and \((\pi/2, \pi/2)\) points of the BZ. For the hole

\[\]
doped cuprates there are two contributions to the in-gap spectral weight: the mean field contribution is given by doping concentration $x$ and the spin-fluctuation contribution is given by the magnon concentration $2n_{sf}$. The latter is temperature dependent resulting in the increasing satellite intensity with the temperature growth.

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