Interplay of pseudo- and superconducting gaps: observable manifestations in cuprates.

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Abstract

Angular dependence of gap, seen in photoemission, its evolution with doping and temperature are interpreted on base t-t'-U Hubbard model in which a pseudogap is a working function for electrons removing from dielectric segments of zone boundary. Tunnel spectra in one-particle approximation display only superconducting gap and too large asymmetry in regions aside from optimal doping. Spectral functions confirm sharp well defined Fermi boundary at \( k_x = k_y \) direction and smoothed destructed one at the \( \Gamma(0,0) - M(\pi,0) - Y(\pi,\pi) \) path. Both tunnel and ARPES data seem require spreading a model to bilayer ones.

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1. Introduction.

Up to now a set of decisive experimental results have been obtained concerning electronic structure of cuprates (see reviews [1, 2, 3]). They include evidence of d-wave superconductivity, discovery of anisotropic normal state pseudogap and "small" Fermi surface (FS) in underdoped (UD) materials accompanied possibly by destruction of FS [4, 5]. Direct measurement of superconducting (SC) gap are provided by tunneling spectroscopy [6]-[9]. Most recent detailed photoemission (ARPES) studies reveal exotic temperature dependence of gap [10, 11] and the doping dependence of its anisotropy in superconducting state [12]. It was revealed the apparent discrepancy between this data and characteristics obtained from penetration depth data. It was shown that angular dependence of superconducting gap \( \Delta(\varphi) \) extracted from ARPES data cannot be adjusted by simple form \( \sim \cos(2\varphi) \) and the shape of gap function depends on doping. In particular, the ratio \( \xi = v_\Delta/\Delta \) of \( v_\Delta = \frac{1}{2}d\Delta(\varphi)/d\varphi \) at \( \varphi = \pi/4 \) to maximum value of gap \( \Delta \) decreases
essentially with doping decrease in UD materials. Finally standard shape of the FS has
been recently revised. It seems to be large partially electron-like FS around \( \Gamma = (0,0) \)
instead the arc around \( Y(\pi, \pi) \) \[13\].

The aim of our paper is to study which of new experiments can or cannot be explained
in simple quasiparticle interpretation of pseudogap origin.

Interpretation of phase diagram and pseudogap have recently \[14\]-\[18\] been proposed
on base of different approaches for description of the correlation mechanism of SC pairing
in cuprates. One of them is the spin-polaron approach in t-t'-J model \[14\]. Another is
variational approach incorporating the correlations of the valence bond (VB) type in t-t'
U Hubbard model \[15, 16\]. In each case the Hubbard splitting of whole band arises due
to long-range antiferromagnet (AF) order and fine details of upper edge of lower Hubbard
band (LHB) determines the low energy phenomena. The hole attraction in d-channel is
shown to be induced by spin-polaron interactions in t-t'-J model or equivalent correlated
hopping interactions due to VB formation in t-t'-U model. According theories \[14\]-\[18\]
the next nearest hopping \( t' \) plays important role in formation of pseudogap and a sign of
\( t'/t \) determines its anisotropy. For systems with \( t'/t > 0 \) a crossing of van Hove singularity
(VHS) by the chemical potential \( \mu \) corresponds to optimal doping and is accompanied by
change in the Fermi boundary topology. The hole pockets around \( k = (\pi/2, \pi/2) \) with
"small" Fermi surface are replaced by large Fermi surface in course of transition from UD
to over-doped (OD) systems. At \( \delta < \delta_{opt} \) the VHS occur below \( \mu \) and some segments of
magnetic Brillouin zone (MBZ) boundary near \( k_M = (\pi, 0) \) become dielectric segments.
According \[16\] the work function \( \mu - E_k > 0 \) for electron removing from this regions of
\( k \) is just a normal state pseudogap observed in ARPES. In difference from standard VHS
scenario \[3\] with united band here we deal with VHS of lower Hubbard subband.

The method and outline of present study are following. We use the variational method
to construct explicitly the correlated state and to test if it could display the observable
properties. Starting from AF state with the VB correlations we explain the supercon-
ducting (SC) and pseudo- gap anisotropy and its temperature and doping dependencies
(Sec.2). Then we calculate the tunnel spectra of system and discuss its distinction from
the observed ones (Sec.3). Manifestation of FS in one-particle spectral functions \( n_k \) and
\( A(k; \omega \to 0) \) and the FS shape are discussed in Sec.4.

2. The doping and temperature dependence of gap anisotropy.
Calculations have been done for t-t'-U-V Hubbard model by method proposed in [16]. Here $t$, $t'$ are the nearest and next nearest hoppings; $U$ and $V$ are the on-site and nearest sites Coulomb-like interactions. The variational correlated state $\Psi = W(\alpha)\Phi$ with the VB-type correlations (the band analogue of the Anderson’s RVB states) is taken as a unitary transformed uncorrelated state $\Phi$. Unitary operator $W(\alpha) = \exp\{\alpha \sum_{<nm>\sigma}(c_{n\sigma}^\dagger n_{m\sigma} - h.c.)(n_{n\sigma} - n_{m\sigma})\}$, $\sigma = -\sigma$, optimizes the covalency of $< nm >$ bonds. A problem with Hamiltonian $H$ in basis of correlated states $\{\Psi\}$ is reduced to a problem with effective Hamiltonian $\tilde{H} = W^\dagger HW \approx H + \alpha[H, Z] + \frac{\alpha^2}{2}[H, [Z, Z]]$ in basis of uncorrelated states $\Phi$. Thus the effective problem $\tilde{H}$ is solved in the mean field (MF) approximation with subsequent minimization of energy over variational parameter $\alpha$ ($\alpha < 0.22$ at $U/t \leq 9$). Most general uncorrelated state $\Phi$ of BCS-type and with double magnetic unit cell allows a testing the possible AF and SC pairing in system. The terms of correlated hopping like $\sim \alpha Uc_{n\sigma}^\dagger n_{m\sigma}n_{n\sigma}n_{m\sigma}$ in $\tilde{H}$ caused by VB formation are responsible for SC order of d-symmetry compatible with AF order. Band energies $E_{k\lambda}$ (eigen values of linearized $\tilde{H}_L$) corresponds to self consistent $\Phi$ and optimal $\alpha$.

The studied homogeneous solutions display the 2D AF spin order in a wide doping range $\delta = |1 - n| \leq \delta_c \sim 0.3$ which is larger than range of the bulk AF order ($\delta_c \sim 0.05$). This implies that finite radius of AF correlations is much larger than lattice constant $a$ and we can use the solutions and a picture of split band as a background in discussing a low energy phenomena. In normal state a LHB has the following structure [16]:

$$E_k = [\epsilon_0 + 4t'c_xc_y + ...] - \sqrt{[Ud_0 + ...]^2 + [2t(c_x + c_y) + ...]^2}$$ (1)

Here only main contributions from lowest harmonics with $c_{x(y)} = \cos k_{x(y)}$ are explicitly written and $d_0 = \langle (-1)^nS_{zn} \rangle$ is the staggered spin. In d-wave superconducting state the self consistent quasiparticle energies are very close to form

$$E_{k\lambda} = \pm \sqrt{(E_k - \mu)^2 + W_k^2}; \quad W_k \sim F_k[k_{11}(c_x - c_y)w_1 + ...]$$ (2)

Here $W_k$ is determined by SC order parameters $w_l = (l_x^2 - l_y^2)^{\dagger} < c_{n\lambda}^\dagger c_{n+l\lambda} >, |l| = 1, \sqrt{5}, 3$ and $F_k$ is determined by structure of one-particle states of LHB. First harmonic gives main contribution to $W_k$ and its angular dependence is close to $W_k \sim (c_x - c_y)$.

The doping dependence $T_c(\delta)$ for Hubbard model with $U/t = 8$, $t'/t = 0.05$ and $V/t = 0.1$ is presented in Fig.1a. (Note, that at $V=0$ the value of $T_c^{\max}$ increases by factor 1.64 [16].) Curve 1 in Fig.1b presents the value $W_M(\delta) = W(k_M)$ of gap function
$W_k$ at $k = k_M = (\pi, 0)$ for the d-wave superconducting pairing calculated at temperature $T/t = 0.002$. But according (2) the quasiparticle energy and the corresponding shift $\Delta = \Delta \omega$ of the edge of photoemission distribution function at $k = (\pi, 0)$ is determined not only by $W_k$, but also by the LHB energy $|E_k - \mu|$ relative to chemical potential. Unlike original unsplit band, the LHB energy $E_k$ is periodic in magnetic Brillouin zone (MBZ) and goes through a maximum on MBZ boundary at any path connecting the points $\Gamma(0, 0)$ and $Y(\pi, \pi)$. This determines the different doping dependence of ratio $\xi = v_\Delta/\Delta_M$ in UD and OD presented in Fig.1c. Here $v_\Delta = \frac{1}{2}d\Delta/d\varphi$ at $\varphi = \pi/4$ and $\Delta_M$ is the $\Delta$ at $k = (\pi, 0)$.

In OD regime each path $\Gamma - Y$ crosses a "large" Fermi-boundary: $E_k - \mu = 0$ at $k = k_F$ and $E_k - \mu > 0$ at all values $k$ at MBZ boundary. In this case a gap $\Delta(\varphi)$ in excitation spectrum for $k$ changing along any path $\Gamma - Y$ is determined only by d-wave SC gap $W_k$ at $k_F$. Therefore the gap anisotropy $\Delta(\varphi)$ coincides with $\Delta(\varphi) = W_k(\varphi) \sim z(\varphi) = 0.5(cos k_x - cos k_y)$ at $k_F$. Corresponding ratio $\xi = v_\Delta/\Delta_M$ measured at $k = k_M$ in [12] is equal to $\xi = \frac{1}{2}(dW_k/d\varphi)/W_M$. It is close to constant value $\sim 0.7$ expected for pure d-wave SC order without pseudogap.

In UD systems with $t'/t > 0$ a "small" Fermi boundary around the hole pockets at $k = (\pi/2, \pi/2)$ is formed whereas the segments of MBZ boundary near $M(\pi, 0)$ become dielectric segments on which $E_k - \mu < 0$. A shift $\Delta(k_M)$ of photoelectron distribution function in ARPES at $k_M = (\pi, 0)$ is equal to $\Delta(k_M) = \sqrt{\Delta^2_N + W^2_M}$. Here $W_M$ is $W_k$ at $k_M$ and the value $\Delta_N = |E_k - \mu|$ at $k_M$ is the normal state pseudogap equal to work function for the electron removing from $k = k_M$ in normal state. Value $\Delta_N$ increases with doping decrease. For the same reason the anisotropy of total shift $\Delta(\varphi) = \sqrt{\Delta^2_N(\varphi) + W^2_k(\varphi)}$ of photoemission edge at the dielectric segments of MBZ boundary differs significantly from anisotropy of $W_k(\varphi)$ only. In UD region ($\Delta_N \neq 0$) one obtains $\xi \sim 0.5[W'(\pi/4)]/\sqrt{\Delta^2_N + W^2_M}$, where $W'(\varphi) = dW_k/d\varphi$ at $\varphi = \pi/4$. Value $\xi$ sharply decreases ($W_k \to 0$) with doping decrease in full accordance with experimental behavior of $\xi(\delta)$ [12]. In contrast to $\xi(\delta)$, a quantity $\xi_W(\delta) = v_\Delta/W_M$ with pure superconducting gap function in denominator remains almost constant (curve 2 in Fig.1c).

Fig.1d presents the results for anisotropic shift $\Delta(\varphi)$ of photoemission edge for strongly UD system ($\delta = 0.14, T_c/T_{c_{max}}^{OD} = 0.55$). Dependencies $\Delta(\varphi)$ are taken at $k$ moving from $k_x = k_y$ to $M(\pi, 0)$ along generalized Fermi boundary consisting of nonshadow part of
small Fermi boundary and dielectric segments of MBZ (see [16]). Several features of calculated anisotropy $\Delta(\varphi)$ have a correspondence with experimental anisotropy features. 1) Deflection of $\Delta(\varphi)$ from linear dependence $\Delta(\varphi) \sim z(\varphi)$ have really been observed in UD Bi-Sr-Ca-Cu-O (BSCCO) [12] and the observed sign of next harmonics in it is the same as in calculated curves. 2) The region of gap $\Delta_k$ near its nodes occurs more sensitive to temperature than at $k \sim (\pi, 0)$. A shift $\Delta(\varphi)$ at $\varphi \sim \pi/4$ disappears with $T \to T_c$ whereas the pseudogap of normal state in region $k \sim (\pi, 0)$ retains nonzero value $\Delta_M = \Delta_N = \mu - E(\pi, 0) > 0$ at $T > T_c$. This feature also corresponds to experimentally observed different temperature sensitivity of $\Delta(\varphi)$ at different $\varphi$ [10, 11]. Finite $k$-resolution in ARPES may be a reason of more smooth observed dependence $\Delta(\varphi)$ in compare with calculated one. Besides, the latter is obtained in neglecting the energy dispersion over $k_z$. 3) The calculated ratio $\eta = 2\Delta_M/kT_c$ have very large values in underdoped case. Thus for $\delta = 0.16$ ($T_c = 0.9T_c^{\text{max}}$) it is $\eta = 9.5$. At the same time for optimal and over- doping the whole gap is determined only by superconducting part $\Delta = W(k_F)$ and the ratio is about $\eta \approx 5$. This value is close to $\eta = 4.5$ obtained from empirical BCS models with d-wave pairing. Decrease of $2\Delta/kT_c$ with doping increase is consistent with experiment [1].

Independent estimations of gap anisotropy near the nodes have been obtained in [12] from behavior of superfluid density $\rho_s$ at low temperature on base of relation between $v_\Delta$ and penetration length at $T \to 0$. This relation $d\rho_s(T)/dT \sim d(\lambda^{-2})/dT \sim 1/v_\Delta$ gives the doping dependence of $v_\Delta$ different from the mutually consistent dependencies $v_\Delta(\delta)$ obtained from ARPES data and our calculations. Origin of distinction is unclear and question arises whether the temperature dependence of $1/\lambda^2$ at $T \to 0$ may be controlled not only by low energy Fermi excitations near the nodes of SC gap, but also by the low frequency spin excitations which adiabatically change the overall spectrum of Fermi system. Important role of spin wave fluctuations has recently been confirmed in [20].

3. Tunneling spectra for AF+VB correlated states

Tunneling spectra can provides a sensitive test for the obtained simple homogeneous solutions of $t - t' - U$ Hubbard model which take into account the AF and VB correlations. Recent reliable experimental results in tunnel spectroscopy [3]-[4] give the base for such testing.
Consider so-called SIN (superconductor-insulator-normal metal) tunneling typical for STM measurements. Total tunnel current \( I(V) = e(W_I - W_{II}) \) is determined by probabilities \( W_I(n - n_0) \) of electron transfer from superconductor to normal metal and vice versa. These probabilities are found in first order in tunnel interaction \( V_{\text{tun}} \sim \sum_{\sigma,n} G(n - n_0) (c_{\sigma n}^\dagger d_{\sigma} + \text{h.c.}) \). Here \( d_{\sigma} \) are the Fermi operators of normal metal (a tip of STM). A "tip formfactor" \( G(n - n_0) \) characterizes the extension of surface-tip interaction centered at some site \( n_0 \). As usually the constant density of state (DOS) for normal metal (tip of STM) and the energy independent formfactor are assumed.

For state with AF+VB correlations and d-wave SC order the quasiparticle operators \( \chi_{k \lambda}^\dagger = b_{k i}^\dagger U_{i \lambda}, \; i, \lambda = 1, \ldots, 4 \), are eigen operators of linearized effective Hamiltonian \( \tilde{H}_L \). Here a basis set of Fermi operators is \( b_{k i}^\dagger = \{ c_{k+}^\dagger, c_{k}^\dagger, c_{-k+}, c_{-k}^\dagger \} _i, \; \tilde{k} = k - (\pi, \pi) \), and \( k \in F \) varies inside MBZ \( |k_x \pm k_y| \leq \pi \). With taking into account the structure and spectrum \( E_{k \lambda} \) of quasiparticles the differential tunnel current takes the form

\[
\frac{dI(V)}{dV} = -\frac{1}{N} \sum_k F \left\{ [RU_{1 \lambda}^2 + \tilde{R}U_{2 \lambda}^2] f'(E_{k \lambda} - eV) + [RU_{3 \lambda}^2 + \tilde{R}U_{4 \lambda}^2] f'(E_{k \lambda} + eV) \right\} \tag{3}
\]

Here \( R = G^2(k), \; \tilde{R} = G^2(\tilde{k}) \) and \( f'(E) = df/dE \) is derivative of Fermi function. Deducing of Eq.(5) includes the averaging over the position of "tip center" \( n_0 \) among two magnetic sublattices of AF state. Sign of \( V \) is chosen so that negative \( V \) corresponds to occupied levels in the sample spectrum. The matrix elements \( U_{i \lambda} \) are the analogues of the coherence factors in simple BCS theory. As in [21] they are retained in explicit form in Eq.(5) since the normal state DOS of superconductor sharply depends on energy near VHS. Note, that here we deals with VHS of LHB instead of VHS of whole unsplit band as in [21].

Figures 2,3 present the tunnel spectra (3) for nearly optimal doping and for UD and OD systems at temperatures lower and higher \( T_c \) for one of studied variants of "tip formfactor". In complete accordance with expectation at temperature lower than \( T_c \) the SC gap (not pseudogap) displays in differential tunnel current. The distance between peaks asides main dip at \( V=0 \) corresponds to gap \( 2\Delta_{SC}(\delta) \) whose values and doping dependence at small \( T \) are close to dependence \( 2W_M(\delta) \) in Fig.1b and is characterized by maximum at optimal doping.

In OD region the calculated gap behavior \( 2\Delta_{SC}(\delta) \) is in accordance with gap behavior measured by STM in BSCCO [3]. In both cases the gap decreases with doping at \( \delta > \delta_{opt} \). In UD samples the observed tunnel gap seems to include the pseudogap which does not
vanish at \( T > T_c \). This result is not reproduced by calculations. Besides, at all doping the observed spectra retain almost symmetrical form close to calculated spectrum for optimal doping (Fig.2). However a tunnel current \( dI/dV \) becomes highly asymmetric in UD and OD systems. At low temperatures sharp peak in function \( dI/dV \) at \( V < 0 \) or \( V > 0 \) for UD and OD doping correspondingly reflects the VHS in the normal state DOS. The asymmetry of observed spectra remains almost invariable at slight variations of doping around optimal value \([3, 4]\). The shape of DOS determines also asymmetric nonlinear background of tunnel current at large \( V \) (see inset in Fig.2). However the one-particle approximation (3) used is unsuitable at large \( V \). It cannot describe secondary wide peaks in observed tunnel spectra at large \( V \). These peaks (as well as similar patterns in ARPES data) are connected by many authors with spin-wave excitations \([22]\). Possible origin of VHS broadening or splitting removing too sharp asymmetry may consist in interlayer coupling of \( CuO_2 \) planes. We neglect this coupling. The split of VHS in bilayer system and position of \( \mu \) between two VHS might manifest as two almost symmetric peaks in tunnel spectra which retains as pseudogap even at \( T > T_c \).

Additional foundation for hypothesis on the bilayer-split have been obtained recently from dependencies of spectral functions \( A(k, \omega) \) on photon energy in ARPES data \([13]\). The observed spectral features are discussed in terms of united band without huge gap between Hubbard subband which are implied in our calculations. One must also keep in mind possible inequivalence of \( CuO_2 \) planes closest to surface and those in bulk caused by uncompensated fields of the charged BiO plane at cleavage in STM experiment.

4. Manifestation of Fermi surface and influence of spin fluctuations.

One of open question in correlated variational approach \([15]\) was how to concert the ARPES data with predicted shape of nonshadow FS for OD models. For such models "large" FS around point \( \Gamma(0, 0) \) with electron- like segments near \( (\pi, 0) \) was obtained. This was in contradiction with widely recognized shape of FS as an arc around \( Y(\pi, \pi) \) \([2]\). But recent new reexamination of FS shape for BSCCO shows the possibility of the electron-like FS crossing on line \( \Gamma - M(\pi, 0) \). Besides the FS shape, it is important to discuss how various sections of FS should manifest in spectral functions.

The second question is about a role of spin fluctuations. Important influence of low frequency collective spin-wave on Fermi spectrum of correlated system is wide spread
known (see [20] among last publication). Since the spin-wave states are the states with a spiral spin structure, the comparative study of the normal state DOS and the band structure features for AF and spiral states of $t-t'-U-V$ Hubbard model have been carried out here. This study has only qualitative character. For this reason and for sake of simplicity we consider and compare the mean-field (MF) solutions with AF and spiral spin structures but without correlations of the VB type.

Standard MF spiral state $\Psi_Q$ with a spirality vector $Q$ is the MF state with one-electron averages $<c_n^{\dagger}c_n>=b_0\exp[iQn]$. At $Q \rightarrow Q_{AF} = (\pi, \pi)$ it comes to AF state. Neglecting of VB correlations significantly changes the energy of system and shifts to larger value a critical doping at which the MF AF (or spiral) solutions transform to paramagnet ones [16]. For the same reason minimization of MF energy over $Q$ at given $\delta$ leads to overestimated difference between optimal vector $Q(\delta)$ and $Q_{AF} = (\pi, \pi)$. In this connection we study and compare the DOS of spiral states at arbitrary vector $Q$, which does not minimize the MF energy at each doping.

For MF states without VB correlations and SC pairing we define under- and overdoped states as that for which the VHS occurs lower or higher than the chemical potential $\mu$. Then at ”optimal” doping the VHS is just placed at chemical potential. For calculated model with parameters $U/t = 8$, $t'/t = 0.05$, $V/t = 0.1$, such definition gives a value $\delta_{opt} \sim 0.25$ for the ”optimal” doping in case of AF state. It is larger than value $\delta_{opt} = 0.19$ for the same system in the AF+VB state which takes into account the VB correlations.

Fig.4 presents the DOS of LHB for MF AF and spiral states with different directions of $Q$ and $|Q-Q_{AF}| = 0.3$. The single VHS for AF state transforms to split VHS’s for spiral states. Formation of spiral spin structure removes degeneracy of VHS at $k = (\pm \pi, \pm \pi)$ in the same manner as the lattice distortion removes it in usual Jahn-Teller effect [3]. Spiral states provide examples of electronic analogues of Jahn-Teller effect.

It is instructive to compare the influence of spin structure on occupation number $n_k = \frac{1}{2}\sum_\sigma <c_k^{\dagger}\sigma c_k\sigma>$ in momenta space and on the one-particle spectral function $A(k, \omega)$ at low frequency $\omega \rightarrow 0$.

$$A(k, \omega = 0) = \frac{1}{ZN} \sum_\sigma \sum_{i,f} |<f|c_k\sigma|i>|^2 \exp(-E_i/kT) \left(\frac{e^\gamma}{\pi[(E_i - E_f - \omega)^2 + \gamma^2]}\right) |_{\omega=0} (4)$$

Here $E_i$, $E_f$ are energies of initial and final states, $Z$ is partition function of system, and standard $\delta$-function $\delta(E_i - E_f - \omega)$ is replaced by Lorentz function with width $\gamma$. 

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Fig. 5 presents functions $n_k$ and $A(k, \omega = 0)$ calculated for $k$ changing along the counter $Y(\pi, \pi) - \Gamma(0, 0) - M(\pi, 0) - Y$ for under-, optimally and over-doped MF states of $t - t' - U - V$ model at $\gamma = 0.003t$.

Several features, partly well known, of obtained spectral functions must be stressed.

Even in AF state, for which the band energy are periodic in MBZ, functions $n_k, A(k, \omega)$ do not possess such periodicity. Neglecting fine details, one can see that occupied ($n_k > 0.5$) or empty ($n_k < 0.5$) momenta states refer to regions around $\Gamma$ or $Y$ correspondingly, just in same manner as it takes place for noninteracting system. This property is well known and retains for spiral states also.

At $\Gamma - Y$ direction the most sharp fall of $n_k$ is seen at $k_x = k_y < \pi/2$ and corresponds to crossing of nonshadow Fermi boundary with line $\Gamma - Y$. Position of fall corresponds to the standard observed Fermi boundary in form of arc with center at $Y(\pi, \pi)$. Involving the spiral (instead of AF) spin order does not change the position of Fermi boundary at this direction. Corresponding peak in $A(k, \omega = 0)$ is most prominent at any doping and does not influenced by spin fluctuations, i.e. its position does not depend on the spirality vector $Q$. This is in accordance with the observed well defined Fermi surface at $\Gamma - Y$ direction for any doping [1]. The second peak of $A(k, \omega = 0)$ on the same direction and corresponding step in $n_k$ refers to shadow Fermi boundary. The intensity of peak is much less and its position significantly depends on $Q$. So this feature is expected to be smoothed by spin fluctuations.

At any doping in region near $M(\pi, 0)$ the occupation number $n_k$ changes smoothly with $k$ running along $\Gamma - M - Y$ and low-frequency Fermi excitation peaks in $A(k, \omega = 0)$ are sufficiently intensive in whole region near $M$ at any doping, especially at “optimal” doping (Fig.5). This is the same in both cases: at UD when the region near $M$ become dielectric one ($E(\pi, 0) - \mu < 0$) and at OD when the region near M arranges between main and shadow large FS’s ($E(\pi, 0) - \mu > 0$). Similar smoothing or destruction of FS in region $k \sim (\pi, 0)$ has been observed in ARPES data [4,5]. Large summary intensity of photoemission from this region of $k$ have really been observed in [13] for BSCCO. However it occurs visible only at the photon energy 22 eV, but not at 33 eV. In our picture of split Hubbard bands the VHS of LHB is more strong than that expected from tight-binding unsplit band. So additional increase of intensity at $k \sim (\pi, 0)$ is possible. But the singlelayer models of cuprates cannot describe the observed dependence of additional
photoemission on the photon energy [13]. As in discussions about tunnel spectra, we come
to necessity of extending the study on bilayer models.

In conclusion, fine structure of upper edge of LHB in $t$-$t'$-$U$ Hubbard model and vari-
atational correlated state with VB formation can describe some of low-energy phenomena
in cuprates. Doping and temperature dependencies of gap anisotropy obtained from pho-
toemission data [12] are explained by interplay of gap and pseudogap which is working
function for electron removing from dielectric segments of generalized FS. It is shown
that only SC gap, but not pseudogap, is seen in tunnel spectra. At $T \to 0$ differential
tunnel current for optimal doping is similar to observed one, but it displays too sharp
asymmetry in heavily UD (and OD) regimes with peaks at negative (or positive) voltages
caused by normal state VHS. Model seems to need extension on bilayer models. Occu-
pation number $n_k$ and spectral functions calculated in MF approximation confirm the
sharp Fermi boundary at $k_x = k_y$ direction and smoothed (destructed ) Fermi boundary
near $(\pi, 0)$ as it observed in ARPES [4, 5]. Change of FS topology at optimal doping
and large partly electron-like FS at OD case in our model seem to receive confirmation
in reexamined ARPES data [13], but single-layer model cannot explain the dependence
of photoemission spectra on photon energy.

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Captions to Figures

Fig. 1.

a) Doping dependence of SC transition temperature $T_c(\delta)$ in unit [0.01t]. b) Double shift of photoemission edge $2\Delta_M(\delta)$ at $k = (\pi, 0)$ (curve 1) and corresponding SC gap $2W_k(\pi, 0)$ (curve 2) in same units. c) The ratios $\xi = v_\Delta/\Delta_M$ (curve 1) and $\xi_W = v_\Delta/W_k(\pi, 0)$ (curve 2) as function of doping. d) Angular dependence of gap $\Delta(\varphi)$ for various temperatures in heavily UD model $\delta = 0.14$, $T_c/T_{c}^{max} = 0.55$. Rest parameters of model are in text.

Fig. 2. Differential tunnel current for nearly optimal doping $\delta = 0.2$ ($T_c/t = 0.0114$) at temperatures $T/t = 0.002, 0.014, 0.018$. Insets: the same and the current $I(V)$ for $T/t = 0.002, 0.018$ in large voltage regions. Parameters of model are $U/t = 8, t'/t = 0.05, V/t = 0.1$.

Fig. 3. Tunnel current $dI/dV$ at $T/t = 0.002, 0.014, 0.018$ for UD and OD models with $T_c/T_{c}^{max} = 0.743$ and 0.63 correspondingly. Model parameters are same as in Fig. 2.

Fig. 4. DOS of LHB for the MF AF state (curve 1) or for spiral states with $Q_2 = (0.9\pi, \pi)$ and $Q_3 = (0.93\pi, 0.93\pi)$ (curves 2 and 3).

Fig. 5. Occupation number $n_k$ (solid lines) and $A(k, \omega = 0, \gamma)$ with $\gamma = 0.003t$ (dotted lines) for MF AF state and spiral states of UD and OD models. Vector $k$ runs along path $Y - \Gamma - M - Y$. For spiral states vectors $Q$ are determined by values $q' = 0.8\pi$ and $q = 0.86$. Dashed dotted curves on segments $\Gamma - M - Y$ (upper graphics) correspond to AF state at nearly "optimal" doping $\delta = 0.3$. 

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$2\Delta_M/T_c$ and $2\Delta(\phi)/T_c$ as functions of $\delta$ for $T/T_c = 0.4, 0.6, 0.8, 0.9, 1.2$, with $\delta = 0.14$.

$Z(\phi) = (\cos k_x - \cos k_y)/2$.
Underdoped
n=0.85

Overdoped
n=0.78
Underdoping ($n=0.85$), $q'=0.8\pi$

- $Q=(\pi,\pi)$
- $Q=(q',\pi)$
- $Q=(q,q)$

Overdoping ($n=0.65$), $q'=0.8\pi$

- $Q=(\pi,\pi)$
- $Q=(q',\pi)$
- $Q=(q,q)$