On the nature of pseudogap anomalies in HTSC

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Abstract. We proposed the model of HTSC where the interaction of electrons from oxygen band with the diatomic negative U-centers (NUC) on pairs of Cu ions in CuO2 plane is assumed to be responsible for the superconducting pairing. As follows from the model the occupation $\eta$ of NUC with real electrons reduces superconducting order parameter due to decreasing of number of states available for scattering of electron pairs. The charge fluctuations between NUC and valence band will result in fluctuations of pairing interaction. In clusters, containing small number of NUC’s, where the relative fluctuations of $\eta$ are great enough, the superconducting gap may open at $T^*>T_{c\infty}$ and close at $T_{c}<T_{c\infty}$, where $T_{c\infty}$ is the temperature of superconducting transition for infinite cluster. The doping dependences of $T^*$ and $T_c$ for YBa$_2$Cu$_3$O$_{6+\delta}$ are calculated as two roots of the same square equation. The obtained results demonstrate the impressive agreement with experiment.

1. Introduction

Earlier [1-3] we have shown that the energy of two excitations (that corresponds to the transition of one electron from $O^{2-}$ to nearest Cu$^{2+}$) can be lowered if they are side-by-side. This is possible due to formation of a bound state (of the Heitler-London type) of two electrons and two holes that occur in the immediate vicinity of this pair of Cu ions. As follows from the model each pair of neighboring Cu ions in CuO$_2$ plane is the potential NUC.

The NUC activation takes place under doping. The mechanism is based on the assumption of rigid localization of doped charge in the close vicinity of doped ion. This localization results in local variation of electronic structure of the parent charge-transfer insulator that depends on the local mutual arrangement of the doped charges. As follows from [1-3] NUC is formed in YBa$_2$Cu$_3$O$_{6+\delta}$ on a given pair of Cu ions in CuO$_2$ plane when three in a row oxygen sites in CuO-chain over (under) this Cu pair are occupied (figure 1a). The concentration of such triplets at random distribution of oxygen ions in CuO-chains is equal to $\delta^3$ per unit cell.

Figure 1. a) NUC (shaded) is formed in YBa$_2$Cu$_3$O$_{6+\delta}$ on a given pair of Cu ions in CuO$_2$ plane when 3 in a row oxygen sites in CuO-chain over (under) this Cu pair are occupied; b) formation of continuous NUC clusters in CuO$_2$ planes by the row of oxygen ions in CuO-chain.
Isolated triplet of oxygen ions in chain forms two NUC’s, one NUC in each of two CuO$_2$ planes (Figure 1a). If the number of consecutive oxygen ions in a chain $N_0 > 3$, only every second triplet can form separated NUC (without common Cu ions) in each of CuO$_2$ planes (Figure 1b). So, we may take that for $N_0 > 3$ each triplet forms one NUC but only in one CuO$_2$ plane.

The continuous sets of oxygen ions belonging to adjacent chains we assume to form united 2D-cluster of NUC’s provided that they touch over 3 or more oxygen ions in adjacent chains (that is the percolation over NUC’s takes place). This will correspond to the formation of continuous 2D-clusters of NUC’s in both CuO$_2$ planes. Figure 2 shows the random distribution pattern for oxygen ions in chains for the 40×40 square lattice obtained for $\delta=0.3$ and $\delta=0.6$.

Figure 2. Pattern of chain oxygen clusters forming a finite clusters of NUC’s in CuO$_2$ planes for random distribution of oxygen ions in chains: (a) $\delta=0.3$ and (b) $\delta=0.6$. Open circles are oxygen ions in chains. Clusters containing more than 3 oxygen ions are dashed.

2. Generation of additional hole carriers

The total number of NUC’s in clusters (for both CuO$_2$ planes) per one unit cell of YBa$_2$Cu$_3$O$_{6+\delta}$ at random distribution of oxygen ions is equal to $N_U = \delta^3 + N_3(\delta)$, where $N_3(\delta)$ is the $\delta$-dependent number of isolated triplets of oxygen ions in chains equal to $N_3(\delta)=\delta^3(1-\delta)^2$. Respectively, $N_U(\delta)=\delta^3\{1+(1-\delta)^2\}$. At $\delta<\delta_c$, NUC’s form finite clusters of various sizes. Within each cluster the NUC occupation number $\eta$ depends on temperature and equals [1,2] to $\eta=2T/(T+T_0)$.

The volume concentration of NUC’s $P=N_U/V_{UC}=\delta^3\{1+(1-\delta)^2\}/V_{UC}$, where $V_{UC}=173\text{Å}^3$ is the volume of unit cell for YBa$_2$Cu$_3$O$_{6+\delta}$. Accordingly, the volume concentration of hole carriers $n$, generated in CuO$_2$ planes as electrons occupied NUC is equal to $n=\eta P$ and Hall coefficient is

$$R_{H}(\delta,T)=\frac{1}{ne}=(1/2e)(V_{UC}/\delta^3\{1+(1-\delta)^2\})\frac{T+T_0}{T},$$

where $e$ is the electron charge. Figure 3a,b shows the temperature and doping dependences of Hall coefficient for YBa$_2$Cu$_3$O$_{6.95}$ single crystals from [4]. As is seen all present data can be approximated successfully by (1) with $T_0\approx 390$ K.

Figure 3. Hall coefficient of CuO$_2$ plane of twin-free YBa$_2$Cu$_3$O$_{6+\delta}$ single crystal depending on temperature and doping: (a) open squares - $R_H(T)$ for $\delta=0.95$ [4]; (b) open rhombuses - $R_H(\delta)$ at $T=300$K [4]. Solid line on both figures is the dependence (1) with $T_0=390$ K.
3. The nature of pseudogap- and 60K-phases

In conventional BCS superconductor the superconducting gap vanishes due to the thermal excitations over the Fermi surface, which decrease the number of unoccupied states available for the electron pair scattering. Analogously the mechanism of superconducting gap suppression in our case is the occupation of NUC’s by real electrons. Therefore fluctuation-induced reduction of pair level occupation will amplify the superconducting interaction and can result in fluctuation-induced turning on superconductivity at $T^* > T > T_c$ (here $T_c$ is equilibrium value of $T_c$ for infinite cluster of NUC’s). Opposite, the increasing of pair level occupation owing to fluctuation will reduce the superconducting interaction and can result in fluctuation-induced turning off superconductivity at $T_c < T < T_{c\infty}$.

Large relative fluctuations of NUC occupation, corresponding to substantial deviation of $T^*$ and $T_c$ from $T_c\infty$ can happened in the underdoped samples when the significant number of NUC’s belongs to small finite clusters. The mean size of finite clusters decreases with doping reduction and relative fluctuations of NUC occupation increase in these clusters (i.e. $T^*$ goes up and $T_c$ goes down). On the ground of the proposed model it is possible to deduce the dependences of $T^*$ and $T_c\infty$ on doping $\delta$ for YBa$_2$Cu$_3$O$_{6+\delta}$. At $\delta < \delta_c$, when NUC’s form finite clusters of various sizes, the sample should be defined as Josephson media, where superconductivity is realized over the whole volume thanks to the Josephson links between superconducting clusters.

The number of Cu ions included in cluster of NUC in CuO$_2$ plane we will take as a size of cluster, $S$. According to [1,2], the number of electrons on NUC’s in a given cluster at temperature $T$ is equal $N=T S/(T+T_0)$. This number can be changed on $\pm \sqrt{N(T)}=\pm (TS/(T+T_0))^{1/2}$ due to fluctuations. The condition for turning superconductivity on (off) in a given cluster at temperature $T^*$ ($T_c$) is $N(T)=\sqrt{N(T)}=N_c$, where $N_c=T_c\infty S/(T_c\infty+T_0)$ – the number of electrons on NUC at the superconducting transition temperature $T_{c\infty}$ for the infinite cluster. Hence,

$$T S/(T+T_0) = (TS/(T+T_0))^{1/2} = T_{c\infty} S/(T_{c\infty} + T_0)$$

Solving Eq.(2) with $T_0=390$ K and $T_{c\infty}=92$ K we find $T^*$ and $T_c$ as a function of $S$ (figure 4).

As it seen from figure 4, the fluctuation effect on $T_c$ decreases with cluster size increasing and becomes to be negligible in clusters of NUC with more than 1500 Cu ions. It is notable that there is minimal $S$ value, below that the cluster does not remain superconductive even at $T\to0$ due to fluctuations of NUC occupation. Since the NUC occupation is $\rho=2/5$ at $T=T_{c\infty}$ any fluctuation in cluster with $N_U<5$ (or $S<10$) that increases the number of electrons on NUC by 2 will result in the destruction of superconducting state. In order to find $T^*(\delta)$ and $T_c(\delta)$ dependences it is necessary to know $\delta_c$ corresponding to the percolation threshold over NUC and the statistics of finite clusters of
NUC depending on $\delta$. These values can be found for the random distribution of oxygen atoms in chains by Monte Carlo method. The value $\delta_c=0.80\pm0.02$ has been determined by this method. It means that $T_c$ would be equal $T_c^{\infty}$ at $\delta > \delta_c$. To simplify the determination of $T^*(\delta)$ and $T_c(\delta)$ dependences we suppose that all finite clusters have the same sizes equal to $S_m$. The dependence $S_m(\delta)$ was also determined for random distribution of oxygen atoms in chains.

Fig. 5. The comparison of calculated dependences of $T^*(\delta)$ (solid triangles down) and $T_c(\delta)$ (solid triangles up) for YBa$_2$Cu$_3$O$_{6+\delta}$ single crystals. Open squares show the experimental results [5] for the single crystals. Open rhombuses are the results of $T_c$ measurements for YBa$_2$Cu$_3$O$_{6+\delta}$ single crystals [6]. Solid lines are drawn by eye. The dotted line of $T_c(\delta)$ at $\delta < 0.5$ corresponds to the area where the mean size of cluster of NUC’s $S_m < 5$.

Substituting the obtained values of $S_m(\delta)$ in the quadric equation (2) we get $T_c(\delta)$ and $T^*(\delta)$ for YBa$_2$Cu$_3$O$_{6+\delta}$ as two solutions of this equation. Both solutions are shown in figure 5 by triangles up and down, correspondingly. As follows from the model the area between these curves is the area of fluctuations, where the finite clusters fluctuate between superconducting and normal states due to fluctuations of occupations of NUC’s. The experimental dependences $T^*(\delta)$ [5] and $T_c(\delta)$ [6] for YBa$_2$Cu$_3$O$_{6+\delta}$ single crystals are shown for comparison. As is seen from figure 5 the agreement can be considered as good in spite of convention of their definition.

4. Summary
In the framework of the model assuming the formation of NUC on the pairs of Cu ions in CuO$_2$ plane the mechanism of hole carrier generation is considered and the interpretation of pseudogap and 60 K-phases in YBa$_2$Cu$_3$O$_{6+\delta}$ is offered. The calculated dependences of hole concentration in YBa$_2$Cu$_3$O$_{6+\delta}$ on doping $\delta$ and temperature as well as $T^*(\delta)$ and $T_c(\delta)$ dependences are found to be in a good quantitative agreement with experimental data. The results may serve as important arguments in favor of the proposed model of HTSC.

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