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NEW METAL/SUPERCONDUCTOR-INSULATOR TRANSITIONS AND THEIR EFFECTS ON HIGH-T_C SUPERCONDUCTIVITY IN UNDERDOPED AND OPTIMALLY DOPED CUPRATES

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Abstract. *A new approach to the metal/superconductor-insulator transition in doped cuprates by studying the polaron formation and localization of doped charge carriers (holes) in them and the possibility of transforming a metallic or superconducting system into an insulator was developed. A more suitable criterion for such a phase transition by comparing the bandwidth (or Fermi energy) of large polarons with their binding energies in the cuprates was derived. The possibility of the metal/superconductor-insulator transition and phase separation in doped cuprates resulting in the formation of competing metallic/superconducting and insulating phases in underdoped, optimally doped and even in overdoped high-*T_c *cuprates was predicted. Then the possible detrimental and beneficial effects of the different disorders (e.g. polaron formation and charge-density-wave transition) and the coexisting insulating and superconducting phases on the critical temperature* T_c *of the superconducting transition of underdoped and optimally doped cuprates was examined. The actual superconducting transition temperature* T_c *in these materials using the theory of Bose-liquid superconductivity, and not the Bardeen-Cooper-Schrieffer-like theory of Fermi-liquid superconductivity, which is incapable of predicting the relevant value of* T_c *in high-*T_c *cuprates was determined. We find that the suppressing of the polaronic and charge-density-wave effects in optimally doped cuprates results in the enhancement of* T_c*, while some lattice defects (e.g., anion vacancies) in the cuprates may strongly affect, on* T_c *and enhance high-*T_c *superconductivity in them.*

Keywords: polaron formation and charge density waves, metal/superconductor-insulator transition, cuprates, Bose-liquid superconductivity, different disorders, suppression and enhancement of high-T_c superconductivity.

1. Introduction

The Mott-Hubbard model is considered appropriate for explaining the metal-insulator transition in undoped cuprates, which are charge-transfer type insulators [1, 2], but not in doped cuprates [2, 3]. Doped cuprates are unique insulators, metals, and superconductors in the intermediate doping regime because they are substantially more complicated systems [1, 2, 4]. The intriguing insulating, metallic, and superconducting properties are particularly seen in underdoped and optimally doped cuprates. These properties cannot be explained by the theories of the Mott and Anderson metal-insulator transitions [1] or the Fermi-liquid superconductivity theory proposed by Bardeen-Cooper-Schrieffer (BCS) [5]. As a result, as the physics of these novel superconducting materials have advanced, so too has interest in the characteristic metal-insulator and superconductor-insulator transitions in doped cuprates [1-3, 6-8]. It is anticipated that numerous deviations in the superconducting behaviors of high-temperature cuprates noted in underdoped and optimally doped regions are intricately linked to transitions between metal/superconductor and insulator states, phase separation, and the coexistence of competing superconducting and insulating phases [6-11]. The physics of these high-T_c materials has advanced significantly (refer to Refs. [1,4,7,12]), but our knowledge of the strange properties of underdoped and optimally doped cuprates in their superconducting state, as well as the distinctive metal/superconductor-insulator transitions in doped cuprates, remains very incomplete. In particular, yet unanswered concerns include the development of competing metallic/superconducting and insulating phases in underdoped and optimally doped cuprates, as well as the causes of the suppression and amplification of high-T_c superconductivity in these substances.

Here, we investigate the effects of the metal/superconductor-insulator transitions in doped cuprates, which are fueled by strong electron-phonon interactions and polaronic formation at the self-trapping of doped charge carriers on high-T_c superconductivity in both optimally and underdoped cuprates. A more relevant criterion for such transitions in doped cuprates, which occur in the doping range from underdoped to overdoped regime and are accompanied by the phase separation into the competing metallic/superconducting and insulating phases was derived. The critical temperature of the superconducting transition T_c in underdoped and optimally doped cuprates using the theory of Bose-liquid superconductivity and the reasons of the suppression and enhancement of high-T_c superconductivity in them was determined. The competing superconducting and insulating phases strongly affect on T_c especially in underdoped cuprates was found. We investigate the possible detrimental and beneficial effects of different disorders (e.g. the polaron formation or charge-density-wave (CDW)) transition and the radiation defects on the superconducting properties (i.e. critical values of the superconducting transition temperatures T_c) of high-T_c cuprates and show that the suppression of the polaronic and CDW effects are accompanied by increasing of T_c, while radiation-induced defects (e.g. anion vacancies) in these materials may also strongly affect on T_c and enhance high-T_c superconductivity.

2. Materials and research methods

The quasi-free holes carriers introduced to the polar cuprate materials by doping are self-trapped spontaneously at their strong interactions with lattice vibrations and therefore, these doped hole carriers are dressed by the local lattice distortions and become large polarons with effective masses $m_p \simeq (2-3)m_e$ [13,14] (where m_e is the free electron mass). At low doping levels, such polaronic carriers are localized and immobile. When the doping level increases towards underdoped region, the ordering of large polarons results in the formation of their superlattice and a narrow energy band. In doped cuprates the width of the polaronic band increases with increasing the doping level and is sufficiently broadened in underdoped cuprates in which the polaronic transport becomes metallic. The width of such a polaronic band is determined by using the tight-binding method. One can expect that when the doping level increases up to a certain underdoping regime, a doped cuprate material may undergo a phase transition from an insulator to a metallic state. Below T_c, such a metal-insulator transition occurs as a superconductor-insulator transition.

3. Results and discussion

3.1. Localization of doped charge carriers and metal/superconductor-insulator transitions in underdoped and optimally doped cuprates

We now develop a new approach and obtain the relevant criterion for the metal/superconductor-insulator transition in doped cuprates. It is natural to assume that the transition of a hole carrier from the localized (polaronic) state to a delocalized itinerant (metallic) state becomes possible when the kinetic energy (or Fermi energy ε_F) of hole polarons is larger than their binding energy E_p.

Using the relation (1) and Eq. (2) in Ref. [15], we can determine the critical doping level $n = n_c$ (n is the density of large polarons) corresponding to the metal/superconductor-insulator transition in the cuprates from the expression

$$n_c = \frac{1}{3\pi^2}\left[\frac{2m_pE_p}{\hbar^2}\right]^{3/2}. \tag{1}$$

Then the relevant criterion for the metal/superconductor-insulator transition in doped cuprates can be written as

$$x \gtrsim x_c = \frac{n_c}{n_a} = \frac{1}{3\pi^2\hbar^3 n_a}\left[2m_pE_p\right]^{3/2}, \tag{2}$$

where $n_a = 1/V_a$ is the concentration of lattice atoms or CuO_2 molecules, V_a is the volume per CuO_2 formula unit in the cuprate materials.

This newly established criteria for the metal/superconductor-insulator transitions enables us to forecast the likelihood of achieving such phase transitions in underdoped and optimally doped cuprates, driven by the strong electron-phonon interactions and polaronic formation. Firstly, we investigate whether the new metal/superconductor-insulator transitions are possible in these cuprate materials. We consider the effects of both the variation of ε_∞ and the large ionicity of the cuprates $\eta = \varepsilon_\infty/\varepsilon_0 \ll 1$ (where ε_0 and ε_∞ are the static and high frequency dielectric constants, respectively).

Now we calculate the critical doping levels x_c for metal/superconductor-insulator transitions in La- and Y-based high-T_c cuprates $La_{2-x}Sr_xCuO_4$ (LSCO) and $YBa_2Cu_3O_{7-\delta}$ (YBCO). In so doing, we taking the calculated values of $E_p \simeq 0.078 - 0.2$ eV at $\varepsilon_\infty = 2.5 - 4.0$ and $\eta = 0.04$ [16] and the observed values of $m_p \simeq (2-3)m_e$ [17]. The values of V_a can be determined approximately as $V_a \simeq 190$ Å^3 in LSCO and $V_a \simeq 100$ Å^3 in YBCO, so that the values of n_a are equal roughly to $0.53 \cdot 10^{22} cm^{-3}$ (in LSCO) and $10^{22} cm^{-3}$ (in YBCO). For LSCO using the values of parameters $m_p = 2.2m_e$, $E_p = 0.078 - 0.2\, eV$ and $n_a \approx 0.53 \cdot 10^{22} cm^{-3}$, we find the values of critical doping for metal/superconductor-insulating transitions $x_c = 0.060 - 0.249$ in this system. Then, we use the other values of parameters $m_p = 2.8m_e$, $E_p = 0.078 - 0.2\, eV$ and $n_a \approx 10^{22} cm^{-3}$ for YBCO, we obtain the values of critical doping for metal/superconductor-insulating transitions $x_c = 0.046 - 0.189$ in this cuprate material. Further, the variations of x_c with decreasing ε_∞ in LSCO and YBCO are shown in Figs.1 and 2 for $\eta = 0.04$.

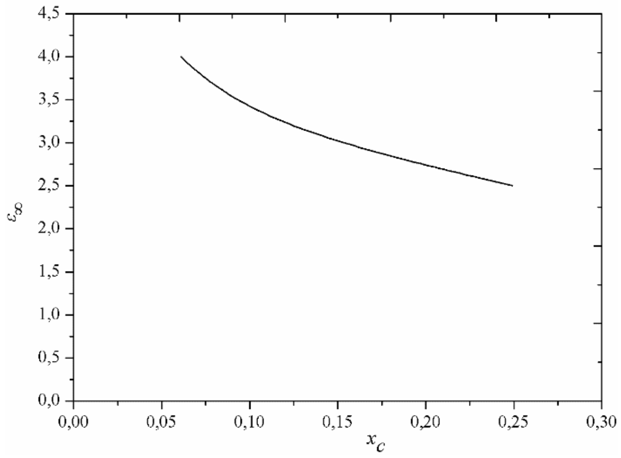

Fig.1. The variation of x_c with decreasing ε_∞ in LSCO for $\eta = 0.04$.

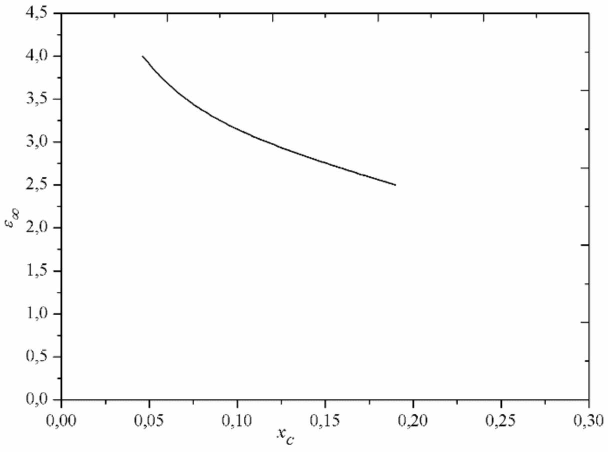

Fig.2. The variation of x_c with decreasing ε_∞ in YBCO for $\eta = 0.04$.

The above presented theoretical results for metal/superconductor-insulator transitions agree well with experimental data on the same transitions in underdoped and optimally doped cuprates [9,11,18-20]. Particularly, our novel and significantly results show that in YBCO the metal/superconductor-insulator transitions and phase separation into competing metallic/superconducting-insulating phases occurs in the doping range $0.05 \lesssim x \lesssim 0.19$ in accordance with experimental observations [9,11]. As a result, the metallic/superconducting and insulating phases will compete with each other in underdoped and optimally doped high-T_c cuprates.

3.2. Possible effects of the competitions between the insulating and superconducting phases on high-T_c superconductivity in underdoped and optimally doped cuprates

Based on the given information, it can be inferred that the insulating and metallic or superconducting phases compete in underdoped and optimally doped cuprates, where the non-superconducting (i.e. immobile) and superconducting hole carriers below T_c reside in carrier-poor (insulating) and carrier-rich (superconducting) domains, respectively. We argue that the hole carriers residing in an adequately broadened polaronic band may become mobile and their Cooper pairing would occur in momentum (k-) space and leads to the formation of polaronic (i.e. tightly-bound) Cooper pairs above T_c, which behave like Bose particles and condense into a superfluid state below T_c. Actually, such preformed Cooper pairs would exist in doped high-T_c cuprates at $\varepsilon_F \sim \varepsilon_A$ (where ε_A is the energy of the attractive interaction among two polaronic carriers). Since the pairing interaction mechanism between large polarons in the energy range $\{-\varepsilon_A, \varepsilon_A\}$ is much stronger than in the usual BCS model [5]. In the present case the pair Hamiltonian of the strongly interacting polaronic Fermi gas can be diagonalized by the Bogoliubov transformation of Fermi operators. Then, we use the model interpolaron interaction potential [21] and get the following BCS-like gap equation for determining the onset temperature T^* of the Cooper pairing of polarons:

$$\frac{1}{\lambda_F} = \int_0^{\varepsilon_A} \frac{d\xi}{\sqrt{\xi^2+\Delta_F^2(T)}} tanh \frac{\sqrt{\xi^2+\Delta_F^2(T)}}{2k_BT}, \qquad (5)$$

where $\xi = \varepsilon(k) - \varepsilon_F$ is the energy of large polarons measured from their Fermi energy ε_F $\varepsilon(k)$ is the kinetic energy of these polarons; $\lambda = D(\varepsilon_F)\tilde{V}_F$ is the BCS-like coupling constant, $D(\varepsilon_F)$ is the density of states on the Fermi surface, $\tilde{V}_F = V_A - V_C$, $\tilde{V}_F = V_C/[1 + D(\varepsilon_F)V_C \ln(\varepsilon_C/\varepsilon_A)]]$ is the screened Coulomb interaction between two fermions, V_A and V_C are the interfermion attractive interaction potential and Coulomb interaction potential appropriate to the cutoff energies ε_C and ε_A, respectively, $\Delta_F(T)$ is the BCS-like gap.

At $T \to T^*$energy gap $\Delta_F(T)$ in the excitation spectrum of an interacting Fermi-gas of polarons tends to zero. When $\varepsilon_A \gg k_BT^*$, Eq. (5) gives

$$k_BT^* \simeq 1.134\varepsilon_A \exp[-1/\lambda_F]. \qquad (6)$$

The underdoped and optimally doped cuprates have low Fermi energies $\varepsilon_F \simeq (0.1 - 0.3)eV$ [22]. For these materials we can take $\varepsilon_A = E_p + \hbar\omega_0$, where $\hbar\omega_0$ is the energy of optical phonons. By taking $\lambda_F \simeq 0.4$ and $\varepsilon_A \simeq 0.15eV$ (assuming that $E_p \simeq 0.1\,eV$ and $\hbar\omega_0 \simeq 0.05\,eV$) for underdoped cuprates, we find, $T^* \simeq 162K \gg T_c$ (possible values of T_c for underdoped cuprates $YBa_2Cu_3O_{7-\delta}$ and $Bi_2Si_2CaCu_2O_{8+\delta}$ accordingly will be less than 90 K and 100 K) fully consistent with the results of the experiments for T^* in such high-T_c cuprates [23, 24]. If the preformed polaronic Cooper pairs in high-T_c cuprates behave like bosons, then their transition to superconducting state is not described by BCS-like theories of Fermi-liquid superconductivity. For these cuprate materials, the BCS-like theory becomes ineligible for the determination of T_c. Only the alternative Bose-liquid theory for superconductivity [21] might be adequate for describing the high-$T_c$superconductivity in underdoped and optimally doped cuprates. According this theory, T_c in the weak interboson coupling is determinated from the relation

$$T_c \simeq T_{BEC}\left[1 + c\gamma_B\sqrt{k_BT_{BEC}/\xi_B}\right] \qquad (7)$$

where γ_B is the interboson coupling constant, $T_{BEC} = 3.31\hbar^2\rho_B^{2/3}/2k_Bm_B$ is the Bose-Einstein condensation temperature of an ideal Bose gas of polaronic Cooper pairs, ρ_B is the density of the attracting bosons, $m_B = 2m_p$ is the mass of bosonic Cooper pairs, k_B is the Boltzmann constant, ξ_B is the characteristic thickness of the condensation layer including the attracting bosonic Cooper pairs, $c = \pi^{3/2}/3.918$, $\gamma_B \ll 1$.

According to the above proposed microscopic picture of the superconductor-insulator transition and evolution of competing superconducting and insulating phases, the insulating regions in underdoped cuprates are gradually narrowed with increasing doping and would persist as small islands in optimally doped cuprates and finally disappear above the doping level $x = 0.19$. This more realistic image shows that only Cooper pairs residing in metallic regions condense in a Bose superfluid below T_c and are involved in high-T_c superconductivity, while the other Cooper pairs progressively become localized in carrier-poor regions due to transition from a superconducting phase to an insulating phase and therefore, they become immobile and non-superconducting. In high-T_c cuprates, T_c determined from the expression (7) reaches the maximum T_c^{max} at some optimal doping close to overdoped (OD) regime when the insulating regions disappear at this doping level. However, at doping levels $x \lesssim 0.16$ the critical temperature T_c becomes less than T_c^{max} and is ascertained based on the expression

$$T_c = \frac{1}{1+f_I} T_c^{max}, \tag{8}$$

where $f_I = V_I/V_S$ is the fraction of the insulating phase, V_I is the volume of the insulating regions in the cuprates, V_S is the volume of the superconducting regions of these materials.

The variation of the ratio T_c/T_c^{max} in high-T_c cuprates with insulating volume fraction f_I is shown in Fig.3.

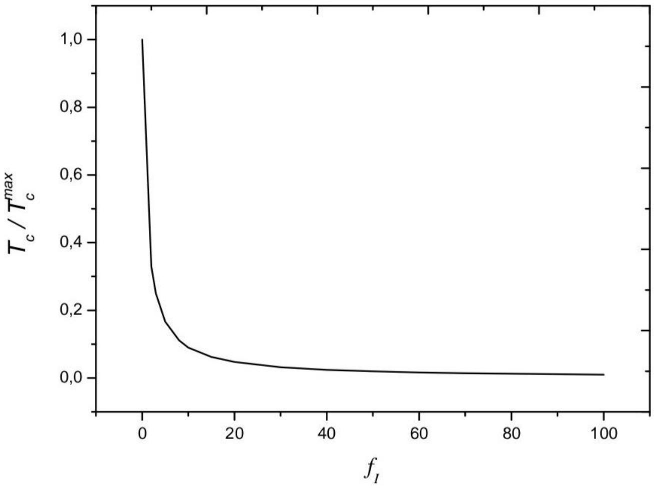

Fig.3. – The variation of T_c/T_c^{max} in high-T_c cuprates with increasing f_I.

Now, we use the expression (7) and can estimate the value of T_c^{max} in optimally doped YBCO. Assuming that $m_B = 4m_e, \gamma_B = 0.25$, $k_B T_{BEC}/\xi_B \simeq 0.15$ and $\rho_B \simeq 6 \cdot 10^{19} cm^{-3}$, we find $T_{BEC} \simeq 112.3\,K$ and $T_c^{max} \simeq 92\,K$ for optimally doped YBCO. For the underdoped (UD) system YBCO ($x \lesssim 0.14$), we can take $f_I = 0.25$. Then we obtain $T_c = T_c^{max}/1.25 \approx 74\,K$, which is in agreement with the experimental information for YBCO [25]. In YBCO the insulating volume fraction f_I is small enough at $x > 0.15$ and T_c changes little between $x_{UD} \simeq 0.15$ and $x_{OD} \simeq 0.16$. The experimental observations in YBCO confirm the predicted behaviour of T_c [25]. If we assume that the ratio V_I/V_s in underdoped LSCO is of order 0.2 at $x \lesssim 0.13$, then we obtain $T_c \simeq 0.83 T_c^{max} \simeq 32K$ which agrees well with experimental results (e.g., at x=0.13 the value of T_c is about $32K$ Ref. [23]). In underdoped and optimally doped cuprates, some part of metallic/superconducting regions goes over to insulating state at the doping level $x < 0.16$.

Therefore, a marked suppression of superconductivity will occur in underdoped cuprates due to more stronger polaronic effect and due to an increase of the insulating volume fraction at the expense of the volume of superconducting regions. The experimental findings depicted in Ref. [17] give evidence that the polaronic effect weakens with increasing doping towards overdoped regime. This means that superconductivity is strongly enhanced in optimally doped regime due to the weakening of the polaronic effect and the decreasing of the mass m_p of polarons entering the expression (7).

The strong electron-phonon coupling in the cuprates also results in the formation of the CDWs which hinder high-T_c superconductivity in underdoped cuprates. Since the formation of CDWs is also accompanied by a lattice distortion [26] and is similar to the polaron formation. Further, the irradiation-induced disorders (i.e. lattice defects) in the cuprates may strongly affect on T_c and enhance superconductivity, since the anion vacancy-enhanced Coulomb repulsion hinders the polaron formation. Actually, it has been found experimentally that disorder created in the cuprate superconductor $La_{1.875}Ba_{0.125}CuO_4$ by proton irradiation increases the superconducting critical temperature T_c by 50 % while suppressing the CDW state [26].

4. Conclusions

The possibilities of metal/superconductor-insulator transitions, which are caused by the strong electron-phonon interactions and polaronic formation were studied. This process is accompanied by phase separation into the competing metallic/superconducting and insulating phases in underdoped and optimally doped cuprates. We have argued that the strong hole-lattice interactions in doped cuprates result in the formation of large polarons and the localization of doped hole carriers transforming a metallic or superconducting system into an insulator. We have found that the metal/superconductor-insulator transitions in doped cuprates occur in the doping range from underdoped to overdoped regime ($0.05 < x < 0.19$) and are accompanied by the phase separation and formation of competing superconducting and insulating phases in underdoped, optimally doped and even overdoped high-T_c cupretes. In so doing, we have established that in doped cuprates the metal/superconducting-insulator transitions occur at low doping levels ($x \lesssim 0.05 - 0.06$) for $\varepsilon_\infty \gtrsim 3.5$ and $\eta = 0.04$, but such phase transitions take place at high doping levels ($x \simeq 0.19 - 0.25$) for $\varepsilon_\infty \lesssim 2.5$ and $\eta = 0.04$. We have predicted the possible detrimental and beneficial effects of the different disorders (e.g. polarons and CDWs) and the evolution of the competing insulating and superconducting phases on T_c in underdoped and optimally doped cuprates. We have determined T_c in these unconventional superconductors using the theory of Bose-liquid superconductivity. Unlike the BCS-like theories of Fermi-liquid superconductivity, this alternative theory of unconventional superconductivity is capable of predicting the actual T_c in underdoped and optimally doped cuprates. We conclude that the suppressing of the polaronic and CDW effects is accompanied by enhancement of high-T_c cuprate superconductivity, while some lattice defects (e.g. anion vacancies) in the cuprates may also affect on T_c and strongly enhance high-T_c superconductivity in them.

Conflict of interest statement

The authors declare that they have no conflict of interest in relation to this research, whether financial, personal, authorship or otherwise, that could affect the research and its results presented in this paper.

CRediT author statement:

Kurbanov U.T.: Validation, Formal analysis; Zhumabaeva G.K.: Investigation; Dzhumanov S.: Supervision, Writing - Original Draft. The final manuscript was read and approved by all authors.

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