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Pseudogap and Local Pairs in High-T_c Superconductors

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The temperature (T) dependence of pseudogap (PG) $\Delta^*(T)$ is calculated for Bi2201 within the local pair (LP) model [1, 2]. The model is based on analysis of the excess conductivity derived from resistivity experiments in high-temperature superconductors (HTSs) and supposes the local pairs, which are formed in HTSs at T well above T_c, to generate a pseudogap. To confirm the conclusion, $\Delta^*(T)$ is compared with the temperature dependence of the loss of the spectral weight $W(E_F)(T)$ measured by ARPES for the same Bi2201 sample [3]. A good agreement between $\Delta^*(T)$ and $W(E_F)(T)$ is found, confirming the local pairs to be one of the most likely cause for the PG formation.

Температурну залежність псевдощілини $\Delta^*(T)$ розраховано для Bi2201 в межах моделю локальних пар [1, 2]. Цей модель засновано на аналізі надлишкової провідности, яка одержується з експериментів щодо питомого опору у високотемпературних надпровідниках (ВТНП), і припускає наявність локальних пар, що мають утворюватися у ВТНП за температур T, набагато більш високих, ніж T_c, формуючи псевдощілину. Для підтвердження цього висновку $\Delta^*(T)$ порівнюється з температурною залежністю втрати спектральної ваги $W(E_F)(T)$, що вимірюється ARPES в тому ж самому зразку Bi2201 [3]. Одержано хороший збіг $\Delta^*(T)$ і $W(E_F)(T)$, який підтверджує, що локальні пари є однією з найбільш ймовірних причин утворення псевдощілини.

Температурная зависимость псевдощели $\Delta^*(T)$ рассчитана для Bi2201 в рамках модели локальных пар [1, 2]. Эта модель основана на анализе избыточной проводимости, которая получается из экспериментов по удельному сопротивлению в высокотемпературных сверхпроводниках (ВТСП), и подразумевает наличие локальных пар, которые должны образовываться в ВТСП при температурах T, намного более высоких, чем T_c, формируя псевдощель. Для подтверждения этого вывода $\Delta^*(T)$ сравнивается с температурной зависимостью потерь спектрального веса $W(E_F)(T)$, измеряемого ARPES в том же самом образце Bi2201 [3]. Получено хорошее совпадение $\Delta^*(T)$ и $W(E_F)(T)$, подтверждающее, что локальные пары являются одной из наиболее вероятных причин образования псевдощели.

Key words: high-temperature superconductors, conductivity, spectral gap, spectral weight.

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1. INTRODUCTION

Up to now, the pseudogap (PG) observed mostly in underdoped (UD) cuprates remains the most intriguing and controversial property of high-temperature superconductors (HTSs). Below, any representative temperature $T^* >> T_c$, for reasons, which have still not been finally established, the density of quasi-particle states at the Fermi level starts to decrease [4–6]. That is why the phenomenon has been named a 'pseudogap'. Thus, below T^*, the HTSs goes into the PG regime, which is characterized by many unusual features [1, 7–10].

The paper addresses the problem of the PG, which is believed to appear most likely due to the ability of a part of conduction electrons to form paired fermions (so called local pairs) in HTSs at $T \leq T^*$ [13, 15]. The possibility of the long-lived pair states formation in HTSs in the PG temperature range was justified theoretically in [2, 18–20]. In accordance with proposed local pair (LP) model [1], at high temperatures ($T \leq T^*$), the local pairs are known to be in the form of strongly bound bosons (SBB), which satisfy the theory of Bose–Einstein condensation (BEC) [13, 15–20]. In accordance with this theory, the SBB are extremely short but very tightly bound pairs. As a result, the SBB cannot be destroyed by thermal fluctuations. Besides, they have to be local (*i.e.* not interacting with one another) objects since the pair size is much less than the distance between the pairs. The important point here is that the SBB may be formed only in the systems with low and reduced density of charge carriers n_f [15–19]. This condition is realized just in the UD cuprates [2, 7, 11, 13] and new FeAs-based superconductors [21, 22] resulting, in our opinion, in the PG formation. But, strictly speaking, the presence or absence of a PG in FeAs-based HTSs still remain controversial [21, 23].

It is worth to emphasize that the coherence length $\xi_{ab}(T) = \xi_{ab}(0)(T/T_c - 1)^{-1/2}$, which actually determines the pair size, is extremely short in HTSs [7, 8, 11–13, 15]. At the same time, the energy of a bound state of two fermions in the pair, $\varepsilon_b \propto \xi(T)^{-1}$, where $\xi(T)$ is the coherence length of the superconductor, is very large. This is an additional requirement for the formation of the SBB [15–18, 24]. Eventually, just the value of $\xi_{ab}(T)$ will determine the system behaviour [13, 15–17, 24]. On cooling, $\xi_{ab}(T)$ increases, whereas ε_b decreases. As a result, the local pairs have to change their state from the SBB into fluctuating Cooper pairs, which satisfy the BCS theory and behave in a good many ways like those of conventional superconductors [15, 18, 20, 24]. Thus, with decrease of temperature, there must be a transition from BEC to BCS state. Precisely how this happens is one of the challenging questions in strongly correlated electron systems. Nevertheless, the transition was predicted theoretically in [16, 17] and in more explicit form in Ref. [24], and approved in our experiments [13, 25]. This fact has to confirm our assumption as for existence of the local pairs in HTSs, which also has found a theoretical background in Ref. [2].

2. RESULTS AND DISCUSSION

Within the proposed LP model, the PG in YPrBCO films [27], FeAs-based superconductor $SmFeAsO_{0.85}$ with $T_c = 55$ K [22], and in slightly doped HoBCO single-crystals [28] is studied for the first time. But the basic results have been obtained from the analysis of the resistivity data for a set of four YBCO films with different oxygen concentrations [13, 25]. The films were fabricated at Max Plank Institute (MPI) in Stuttgart by pulse laser deposition method [29]. All samples were the well-structured *c*-oriented epitaxial YBCO films, as it was confirmed by studying the corresponding X-ray and Raman spectra. Using the LP model, the temperature dependences of Δ^* for every film were analysed. The main common feature of every found $\Delta^*(T)$ dependence is a maximum of $\Delta^*(T)$ observed at the same $T_{\max} \approx 130$ K. The important point here is that $\xi_{ab}(T_{\max})$ was found to be the same for every studied film, namely, $\xi_{ab}(T_{\max}) \approx 18$ Å [13, 25].

Above 130 K, $\xi_{ab}(T)$ is very small ($\xi_{ab}(T^*) \approx 13$ Å), whereas the coupling energy ε_b is very strong. It is just the condition for the formation of the SBB [15–18]. It was found [25] that at $T_{\max} < T < T^*$ every experimental $\Delta^*(T)$ curve can be fitted by the Babaev–Kleinert (BK) theory [19] in the BEC limit (low n_f), in which the SBB have to form [15–20]. This finding has to confirm the presence of the local pairs in the films, which are supposed to exist at high temperatures just in the form of SBB. As SBB do not interact with one another, the local pairs demonstrate no superconducting (SC) (collective) behaviour in this temperature interval. It has subsequently been shown to be consistent with the tunnelling experiments in Bi2223 [30], in which the SC tunnelling features are smeared out above $T_{\max}$. Thus, above $T_{\max}$, it is the so-called non-superconducting part of the PG.

On cooling, $\xi_{ab}(T)$ continues to increase, but $\varepsilon_b(T)$ becomes smaller.

Finally, at $T \le T_{\max} \approx 130$ K, where $\xi_{ab}(T) > 18$ Å, the local pairs begin to overlap and acquire the possibility to interact. Besides, they can be destroyed by the thermal fluctuations now, *i.e.*, transform into fluctuating Cooper pairs, as discussed above. The SC (collective) behaviour of the local pairs in this temperature region is distinctly seen in many experiments [27, 30–33]. Recently, the direct imaging of the local pair SC clusters persistence up to $\cong 140$ K in Bi2212 is reported [9]. Thus, below $T_{\max}$, it is the SC part of the PG. Moreover, we consider $\xi_{ab}(T_{\max}) \approx \approx 18$ Å to be the critical size of the local pair, at least in YBCO [13, 25]. Thus, the local pairs behave like SBB, when $\xi_{ab}(T) < 18$ Å, and transform into fluctuating Cooper pairs, when $\xi_{ab}(T) > 18$ Å below $T_{\max}$. The possibility of this BEC–BCS transition is the main assumption of the LP model.

Consequently, it can be concluded that the PG description in terms of local pairs gives a set of reasonable and self-consistent results. However, to justify the conclusion, it would be appropriate to have independent results of other research groups, who have measured straightforwardly the PG or any other related effects. But, for a long time, there was a lack of indispensable data.

Fortunately, analysis of the pseudogap in $(Bi,Pb)_2(Sr,La)_2CuO_{6+\delta}$ (Bi2201) single-crystals with various T_c's by means of ARPES spectra study was recently reported [3]. The study of Bi2201 allows avoid the complications resulting from the bilayer splitting and strong antinodal bosonic mode coupling inherent to Bi2212 and Bi2223 [32, 33]. Symmetrised energy distribution curves (EDCs) were found to demonstrate the opening of the pseudogap on cooling below T^*. It was shown that T^* obtained from the resistivity measurements agrees well with one determined from the ARPES data using a single spectral peak criterion [3].

Finally, from the ARPES experiments, information about temperature dependence of the loss of the spectral weight close to the Fermi level, $W(E_F)$, was derived [3]. The $W(E_F)$ versus T measured for optimally doped OP35K Bi2201 ($T_c = 35$ K, $T^* = 160$ K) turned out to be rather unexpected, as shown in Fig. 1, *a* taken from Ref. [3]. Above T^*, the $W(E_F)$ is nonlinear function of T. But, below T^*, over the temperature range from T^* to $T_{\rm pair} = 110 \pm 5$ K (Fig. 1, *a*), the $W(E_F)(T)$ decreases linearly that is considered as a characteristic behaviour of the 'proper' PG state [3]. However, no assumption as for physical nature of this linearity as well as for existence of the paired fermions in the PG region is proposed. Below $T_{\rm pair}$, the $W(E_F)$ *vs* T noticeably deviates down from the linearity (Fig. 1, *a*). The deviation suggests the onset of another state of the system, which likely arises from the pairing of electrons, since the $W(E_F)(T)$ associated with this state smoothly evolves through T_c (Fig. 1, *a*).

To compare results and justify our LP model, the ρ_{ab} *vs* T of the OP35K Bi2201 reported in the Supplementary to Ref. [3] was studied

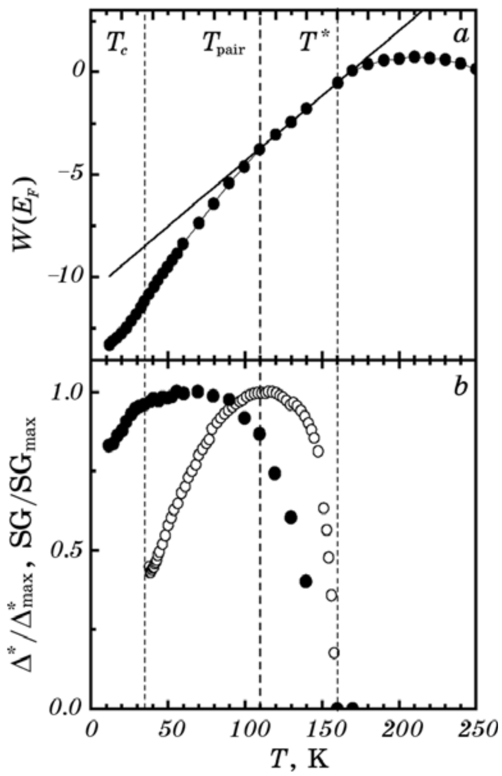

Fig. 1. Spectral weight $W(E_F)$ *vs* T (dots) for OP35K Bi2201 (*a*). Pseudogap $\Delta^*(T)/\Delta^*_{max}$ (circles) and spectral gap $SG(T)/SG_{max}$ (dots) for the same sample (*b*).

within the model. Resulting $\Delta^*(T) = \Delta^*_{max}$ is plotted in Fig. 1, *b* (circles). The $\Delta^*(T)$ was calculated, using equation

$$\Delta^* = T\ln\left[\frac{e^2 A_4\left(1-\dfrac{T}{T^*}\right)}{16\sigma'(T)\hbar\xi_c(0)\sqrt{2\varepsilon^*_{c0}\sinh(2\varepsilon/\varepsilon^*_{c0})}}\right] \tag{1}$$

proposed in Ref. [25] with respect to the LP model. Here, A_4 is a numerical factor, which has the meaning of the C-factor in the fluctuation conductivity theory [13]. All other parameters, including the coherence length along c-axis $\xi_c(0)$ and the theoretical parameter $\varepsilon_{c0}{}^*$, directly come from the experiment. To find A_4, we calculate $\sigma'(\varepsilon)$ and fit it to the experiment in the range of 3D Aslamazov–Larkin (AL) fluctuations near T_c [13, 25] where $\ln\sigma'(\ln\varepsilon)$ is a linear function of the reduced temperature, $\varepsilon = (T - T_c{}^{mf})/T_c{}^{mf}$, with a slope $\lambda = -1/2$. $T_c{}^{mf}$ is a mean-field critical temperature [26]. Equation (1) was solved with the following reasonable set of parameters: $T_c = 35$ K, $T_c^{mf} = 36.9$ K, $T^* = 160$ K, $\xi_c(0) \approx 2.0$ Å, $\varepsilon_{c0}{}^* = 0.89$, and $A_4 = 59$. The $\sigma'(T)$ is the experimentally measured excess conductivity derived from the resistivity data [13].

As expected, the shape of the $\Delta^*(T)$ curve, with a maximum at $T_{\max} \approx \approx 100$ K (Fig. 1, *b*), is similar to that found for YBCO films [13, 25]. Moreover, the maximum of $\Delta^*(T) = \Delta^*_{\max}$ at $T_{\max}$ (Fig. 1, *b*) coincides with T_{pair} (Fig. 1, *a*) that seems to be reasonable. In fact, in accordance with our logic, $T_{\max}$ is just the temperature, which divides the PG region on SC and non-SC parts depending on the local pair state, as discussed above. Let us remind that above $T_{\max}$ the local pairs are expected to be in the form of SBB. Most likely just the specific properties of the SBB cause the linear $W(E_F)(T)$ in this temperature range (Fig. 1, *a*). The two facts are believed to confirm the conclusion. First, when SBB disappear above T^*, the linearity disappears too. Second, below $T_{\max}$, or below T_{pair} in terms of Ref. [3], the SBB have to transform into fluctuating Cooper pairs giving rise to the SC (collective) properties of the system. This argumentation coincides with the conclusion of Ref. [3] as for SC part of the pseudogap below T_{pair}. As SBB are now also absent, the linearity of $W(E_F)(T)$ disappears too. Thus, we consider the $\Delta^*(T)$ calculated within the LP model (Fig. 1, *b*) to be in a good agreement with the temperature dependence of the loss of the spectral weight $W(E_F)$ (Fig. 1, *a*) obtained from the ARPES experiments performed on the same sample. In this way, the results of ARPES experiments reported in Ref. [3] are believed to confirm our conclusion as for existence of the local pairs in HTSs, at least in Bi2201 compounds.

The normalized spectral gap (SG(T)) (dots), which is equal to the energy of the spectral peaks of EDCs measured by ARPES, is also plotted in Fig. 1, *b* [3]. In this case, it is important that SG(T) smoothly evolves through both T_{pair} and T_c. This fact is believed to confirm the local pair presence above T_{pair} assumed in the LP model. But, there are at least two differences between the curves shown in Fig. 1, *b*. First, there is no direct correlation between the SG(T) and the $W(E_F)(T)$ (Fig. 1, *a* and *b*). Why the maximum of SG(T) is shifted toward low temperatures compared to T_{pair} is not known now. The second difference is the absolute value of the SG compared to the PG. The spectral gap has $\text{SG}_{\max} \approx 40$ meV and $\text{SG}(T_c) \approx 38$ meV [3]. It gives $2\text{SG}(T_c)/(k_BT_c) \approx 26$, which is apparently too high. The PG values are $\Delta^*_{\max} \approx 16.5$ meV and $\Delta^*(T_c) \approx 6.96$ meV, respectively. It gives $2\Delta^*(T_c)/(k_BT_c) \approx 6.4$, which is a common value for the Bi compounds [34] with respect to relatively low T_c in considered case. Thus, no direct coincidence between the SG and PG is found.

3. CONCLUSION

We present a detailed consideration of the LP model developed to study the PG in HTSs. In accordance with the model, the local pairs have to be the most likely candidate for the PG formation. At high temperatures ($T_{pair} < T \leq T^*$), we believe that the local pairs should have the form of SBB, which satisfy the BEC theory (non-SC part of a PG). Below T_{pair}, the local pairs have to change their state from the SBB into fluctuating Cooper pairs, which satisfy the BCS theory (SC part of a PG). Thus, with decrease of temperature, there must be a transition from BEC to BCS state [13, 15–18, 25]. The possibility of such a transition is considered to be one of the basic physical principles of the high-T_c superconductivity. The transition was predicted theoretically in Refs [16, 17, 24] and corroborated by our experiments.

A key test for our consideration is the comparison of $\Delta^*(T)$ calculated within the LP model with the temperature dependence of the loss of the spectral weight close to the Fermi level $W(E_F)(T)$ measured by ARPES for the same sample [3]. Resulting $\Delta^*(T)$ is found to be in a good agreement with the $W(E_F)(T)$ obtained for OP35K Bi2201 (Fig. 1). It enables us to explain reasonably the $W(E_F)(T)$ both above and below T_{pair} in terms of local pairs. The obtained results are also in agreement with the conclusions of Refs [9, 32, 33] as for SC and non-SC parts of the PG in Bi systems. Besides, formation of local pairs is also believed to explain the rise of the polar Kerr effect and response of the time-resolved reflectivity both observed for Bi systems just below T^* [32]. While, the Nernst effect [9], which is likely caused by the SC properties of the local pairs, is observed only below T_{pair}, or below T_{max} in terms of our model.

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