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Possibility of local pair existence in optimally doped $SmFeAsO_{1-x}$ in pseudogap regime

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We report the analysis of pseudogap Δ^* derived from resistivity experiments in FeAs-based superconductor $SmFeAsO_{0.85}$, having a critical temperature $T_c = 55$ K. Rather specific dependence $\Delta^*(T)$ with two representative temperatures followed by a minimum at about 120 K was observed. Below $T_s \approx 147$ K, corresponding to the structural transition in SmFeAsO, $\Delta^*(T)$ decreases linearly down to the temperature $T_{AFM} \approx 133$ K. This last peculiarity can likely be attributed to the antiferromagnetic (AFM) ordering of Fe spins. It is believed that the found behavior can be explained in terms of Machida, Nokura, and Matsubara theory developed for the AFM superconductors.

PACS: **74.25.–q** Properties of superconductors;
74.40.–n Fluctuation phenomena;
74.78.Fk Multilayers, superlattices, heterostructures;
74.70.–b Superconducting materials other than cuprates.

Keywords: high-T_c superconductivity, FeAs-based superconductors, pseudogap, local pairs.

1. Introduction

Despite of considerable efforts devoted to the study of superconducting pairing mechanism in the new FeAs-based high-T_c superconductors (HTS's) its physical nature still remains uncertain. However, there is growing evidence that it is of presumably magnetic type and all members of the iron arsenide $RFeAsO_{1-x}F_x$ family, where R is a lanthanide, are characterized by the long-range (nonlocal) magnetic correlations [1]. It is well known that upon electron or hole doping with F substitution at the O site [2–4], or with oxygen vacancies [5,6] all properties of parent RFeAsO compounds drastically change and evident antiferromagnetic (AFM) order has to disappear [7–9]. However, the comparison with the present $SmFeAsO_{1-x}F_x$ superconductors points towards an important role of low-energy spin fluctuations that emerge on doping away from an antiferromagnetic state which is of spin-density wave (SDW) type [10,11]. Thus, below 150 K the AFM fluctuations, being likely of spin wave type, are believed to affect noticeably the properties of $RFeAsO_{1-x}F_x$ systems [1,10,11]. As shown by many studies [10–13] the static magnetism persists well into the superconducting regime of ferropnictides. Besides, it was recently shown theoretically that antiferromagnetism and superconductivity can coexist in these materials only if Cooper pairs form an unconventional, sign-changing state [1,13,14].

In $SmFeAsO_{1-x}F_x$ highly disordered but static magnetism and superconductivity both are found to exist in the wide range of doping and prominent low-energy spin fluctuations are observed up to the highest achievable doping le-

vels where T_c is maximal [10]. The analysis of the muon asymmetry [11] demonstrates that the coexistence of magnetism and superconductivity must be nanoscopic, i.e., the two phases must be finely permeated over a typical length scale of few nm. Recently reported results on peculiar magnetic properties of $LaFeAsO_{0.85}F_{0.1}$ at $T_{AFM} \approx 135$ K [15] are likely due to this two-phase structure.

The relation between the SDW and superconducting order is a central topic in the current research on the FeAs-based high-T_c superconductors. However, a nature of the complex interplay between magnetism and superconductivity in FeAs-based HTS's is still rather controversial. As a result, extremely complicated phase diagrams for different FeAs-based high-T_c systems [4,12–14] and especially for $SmFeAsO_{1-x}F_x$ [3,16–19] are reported. For all these HTS's adequately wide temperature region is found in which the superconductivity coexists with SDW regime. For $SmFeAsO_{1-x}F_x$ in a zero magnetic field this temperature region ranges from approximately $x = 0.1$ up to $x = 0.18$ [3,10]. As a result, sufficiently peculiar normal state behavior of the system upon T diminution is expected in this case [3,12–14] when x is, let say, 0.15, as it is in our sample [20].

To shed more light on the problem, in our previous study [20] the fluctuation conductivity (FLC) and $\Delta^*(T)$, referred to as a pseudogap (PG), derived from resistivity measurements on $SmFeAsO_{0.85}$ polycrystal with $T_c \approx 55$ K were analyzed. As expected, the temperature behavior of FLC was found to be rather similar to that observed for YBCO films with nearly optimal oxygen doping [21], whereas $\Delta^*(T)$ has demonstrated several peculiar features [20]. In this contribution we venture to explain found $\Delta^*(T)$ peculiarities in terms of Machida–Nokura–Matsubara (MNM) [22] theory developed for AFM superconductors as well as to compare results with Babaev–Kleinert (BK) theory [23] considering superconductors with different charge carrier density n_f.

2. Results and discussion

To begin with the pseudogap analysis, at first the FLC in $SmFeAsO_{0.85}$ polycrystal with $T_c \approx 55$ K has been thoroughly analyzed [20]. The FLC is a part of a common excess conductivity $\sigma'(T) = \sigma(T) - \sigma_N(T)$ which is usually written as

$$\sigma'(T) = [\rho_N(T) - \rho(T)] / [\rho_N(T)\rho(T)] . \qquad (1)$$

Here $\rho = \rho_{xx}(T)$ is the measured resistivity, and $\rho_N(T) = 1/\sigma_N(T) = aT + b$ determines the resistivity of a sample in the normal state extrapolated towards low temperatures. At the PG temperature $T^* = (175 \pm 1)$ K the longitudinal resistivity $\rho_{xx}(T)$ demonstrates a pronounced downturn from its linear dependence at higher temperatures, thus resulting in the appearance of the excess conductivity.

The excess conductivity $\sigma'(T)$ as a function of the reduced temperature which is defined as $\varepsilon = \ln(T / T_c^{mf}) \approx \approx (T - T_c^{mf}) / T_c^{mf}$ is plotted in Figs. 3 and 4 (see Ref. 20) in a double logarithmic scale. Here $T_c^{mf} \approx 57$ K is the mean-field critical temperature [21]. It was shown that the conventional fluctuation theories by Aslamasov–Larkin (AL) [24] and Hikami–Larkin (HL) [25] well fit the experimental data in the temperature region relatively close to T_c. The result suggests the interband pairing mechanism as dominant one in $SmFeAsO_{0.85}$, as it was theoretically discussed in Ref. 26. It should be also noted that in the HL theory only the Maki–Thompson (MT) fluctuation contribution was used [20].

The MT–AL (2D–3D) crossover is distinctly seen in the $\sigma'(T)$ dependence as T approaches T_c [20]. Taking into account the crossover temperature $T_0 \approx 58.5$ K and the distance between As layers in conducting As–Fe–As planes $d \approx 3.05$ Å, the coherence length along the c axis $\xi_c(T) = d\varepsilon_{c0}^{1/2} = (1.4 \pm 0.005)$ Å was determined [20]. The coherence length $\xi_c(T)$ is an important parameter of the PG analysis [21].

2.1. Pseudogap analysis

To analyse PG we assume that the excess conductivity $\sigma'(T)$ at the temperatures $T_c^{mf} << T << T^*$ arises as a result of the paired fermions organization in the form of the local pairs (strongly bound bosons (SBB)) [21,27], which satisfy the Bose–Einstein condensation (BEC) theory [28–32]. Upon temperature decrease the local pairs transform into fluctuating Cooper pairs as T approaches T_c^{mf} [21]. The conventional fluctuation theories describe experiment only up to $T_{c0} \approx 69$ K [20]. Unfortunately, there is still no fundamental theory to describe the experimental curve in the whole PG region. Nevertheless, the equation for $\sigma'(\varepsilon)$ has been proposed in Ref. 21 as

$$\sigma'(\varepsilon) = \frac{A_4 e^2 [1 - (T/T^*)] \exp(-\Delta^*/T)}{16\hbar\xi_c(0)\sqrt{2\varepsilon_{c0}^* \sinh(2\varepsilon/\varepsilon_{c0}^*)}}, \qquad (2)$$

where A_4 is a numerical factor which has the same meaning as a C-factor in the FLC theory. In this case the fact is important that Eq. (2) contains PG in an explicit form. Besides, the dynamics of pair-creation and pair-breaking below T^* has been taken into account in order to correctly describe experiment [21]. To find coefficient A_4 the curve, calculated with Eq. (2), has to fit the $\sigma'(\varepsilon)$ data in the region of 3D AL fluctuations near T_c [20,21]. All other parameters in Eq. (2) directly come from resistivity and FLC analysis. As it was shown in Ref. 20 the curve constructed using Eq. (2) with parameters $\varepsilon_{c0}^* = 0.616$, $\xi_c(0) = 1.405$ Å, $T_c^{mf} = 57$ K, $T^* = 175$ K, $A_4 = 1.98$ and $\Delta^*(T_c)/k_B = 160$ K describes the experimental data well in the whole temperature interval of interest.

Solving Eq. (2) for Δ^* we obtain [21]

$$\Delta^*(T) = T \ln \frac{A_4 e^2 [1-(T/T^*)]}{\sigma'(T)(16\hbar\xi_c(0)\sqrt{2\varepsilon^*_{c0}\sinh(2\varepsilon/\varepsilon^*_{c0})}}. \quad (3)$$

Here $\sigma'(T)$ is the experimentally measured values of the excess conductivity in the whole temperature range from T^* down to T_c^{mf}. All other parameters are the same as designated above. As all the parameters, including $\sigma'(T)$, are determined from the experiment, $\Delta^*(T)$ can be calculated according to Eq. (3) and plotted now as shown in Fig. 5 of Ref. 20.

Unfortunately, the value of $\Delta^*(T_c)$ and in turn the ratio $2\Delta^*(T_c)/k_BT_c$ in the FeAs-based HTS's remain uncertain. At present it is believed that $SmFeAsO_{1-x}$ has two superconducting gaps, i.e., $\Delta_1(0) \approx 6$ meV (~ 70 K) and $\Delta_2(0) \approx (14\ldots21)$ meV [~ (160…240) K] [33]. Besides we think that $\Delta^*(T_c) \sim \Delta(0)$ [21,34]. That is why, four curves are finally plotted in Fig. 5 (Ref. 20) with $\Delta^*(T_c)/k_B =$ = 160 K ($2\Delta^*(T_c)/k_BT_c \sim 5.82$ close to strongly coupled limit), 140 K ($2\Delta^*(T_c)/k_BT_c \sim 5.0$), 120 K ($2\Delta^*(T_c)/k_BT_c \sim 4.36$) and 100 K ($2\Delta^*(T_c)/k_BT_c \sim 3.63$ close to weakly coupled BCS limit) from top to bottom, respectively. Naturally, different values of coefficients A_4 correspond to each curve whereas the other parameters mentioned above remain unchangeable.

It was found [20] that at $T \le T^*$ the $\Delta^*(T)$ starts to increase rapidly as it was observed for YBCO films with different oxygen concentration [21]. However, an unexpected sharp decrease of $\Delta^*(T)$ at $T_s \approx 147$ K was revealed as clearly illustrate Fig. 1 as well as Fig. 5 in Ref. 20. Usually T_s is treated as a temperature at which a structural tetragonal–orthorhombic transition occurs in SmFeAsO. In the undoped FeAs compounds it is also expected to be a transition to SDW ordering regime [7–9]. Below T_s the pseudogap $\Delta^*(T)$ drops linearly down to $T_{AFM} \approx 133$ K which is attributed to the AFM ordering of the Fe spins in a parent SmFeAsO [7,35]. Below T_{AFM} the slop of the $\Delta^*(T)$ curves apparently depends on the $\Delta^*(T_c)$ [20].

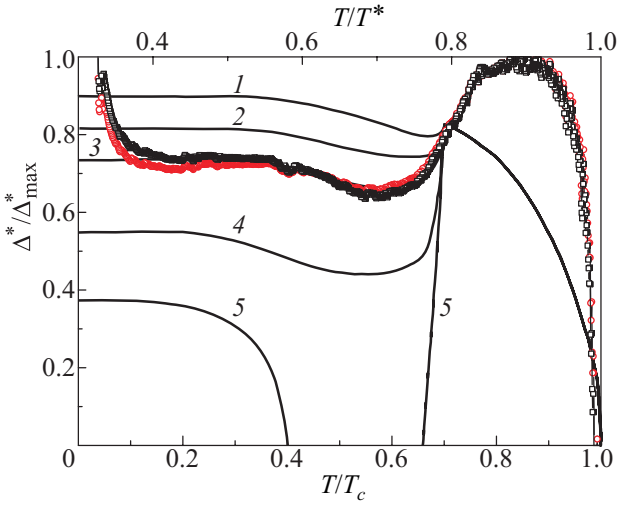

Fig. 1. $\Delta^*(T)/\Delta^*_{max}$ in $SmFeAsO_{0.85}$: $\Delta^*(T_c)/k_B =$ 130 K (□); 135 K (○). Solid curves correspond to MNM theory with different $\alpha \sim 1/[\breve{g}N(0)]$: $\alpha = 0.1$ (*1*), 0.2 (*2*), 0.3 (*3*), 0.6 (*4*), 1.0 (*5*); $T_N/T_c = 0.7$ [22].

Found $\Delta^*(T)$ behavior is believed to be explained in terms of the MNM theory (Fig. 1) [22] developed for the AFM superconductors, in which the AFM ordering with a wave vector Q may coexist with the superconductivity. In the MNM theory the effect of the AFM molecular field $h_Q(T)$ ($|h_Q| << \varepsilon_F$) on the Cooper pairing was studied. It was shown that below T_N the BCS coupling parameter $\Delta(T)$ is reduced by a factor $[1-\text{const}\cdot|h_Q(T)|/\varepsilon_F]$ due to the formation of energy gaps of SDW on the Fermi surface along Q. As a result, the effective attractive interaction $\breve{g}N(0)$, or, equivalently, the density of states at the Fermi energy ε_F, is diminished by the periodic molecular field, that is,

$$\breve{g}N(0) = gN(0)[1-\alpha m(T)]. \quad (4)$$

Here $m(T)$ is the normalized sublattice magnetization of the antiferromagnetic state and α is a changeable parameter of the theory. Between T_c and T_N ($T_c > T_N$ is assumed) the order parameter is that of the BCS theory. Since below T_N the magnetization $m(T)$ becomes nonvanishing, $\breve{g}N(0)$ is weakened that results in turn in a sudden drop of $\Delta(T)$ immediately below T_N. As $m(T)$ saturates at lower temperatures, $\Delta(T)$ gradually recovers its value with increasing the superconducting condensation energy (Fig. 1, solid curves). This additional magnetization $m(T)$ was also shown to explain the anomaly in the upper critical field H_{c2} just below T_N observed in studying of RMo_6S_8 (R = Gd, Tb, and Dy) [22]. However, predicted by the theory decrease of $\Delta(T)$ at $T \le T_N$, was only recently observed in AFM superconductor $ErNi_2B_2C$ with $T_c \approx 11$ K and $T_N \approx 6$ K, below which the SDW ordering is believed to occur in the system [36]. The result evidently supports the prediction of the MNM theory.

Our results are found to be in a qualitatively agreement with the MNM theory as shown in Fig. 1, where the data for $\Delta^*(T_c)/k_B =$ 130 and 135 K are compared with the MNM theory. The curves are scaled at $T/T_c = 0.7$ and demonstrate rather good agreement with the theory below $T/T_c = 0.7$. The upper scale is T/T^*. Both shown $\Delta^*(T)$ dependencies suggest the issue that just $\Delta^*(T_c) = 133$ K would provide the best fit with the theory. Above $T/T_c = 0.7$ the data evidently deviate from the BCS theory. It seems to be reasonable seeing $SmFeAsO_{0.15}$, as well as any ferropnictide, to be not a BCS superconductor.

It is important to emphasize that in our case we observe the particularities of $\Delta^*(T)$ in the PG state, i.e., well above T_c, but just at T_s, below which the SDW ordering in parent SmFeAsO should occur. It seems to be somehow surprising as no SDW ordering in optimally doped

$SmFeAsO_{0.15}$ is expected. On the other hand, the AFM fluctuations (low-energy spin fluctuations) should exist in the system as mentioned above. At the singular temperature T_s these fluctuations are believed to enhance the AFM in the system likely in form of SDW. After that, in accordance with the MNM theory scenario, the SDW has to suppress the order parameter of the local pairs as shown by our results. Thus, the results suggest the existence of paired fermions in the PG region, which order parameter is apparently suppressed by the AFM fluctuations at $T \le T_s$. These fermions have most likely to exist in the form of the local pairs (SBB) [21].

To justify the issue the relation $\Delta^*(T)/\Delta^*_{\max}$ as a function of T/T^* (T/T_c in the case of the theory) is plotted in Fig. 2. The dots and circles represent the studied $SmFeAsO_{0.85}$ with $\Delta^*(T_c)/k_B = 160$ K and the data for YBCO film with $T_c = 87.4$ K, respectively [21]. The solid and dashed curves display the results of the Babaev–Kleinert (BK) theory [23] developed for the superconducting systems with different charge carrier density n_f. For the different curves the different theoretical parameter $x_0 = \mu/\Delta(0)$ is used, where μ is a chemical potential. Curve *1*, with $x_0 = +10$, gives the BCS limit. For curve *2* the value $x_0 = -2$ is taken, for curve *3* parameter $x_0 = -5$. Finally curve *4* with $x_0 = -10$ represents the BEC limit, which corresponds to the systems with low n_f in which the SBB must exist [28–32]. As well as in YBCO film the $\Delta^*(T)/\Delta^*_{\max}$ in $SmFeAsO_{0.85}$ evidently corresponds to the BEC limit suggesting the local pairs presence in the FeAs-based superconductor. Below $\Delta^*(T)/\Delta^*_{\max} \approx 0.4$ both experimental curves demonstrate the very similar slope suggesting the BEC–BCS transition from local pairs to the fluctuating Cooper pairs found for the YBCO films with different oxygen concentration as temperature approaches T_c [21]. But, naturally, no drop of $\Delta^*(T)$ is observed for the YBCO film (Fig. 2) as no antiferromagnetism is expected in this case. This fact accentuates the AFM nature of the $\Delta^*(T)$ linear reduction below T_s in $SmFeAsO_{0.85}$ found in our experiment.

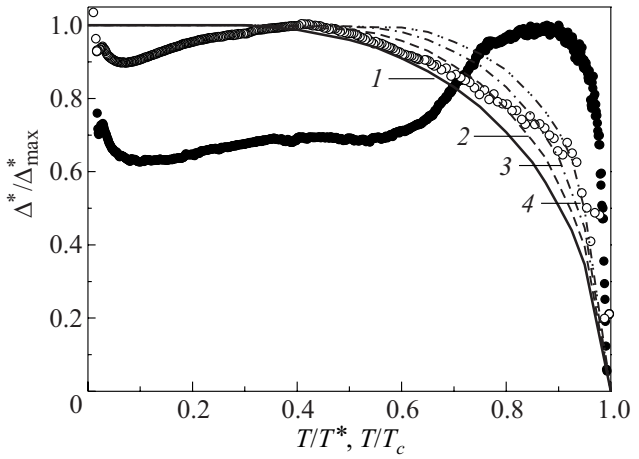

Fig. 2. $\Delta^*(T)/\Delta^*_{\max}$ in $SmFeAsO_{0.85}$ with $\Delta^*(T_c)/k_B = 160$ K (●) and in YBCO film with $T_c = 87.4$ K (○) [13] as a function of T/T^* (T/T_c in the case of the theory). Curves *1–4* correspond to the BK theory [29] with different $x_0 = \mu/\Delta(0)$: *1* — $x_0 = 10$ (BCS limit); *2* — $x_0 = -2$; *3* — $x_0 = -5$; *4* — $x_0 = -10$ (BEC limit).

3. Conclusion

Analysis of the pseudogap $\Delta^*(T)$ in the FeAs-based superconductor $SmFeAsO_{0.85}$ with $T_c = 55$ K based on the systematic study of the excess conductivity $\sigma'(T)$ [20] has been performed. Rather specific temperature dependence of the $\Delta^*(T)$ was found (Figs. 1 and 2). The more striking result is the pronounced decrease of $\Delta^*(T)$ below $T_s \approx 147$ K. As a rule, T_s is treated as a temperature at which a structural tetragonal–orthorhombic transition occurs in SmFeAsO [7–9]. In accordance with recent results [3,16–18] it is expected to be a transition to SDW ordering regime in the undoped Fe–As compounds too. Below T_s the pseudogap $\Delta^*(T)$ is linear down to $T_{AFM} \sim 133$ K, which is attributed to the antiferromagnetic ordering of the Fe spins in SmFeAsO [6–9]. Note that no such peculiarities of $\Delta(T)$ are observed in the superconducting state of $SmFeAsO_{1-x}F_x$ [37] as no pronounced antiferromagnetism in SC state of the FeAs-based compounds is expected [1–9].

Found $\Delta^*(T)$ reduction can be qualitatively explained in the framework of the MNM theory [22], which predicts the suppression of the superconducting order parameter in AFM superconductors. But we have to emphasize that we observe the $\Delta^*(T)$ reduction in the PG state, i.e., well above T_c. The finding suggests the presence of paired fermions in $SmFeAsO_{0.85}$ in the PG region, the order parameter of which $\Delta^*(T)$ is apparently suppressed by the enhanced AFM fluctuations (spin waves) in accordance with the MNM theory. At the same time no unusual drop of $\Delta^*(T)$ is observed for the YBCO film (Fig. 2) as no antiferromagnetism is expected in this case. This fact is to justify the AFM nature of the found $\Delta^*(T)$ reduction in $SmFeAsO_{0.85}$.

As it is clearly seen in Fig. 2, the ratio $\Delta^*(T)/\Delta^*_{\max}$ in $SmFeAsO_{0.85}$ at high temperatures evidently corresponds to the BEC limit. It seems to be reasonable as in FeAs-based compounds n_f is found to be at least an order of magnitude less than in conventional metals [17]. Thus, we may conclude that paired fermions should exist in the PG temperature region of the FeAs-based superconductor $SmFeAsO_{0.85}$. Most likely they should appear in the form of local pairs (strongly bound bosons), as it was found for the YBCO films with different oxygen concentration [21]. Thus, the local pair presence seems to be the common feature of the PG formation in both cuprates and FeAs-based HTS's.

It has to be emphasized that recently reported phase diagrams [3,16–19] apparently take into account a complexity of magnetic subsystem in $SmFeAsO_{1-x}F_x$ and are in much more better agreement with our experimental results. But it has also to be noted that we study the $SmFeAsO_{1-x}$

system whereas the phase diagrams are mainly reported for the $SmFeAsO_{1-x}F_x$ compounds. Is there any substantial difference between the both compounds has yet to be determined. Evidently, more experimental results are required to clarify the question.

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