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Multiple bands – a key to high-temperature superconductivity in iron arsenides?

E. Z. Kuchinskii[1)], *M. V. Sadovskii*[1)]

Institute for Electrophysics, Ural Division RAS, 620016 Ekaterinburg, Russia

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In the framework of four-band model of superconductivity in iron arsenides proposed by Barzykin and Gor'kov we analyze the gap ratios on hole – like and electron – like Fermi – surface cylinders. It is shown that experimentally observed (ARPES) gap ratios can be obtained only within rather strict limits on the values of pairing coupling constants. The difference of T_c values in 1111 and 122 systems is reasonably explained by the relative values of partial densities of states. The multiple bands electronic structure of these systems leads to a significant enhancement of effective pairing coupling constant determining T_c, so that high enough T_c values can be achieved even for the case of rather small intraband and interband pairing interactions.

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The discovery of high-temperature superconductivity in layered FeAs compounds stimulated active experimental and theoretical studies of these new superconductors [1]. The main anomaly of these systems is their multiple bands nature. Electronic structure in a narrow enough energy interval around the Fermi level is formed almost only from the d – states of Fe. In fact, electronic spectrum of iron arsenides was calculated in a number of papers [2 – 6]. The Fermi surface consists of several hole – like and electron – like cylinders and on each of these its "own" superconducting gap can be formed. In the energy interval relevant to superconductivity electronic spectrum is especially simple [7 – 9]. It was used by Barzykin and Gor'kov to formulate a simple (analytic) model of superconducting state of new superconductors [10].

Schematically, the simplified electronic spectrum and Fermi surfaces of these systems are shown in Fig.1 [10]. There are two hole – like Fermi surface cylinders surrounding the Γ point and two electronic pockets around X and Y points in extended Brillouin zone.

Let Δ_i be a superconducting order – parameter (gap) on the i-th sheet of the Fermi surface. The value of Δ_i is determined by self – consistency equation for the anomalous Gor'kov Green's function.

Pairing BCS-like interaction can be represented by a matrix:

$$V = \begin{pmatrix} u & w & t & t \\ w & u' & t & t \\ t & t & \lambda & \mu \\ t & t & \mu & \lambda \end{pmatrix} \quad (1)$$

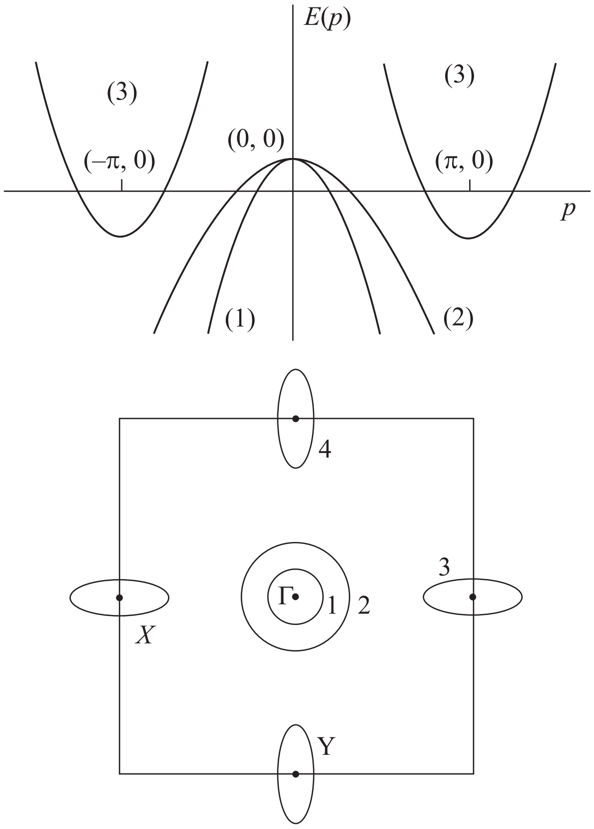

Fig.1. Schematic electronic spectrum and Fermi surfaces of FeAs superconductor in the extended band picture. There are two hole-like cylinders around point Γ, while electron-like cylinders are around X (Y) points [10]

where matrix elements $V^{i,j}$ define intraband and interband pairing coupling constants. For example, $\lambda = V^{eX,eX} = V^{eY,eY}$ determines pairing interactions on the same electronic pocket at point X or Y, $\mu = V^{eX,eY}$

[1)]e-mail: kuchinsk@iep.uran.ru; sadovski@iep.uran.ru connects electrons of different pockets at these points, $u = V^{h1,h1}$, $u' = V^{h2,h2}$ and $w = V^{h1,h2}$ characterize BCS interactions within two hole – like pockets – the small one ($h1$) and the large one ($h2$), as well as between these pockets, while $t = V^{h,eX} = V^{h,eY}$ couple electrons at points X and Γ. In Ref. [10] it was assumed that $u = u' = w$. This assumption seems to be too strong and below we analyze the general case.

Superconducting critical temperature T_c is determined by an effective pairing coupling constant g_{eff}:

$$T_c = \frac{2\gamma\omega_c}{\pi} e^{-1/g_{\text{eff}}}, \tag{2}$$

where ω_c is the usual cut – off frequency in Cooper channel (assumed to be the same for all types of couplings under consideration – a simplification!), while g_{eff} in this model is defined by the solution of the system of linearized gap equations:

$$g_{\text{eff}}\Delta_i = \sum_j g_{ij}\Delta_j, \tag{3}$$

where

$$g_{ij} \equiv -V^{i,j}\nu_j, \quad g_{\text{eff}}^{-1} = \ln\frac{2\gamma}{\pi}\frac{\omega_c}{T_c}. \tag{4}$$

The matrix of dimensionless coupling constants g_{ij} is determined by matrix elements of (1) and partial densities of states on different Fermi surface cylinders – ν_j is density of states per single spin projection on the j-th cylinder.

From symmetry it is clear that $\nu_3 = \nu_4$ and the system (3) possesses solutions of two types [10]:

1) solution corresponding to $d_{x^2-y^2}$ symmetry, when gaps on different pockets at points X and Y differ by sign, while gaps on hole-like pockets are just zero:

$$\Delta_1 = \Delta_2 = 0, \quad \Delta_3 = -\Delta_4 = \Delta, \tag{5}$$

and

$$g_{\text{eff}} = (\mu - \lambda)\nu_3. \tag{6}$$

2)solutions corresponding to the so called $s^{\pm}$ pairing [3], for which gaps on the cylinders at points X and Y are equal to each other: $\Delta_3 = \Delta_4$, while gaps on Fermi surfaces surrounding the point Γ are of different sign in case of repulsive interaction between electron-like and hole-like pockets ($t > 0$), and of the same sign for the case of $t < 0$.

As in this case we have $\Delta_3 = \Delta_4$ and $\nu_3 = \nu_4$, two equations in (3) just coincide and instead of (1), (4) we are dealing with 3×3 matrix of coupling constants of the following form:

$$-\hat{g} = \begin{pmatrix} u\nu_1 & w\nu_2 & 2t\nu_3 \\ w\nu_1 & u'\nu_2 & 2t\nu_3 \\ t\nu_1 & t\nu_2 & 2\bar{\lambda}\nu_3 \end{pmatrix}, \tag{7}$$

where $\bar{\lambda} = (\lambda + \mu)/2$ and (3) reduces to the standard problem of finding eigenvalues and eigenvectors for the matrix of dimensionless couplings g_{ij} (7), which has three solutions, determined by cubic secular equation:

$$\text{Det}(g_{ij} - g_{eff}\delta_{ij}) = 0. \tag{8}$$

Physical solution corresponds to a maximal positive value of g_{eff}, which determines the highest value of T_c.

Under the simple assumption of Ref. [10], when $u = u' = w$, situation simplifies further, as in (3) only two independent equations remain, so that we have 2×2 matrix of coupling constants and (8) reduces to a quadratic equation. Then we easily obtain [10]:

$$\Delta_1 = \Delta_2 = \kappa\Delta, \quad \Delta_3 = \Delta_4 = \Delta, \tag{9}$$

where $\kappa^{-1} = -(g_{\text{eff}} + u(\nu_1 + \nu_2))/t\nu_3$, and maximal effective pairing constant is given by:

$$2g_{\text{eff}} = -u(\nu_1 + \nu_2) - 2\bar{\lambda}\nu_3 + \\ + \sqrt{(u(\nu_1 + \nu_2) - 2\bar{\lambda}\nu_3)^2 + 8t^2\nu_3(\nu_1 + \nu_2)}. \tag{10}$$

Possibility of $s^{\pm}$-pairing in FeAs compounds was first noted in Ref. [3]. This kind of solution qualitatively agrees with ARPES data of Refs. [11–13], except the result $\Delta_1 = \Delta_2$ (9), which contradicts the established experimental fact – the gap on the small hole-like cylinder Δ_1 is approximately twice as large as the gap Δ_2 on the large cylinder. In fact, this contradiction is basically due to an unnecessary limitation to the case of $u = u' = w$ used in Ref. [10].

The system of linearized gap equations determines their ratios on different sheets of the Fermi surface for temperatures $T \to T_c$. In general case, the temperature dependence of gaps is determined by the generalized BCS equations:

$$\Delta_i = \sum_j g_{ij}\Delta_j \int_0^{\omega_c} d\xi \frac{\text{th}\dfrac{\sqrt{\xi^2 + \Delta_j^2}}{2T}}{\sqrt{\xi^2 + \Delta_j^2}}. \tag{11}$$

For $T \to 0$ these equations take the form:

$$\Delta_i = \sum_j g_{ij}\Delta_j F\left(\frac{\Delta_j}{\omega_c}\right), \tag{12}$$

where we have introduced $F(x) = \ln\left(\frac{1+\sqrt{1+x^2}}{|x|}\right)$.

Below we present the results of numerical studies of Eqs. (3) and (12) for typical values of parameters (couplings).

Let us denote the pairing coupling constant on a small hole-like cylinder as $g = g_{11}$. In the following we take $g = 0.2$, which allows us to remain within the limits of weak coupling approximation.

The ratio of partial densities of states for different Fermi surface cylinders in quasi-two-dimensional case can be approximated by effective mass ratio on the same cylinders. These can be estimated from the data for electronic dispersions in symmetric directions in the Brillouin zone, obtained in LDA calculations [7–9]. For REOFeAs series (RE=La,Ce,Nd,Pr,Sm...) (1111) and for $BaFe_2As_2$ (122) from these data we get:

$$\begin{array}{lll} \dfrac{\nu_2}{\nu_1} \approx 1.18, & \dfrac{\nu_3}{\nu_1} \approx 0.64, & \text{for 1111}, \\ \dfrac{\nu_2}{\nu_1} \approx 1.26, & \dfrac{\nu_3}{\nu_1} \approx 0.34, & \text{for 122}. \end{array} \tag{13}$$

We suppose that pairing interactions on hole-like cylinders and between them, as well as on electron-like cylinders and between them, are most probably determined by electron-phonon interaction, the relevance of which is clearly demonstrated by rather strong isotope effect, observed in Ref. [14]. At the same time, interband pairing interaction between hole-like and electron-like cylinders is probably due to antiferromagnetic fluctuations and is repulsive ($t > 0$). It should be noted that parameter t from coupling constants matrix (7) enters Eq. (8), determining $g_{\rm eff}$, only via t^2, i.e. independent of sign. Thus its sign does not change the value of an effective pairing coupling constant and that of T_c. Repulsion between quasiparticles on hole-like and electron-like cylinders does not suppress, but actually enhances superconductivity leading to the increase of $g_{\rm eff}$. Also the sign change of t does not change the absolute values of gaps on different cylinders, though the repulsion between electron-like and hole-like cylinders ($t > 0$) leads to different signs of gaps at these cylinders, while for the case of $t < 0$ both gaps acquire the same sign.

Despite rather large number of free parameters of the model it is not easy to obtain the observable (in ARPES experiments of Refs. [11–13]) values of the ratios $|\Delta_2/\Delta_1| \approx 0.5$ and $|\Delta_3/\Delta_1| \approx 1$. In fact it requires small enough attraction (or even repulsion, $u' > 0$) on the "large" hole-like cylinder (cf. Fig.2). In the following we assume the ratios of pairing coupling constants as $w/u = 1$, $t/u = -1$, $\bar{\lambda}/u = 1$, which guarantees us the ratio $|\Delta_3/\Delta_1| = 1$ for any values of u' and arbitrary ratios of partial densities of states at different cylinders. Another choice of pairing couplings producing $|\Delta_3/\Delta_1| = 1$ is also possible, but in general we

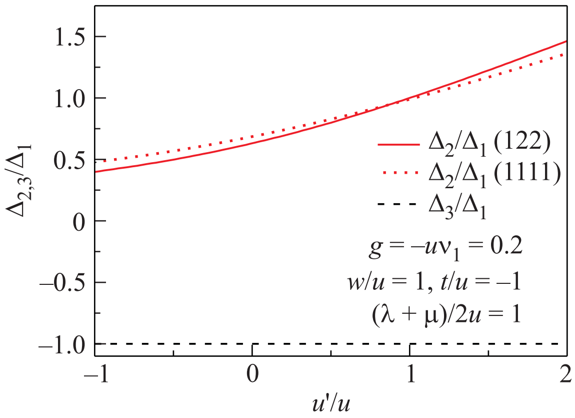

Fig.2. Dependence of gap ratios on different pockets of the Fermi surface on u'/u for $g = 0.2$, $w/u = 1$, $t/u = -1$, $\bar{\lambda}/u = 1$ and partial density of states ratios given by (13)

need larger repulsion on "large" hole-like cylinder to get $|\Delta_2/\Delta_1| \approx 0.5$. In Fig.2 we show the dependences of the gap ratios at $T = 0$ on u'/u, obtained from (12), using the partial density of states ratios on different cylinders (13), characteristic for (1111) and (122) systems. The gap ratios for $T \to T_c$ differ from the values obtained at $T = 0$ rather insignificantly.

In Ref. [15] a two-band model with two hole-like cylinders was analyzed, assuming that only interband coupling exists, i.e. the coupling constants matrix has the form:

$$-g_{ij} = \begin{pmatrix} 0 & w\nu_2 \\ w\nu_1 & 0 \end{pmatrix}. \tag{14}$$

Under this assumption the gap ratio on hole-like cylinders is given by:

$$\frac{\Delta_2}{\Delta_1} = \sqrt{\frac{\nu_1}{\nu_2}} \tag{15}$$

so that for characteristic for $BaFe_2As_2$ value of $\nu_2/\nu_1 \approx$ ≈ 1.26 we obtain $\Delta_1/\Delta_2 \approx 1.12$, which is significantly lower than the experimentally observed value of [11] $\Delta_1/\Delta_2 \approx 2$.

Four-band model somehow similar to that considered above was analyzed in Ref. [16], where temperature dependences of gaps (with proper ratios) on different sheets of the Fermi surface were calculated along with the temperature dependence of superfluid electron density. However, in this work no analysis was made of the important role of multiple bands structure for the increase of T_c, which we shall discuss shortly.

In Fig.3 we show the dependence of an effective pairing coupling constant and superconducting critical temperature on u'/u for both classes of FeAs systems (1111 and 122). It is clearly seen that the effective coupling

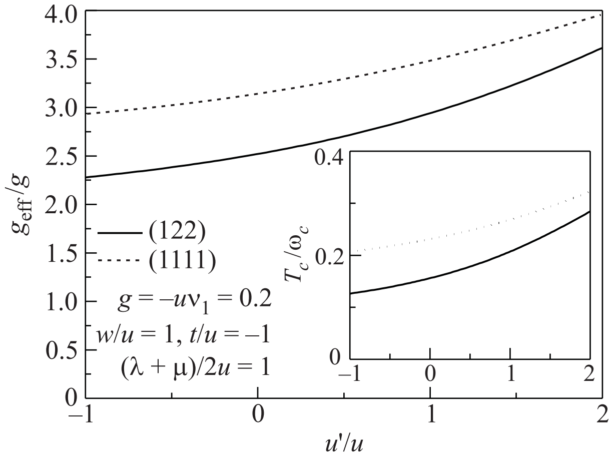

Fig.3. Dependence of effective pairing coupling constant on u'/u for $g = 0.2$, $w/u = 1$, $t/u = -1$, $\bar{\lambda}/u = 1$ and partial density of states ratios on different Fermi surface pockets given by (13). At the insert – similar dependence of the critical temperature

constant g_{eff} is significantly larger than the pairing constant g on the small hole-like cylinder. It can be said that coupling constants from different cylinders effectively produce "additive" effect. In fact this can lead to high enough values of T_c even for relatively small values of intraband [2] and interband pairing constants. Actually, using this type of estimates we can convince ourselves that the critical temperature for superconducting transition with $d_{x^2-y^2}$ gap symmetry, which is determined by an effective pairing constant given by (6), is always smaller (for typical values of parameters) than the critical temperature for $s^{\pm}$ pairing.

To clarify the reasons for the growth of effective pairing coupling it is helpful to analyze the most simple case, when all pairing interactions (both intraband and interband) in (1) are just the same (and equal e.g. to u), and all partial densities of states on all four Fermi surface pockets are also the same (and equal e.g. to ν_1). In this case we obtain $g_{\mathrm{eff}} = 4g = -4u\nu_1$, which simply corresponds to the fact that now the total density of states at the Fermi level is four times partial. However, in real situation the growth of an effective pairing constant does not reduce to this simple summation of partial densities of states. In particular, the effective pairing coupling may be much larger than the simple sum of intraband (diagonal) dimensionless coupling constants, e.g. in case of significant interband pairing interaction, which can be present in iron arsenides, where the pairing interaction between electron-like and hole-like cylinders is most probably attributed to antiferromagnetic fluctuations.

It can be estimated that with the same values of interaction constants in (1) the critical temperature in 1111-type systems is typically larger than in 122 just due to the difference of partial densities of states as given in (13) (cf. insert in Fig.3). For example, in case of $u'/u = 0$ (with the values of parameters for 122-system we get the ratio of gaps $\Delta_2/\Delta_1 \approx 0.6$) the calculated ratio of critical temperatures of 122 and 1111 systems $T_c(122)/T_c(1111) = 0.67$ is very close to the observed ration of maximal critical temperatures obtained for these systems: 38 K/55 K$\approx$ 0.69. Thus the typical difference of T_c's for both classes of new superconductors can be attributed to the different values of partial densities of states on corresponding Fermi surface cylinders, despite the fact that total densities of states at the Fermi level in these systems are practically the same [7 – 9]. Of course, the accuracy obtained should not be taken too seriously, as in real systems rather strong renormalization effects of electronic spectrum (effective masses, bandwidths etc.) in comparison with the results of LDA calculations are definitely present (and observed in ARPES experiments), e.g. due to moderate or probably even strong enough Coulomb correlations [1]. The main conclusion following from our analysis is the simple fact that the value of T_c in multiple bands systems is determined by the relations between partial densities of states on different sheets of the Fermi surface, not by the total density of states at the Fermi level as in the standard BCS model.

It should be noted that for the first time (though only implicitly) the role of multiple bands structure of electronic spectrum as the reason for the increase of superconducting T_c was apparently discussed in relation to superconductivity in multivalley doped semiconductors [17, 18]. In these works the important role of interband electron-phonon pairing mechanism was also stressed. It was noted that such processes with large momentum transfer, leading to reduced screening, may be most relevant for the increase of T_c. This fact can be also important for new superconductors besides the abovementioned role of pairing due to spin fluctuations.

Direct experimental confirmation of the role of multiple bands in new superconductors follows from ARPES measurements on extremely (hole) overdoped system KFe_2As_2 with T_c=3 K [19] and similar heavily (electron) overdoped $BaFe_{1.7}Co_{0.3}As_2$ [20], where superconductivity is just absent. From these measurements it is clearly seen how the disappearance of electronic pockets in the first system and hole-like pockets in the second one leads to strong suppression or even the complete disappearance of T_c.

To conclude, on Fig.4 we show the dependence of $2\Delta/T_c$ ratio on different sheets of the Fermi surface on the ratio of coupling constants u'/u. Here it is important to note that the value of this characteristic

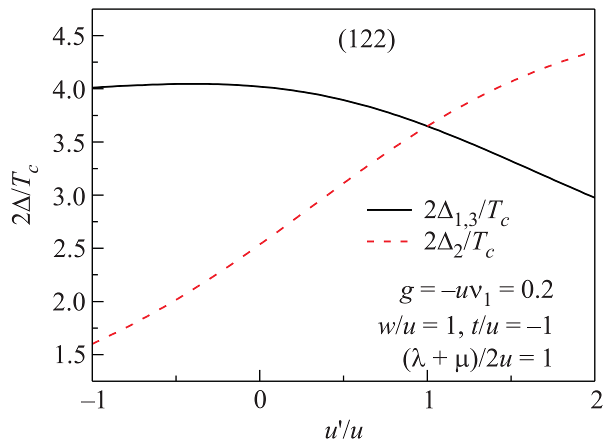

Fig.4. Dependence of $2\Delta/T_c$ ratio on u'/u for 122 – system with $g = 0.2$, $w/u = 1$, $t/u = -1$, $\bar{\lambda}/u = 1$ and partial densities of states ratios on different Fermi surface sheets, as given in (13)

ratio can be significantly different from the standard BCS value $2\Delta/T_c \approx 3.5$. However, the values shown in Fig.4 are much lower than the ratios observed in ARPES experiments [11 – 13], where the typical values are $2\Delta_{1,3}/T_c \approx 7.5$ and $2\Delta_2/T_c \approx 3.7$, which is apparently due to the strong coupling effects important in real systems. Our analysis was limited to the standard BCS-like weak coupling approach. Strong coupling Eliashberg-type analysis of multiple bands effects for new superconductors is yet to be done. Preliminary results on gap ratios in the strong coupling limit for the simple two-band model were derived in Ref. [15].

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