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

E.Z. Kuchinskii, M.V. Sadovskii *

Institute for Electrophysics, Russian Academy of Sciences, Ural Branch, Ekaterinburg 620016, Russia

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ABSTRACT

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 intraband and interband pairing coupling constants. The difference of T_c values in 1111 and 122 FeAs systems is reasonably explained by the relative values of partial densities of states, obtained from LDA calculations. 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, and not only by the total density of states at the Fermi level as in the standard BCS model. The multiple bands electronic structure of iron arsenides 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.

Schematically two-dimensional Fermi surfaces of these systems are shown in Fig. 1 [1,2]. 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 ith sheet of the Fermi surface. In general case BCS-like pairing interaction can be represented by a matrix:

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

Superconducting critical temperature T_c and gap ratios on different Fermi surface cylinders are determined by the solution of the system of linearized gap equations [1,2]:

$$g_{eff}\Delta_i = \sum_j g_{ij}\Delta_j, \qquad (2)$$

$$g_{ij} \equiv -V^{i,j}\nu_j, \quad g_{eff}^{-1} = \ln\frac{2\gamma}{\pi}\frac{\omega_c}{T_c}. \qquad (3)$$

Here ω_c is the cut-off frequency in Cooper channel, and ν_j are partial densities of states on different Fermi surface cylinders. From symmetry it is clear that $\nu_3 = \nu_4$ and below we consider only solutions corresponding to the so called $s^{\pm}$-pairing [1,2]. Eq. (3) in fact reduces to the standard problem of finding eigenvalues and eigenvectors for the matrix of dimensionless couplings g_{ij} and g_{eff} determining T_c given by the root of the secular equation:

$$Det(g_{ij} - g_{eff}\delta_{ij}) = 0. \qquad (4)$$

Despite rather large number of free parameters of the model it is not easy to obtain the observable (in ARPES experiments [3]) 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. In the following we assume $t' = t$ and the ratios of pairing coupling constants $w/u = 1$, $t/u = -1$, $\bar{\lambda}/u = 1$ (where $\bar{\lambda} = \frac{\lambda+\mu}{2}$), which guarantees us the ratio $|\Delta_3/\Delta_1| = 1$ for any values of u' and arbitrary ratios of partial densities of states ν_i at different cylinders. In Fig. 2 we show the dependences of the gap ratios at $T = 0$ on u'/u using density of states ratios on different cylinders, characteristic for (1111) and (122) systems [2].

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). Effective coupling constant g_{eff} is significantly larger than the pairing constant g on the small hole-like cylinder. Typical difference of T_c's

* Corresponding author. Tel.: +7 343 2678786; fax: +7 343 2678794.
E-mail address: sadovski@iep.uran.ru (M.V. Sadovskii).

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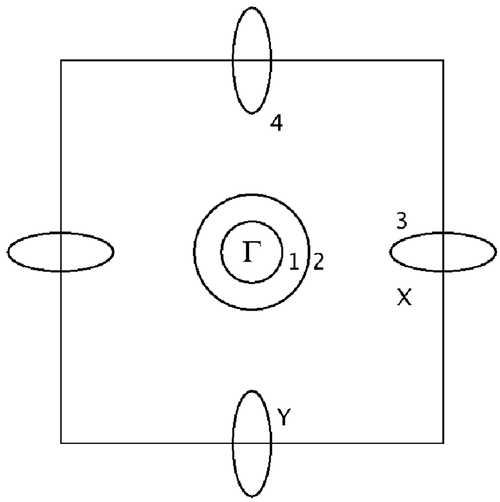

Fig. 1. Two-dimensional Fermi surfaces of FeAs superconductor in the extended band picture. There are two hole-like cylinders around point Γ, while electron-like cylinders are around X (Y) points [1].

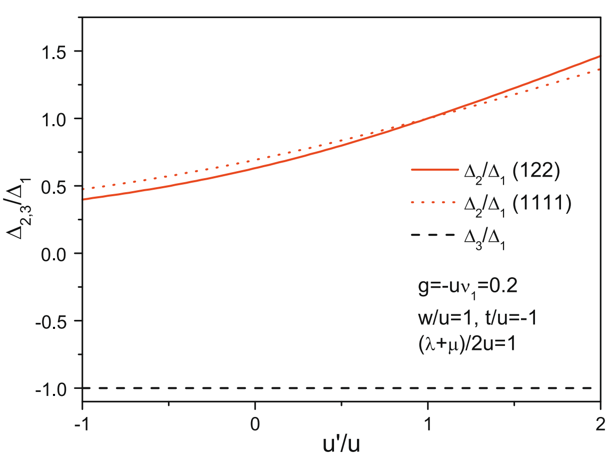

Fig. 2. Dependence of gap ratios on different pockets of the Fermi surface on u'/u for g = 0.2, $w/u = 1, t/u = -1, \bar{\lambda}/u = 1$ and partial density of states ratios typical for 1111 and 122 systems [2].

for different classes of new superconductors can be attributed [2] 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 [4,5]. Consider now briefly the case of $u = u' = w = \bar{\lambda}$ and $t' \neq t$. Gap ratio dependence on t'/t calculated for this case using partial densities of states for 122 system (assuming $g_t = 2t\nu_3 = 0.2$) is shown in Fig. 4. For $u = u = w = \bar{\lambda} \to 0$ the experimental gap ratio $\Delta_{2,3}/\Delta_1 = 0.5$ is obtained with $t'/t = 0.5$. In the general case with nonzero intraband couplings the desired gap ratio is obtained only for interband couplings which are unrealistically large in comparison with intraband couplings, making this case less probable in comparison with that discussed above.

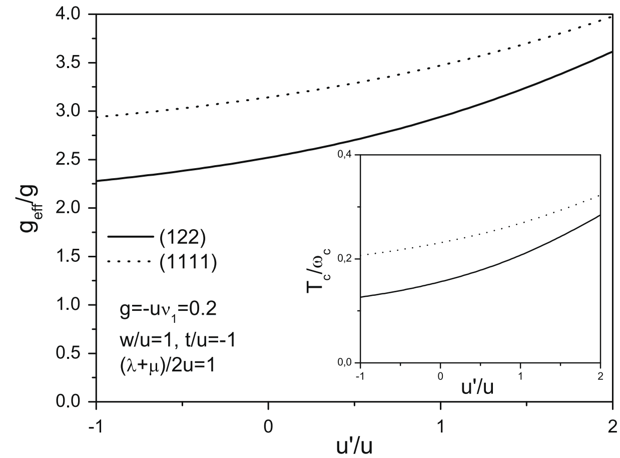

Fig. 3. Dependence of effective pairing coupling constant on u'/u for $g = 0.2$, $w/u = 1, t/u = -1, \bar{\lambda}/u = 1$ and partial density of states ratios on different Fermi surface pockets given estimated for 1111 and 122 systems [2]. At the insert – similar dependence of the critical temperature for $s^{\pm}$-pairing.

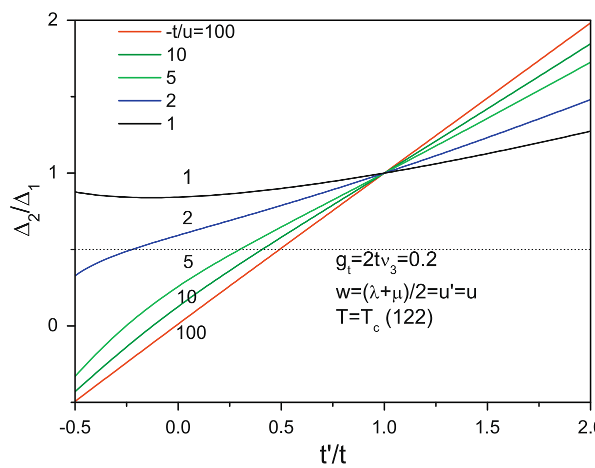

Fig. 4. Dependence of gap ratio on different pockets of the Fermi surface on t'/t for $g_t = 2t\nu_3 = 0.2$, $w = u = u' = \bar{\lambda}$ for different values of the ratio $-t/u$ (122 system).

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