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Particular type of gap in the spectrum of multiband superconductors

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Multiband models are now widely discussed for the new classes of superconductors beginning from YBCO, and more recent MgB_2 and FeAs, FeSe families [1, 2]. Usually the main attention in multiband models is concentrated on the effects of intra- and inter-band interactions (e.g. [3–5]). Interplay of relative signs and values of these interactions leads to superconductivity with order parameters of different signs at different pockets (sheets) of the Fermi surface. In the present paper we should like to draw attention to a quite different effect which takes place even if there is a single Fermi surface and for which interplay of different interactions between the bands is of no importance.

To understand, what unusual for the BCS model spectrum changes are encountered in multiband systems, we consider here the two-band model of a superconductor described by the Hamiltonian

$$\begin{aligned} H = \sum_{\mathbf{k},\alpha} \xi_a(\mathbf{k}) a^+_{\mathbf{k},\alpha} a_{\mathbf{k},\alpha} + \sum_{\mathbf{k},\alpha} \xi_c(\mathbf{k}) c^+_{\mathbf{k},\alpha} c_{\mathbf{k},\alpha} + \\ + \sum_{\mathbf{k},\alpha} (t_{ac}(\mathbf{k}) a^+_{\mathbf{k},\alpha} c_{\mathbf{k},\alpha} + h.c.) - \\ - \sum_{\mathbf{k}} \left(\Delta_a a^+_{-\mathbf{k}\downarrow} a^+_{\mathbf{k}\uparrow} + h.c.\right) - \\ - \sum_{\mathbf{k}} \left(\Delta_c c^+_{-\mathbf{k}\downarrow} c^+_{\mathbf{k}\uparrow} + h.c.\right), \end{aligned} \tag{1}$$

where $a^+_{\mathbf{k},\alpha}$ and $c^+_{\mathbf{k},\alpha}$ are creation operators for electrons with the quasimomentum $\mathbf{k}$ and spin α in bands a and c, respectively, which are generated by atomic orbitals with different kinds of symmetry; $\xi_a(\mathbf{k})$ and $\xi_c(\mathbf{k})$ are the electron energies in the respective bands, and $t_{ac}(\mathbf{k})$ is the matrix element corresponding to the single-particle interband hybridization [6]. The last two terms in Eq. (1) describe the superconducting pairing in the bands. Of course in the multiband superconductors all types of pairing usually exist, but the interband pairing is not crucial for the effect we should like to discuss.

The anomalous averages Δ_a and Δ_c introduced here are defined in the usual way:

$$\Delta_a = -U_a \sum_{\mathbf{k}} \langle a_{\mathbf{k}\uparrow} a_{-\mathbf{k}\downarrow} \rangle, \; \Delta_c = -U_c \sum_{\mathbf{k}} \langle c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow} \rangle. \tag{2}$$

Since a specific mechanism responsible for the superconducting pairing between electrons is not crucial for our aims, we assume for simplicity that the interaction in the both bands is written as in Gor'kov's equations. As a result, the initial order parameters given by Eqs. (2) in the a and c bands are isotropic; i.e., they do not depend on the momentum. For superconductivity to appear it is sufficient to have attraction only in one band. The electron-electron interaction can even be repulsive in the other band as long as this band is much wider (with lesser density of sates). Different signs of the electron-electron interactions within the bands lead to the effective order parameters which are alternating-sign functions of the quasimomentum [6]. At present we need only, that interaction in one or two bands is sufficient for superconductivity to exist.

Because the main part of new superconductors are quasi 2D systems, in what follows we assume that Hamiltonian (1) describes 2D superconductor and present pictures of 2D excitation spectrum, though the gap of the new type exists in 3D system as well.

The excitation spectrum of the model in the superconducting state consists of two branches and has the form

$$\begin{aligned} E^2_\pm(\mathbf{k}) = \frac{\varepsilon^2_a(\mathbf{k}) + \varepsilon^2_c(\mathbf{k})}{2} \pm \\ \pm \frac{1}{2} \sqrt{(\varepsilon^2_a(\mathbf{k}) - \varepsilon^2_c(\mathbf{k}))^2 + 4t^2_{ac}(\mathbf{k})[\xi^2_+(\mathbf{k}) + \Delta^2_-]} \end{aligned} \tag{3}$$

where we denote $\Delta_- = \Delta_a - \Delta_c$,

$$\begin{aligned} \varepsilon^2_a(\mathbf{k}) = \xi^2_a(\mathbf{k}) + \Delta^2_a + t^2_{ac}(\mathbf{k}), \\ \varepsilon^2_c(\mathbf{k}) = \xi^2_c(\mathbf{k}) + \Delta^2_c + t^2_{ac}(\mathbf{k}), \\ \xi_+(\mathbf{k}) = \xi_a(\mathbf{k}) + \xi_c(\mathbf{k}). \end{aligned}$$

As opposed to the standard BCS model with the single gap this spectrum has two gaps appeared due to

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the superconductivity. One opens as usual at the Fermi surface for any k and the second one separates two branches of the spectrum $E_+(\mathbf{k})$ and $E_-(\mathbf{k})$ near the line $\xi_a + \xi_c = 0$. The value of this gap can be estimated from Eq. (3) using expansion in small parameter $|\Delta_c - \Delta_a|/\sqrt{t_{ac}^2(\mathbf{k}) + \xi_c^2(\mathbf{k})}$:

$$E_\pm(\mathbf{k}) \approx \sqrt{t_{ac}^2(\mathbf{k}) + \xi_c^2(\mathbf{k}) \pm |t_{ac}(\mathbf{k})||\Delta_c - \Delta_a|} \approx$$
$$\approx \sqrt{t_{ac}(\mathbf{k})^2 + \xi_c^2(\mathbf{k})} \pm \frac{|t_{ac}(\mathbf{k})||\Delta_c - \Delta_a|}{2\sqrt{t_{ac}^2(\mathbf{k}) + \xi_c^2(\mathbf{k})}}. \qquad (4)$$

We see that this gap appears due to both superconductivity and hybridization and vanishes if either t_{ac} or Δ equals to zero. We can call it a "composite" gap, because hybridization level repulsion and superconductivity make equal contribution to its formation. To avoid misunderstanding we should stress that this gap is not a total energy gap in the density of states, contrary to the gap at the Fermi surface. It separates two branches of the excitation spectrum and its value and position changes along the line $\xi_a(\mathbf{k}) + \xi_c(\mathbf{k}) = 0$ in the Brillouin zone.

The spectrum for the case $\Delta \ll t_{ac}$ is shown in Fig. 1. In this figure we plot the spectrum of Eq. (3)

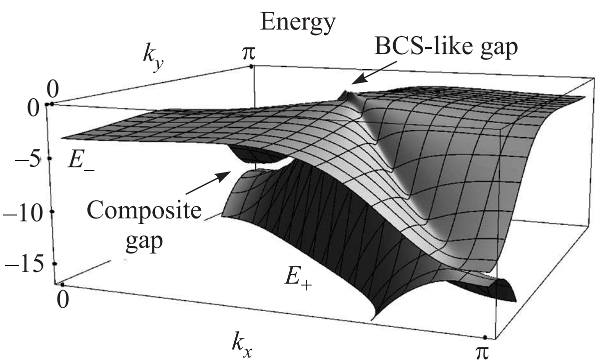

Fig. 1. $E_-(\mathbf{k})$ and $E_+(\mathbf{k})$ branches of the excitation spectrum lying under the Fermi level in superconducting case. A quarter of the Brillouin zone is shown

for the dispersion laws of the two bands typical for the simple cubic lattice: $\xi_a(\mathbf{k}) = t_a(\cos k_x + \cos k_y)$ and $\xi_c(\mathbf{k}) = \varepsilon_{c0} + t_c(\cos k_x + \cos k_y)$. The matrix element of hybridization between the two bands was taken in the form $t_{ac}(\mathbf{k}) = t_{ac}^0(\cos k_x - \cos k_y)$ [6], which corresponds to different types of symmetry the orbitals. (It is not crucial for the discussed here effect but it is closely related to our previous results [7]).

The impact of this particular gap on physical observables depends on the shape of the spectrum and on the position of this gap. We can give now qualitative explanations of our previous results for the density of states behavior in the two band model discussed in [7]. Unexpectedly strong deviations between the superconducting and normal densities of states at the energies of $(12 \div 14)\Delta$ from the Fermi level is the direct consequence of the new composite gap opening.

Eq. (4) shows that this new gap diminishes as $t_{ac}\Delta/\xi_c$ where ξ_c approximately determines the distance of the gap position from the Fermi level.

It can be easily estimated that relative changes of the density of states and conductivity are also of the order of this parameter $t_{ac}\Delta/\xi_c \simeq t_{ac}\Delta/(E - E_\mathrm{F})$. This linear dependence on the parameter $\Delta/(E - E_\mathrm{F})$ is much slower than usual for the BCS model square-low dependence $(\Delta/(E - E_\mathrm{F}))^2$.

This means, for example, that optical conductivity should change noticeably in a spectral range much greater than Δ in quite conventional superconductors with initial isotropic s-wave pairing mechanism which is in accord with mentioned above experimental studies [8, 9]. So just this general mechanism of the composite gap opening qualitatively explains our previous results for slow increase of the conductivity spectral weight with frequency cutoff growing in the two-band model [7].

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