Anomalous density of states in multiband superconductors near the Lifshitz transition

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Anomalous density of states in multiband superconductors near Lifshitz transition

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We consider a multiband metal with deep primary bands and a shallow secondary one. In the normal state the system undergoes Lifshitz transition when the bottom of the shallow band crosses the Fermi level. In the superconducting state Cooper pairing in the shallow band is induced by the deep ones. As a result, the density of electrons in the shallow band remains finite even when the bottom of the band is above the Fermi level. We study the density of states in the system and find qualitatively different behaviors on the two sides of the Lifshitz transition. On one side of the transition the density of states diverges at the energy equal to the induced gap, whereas on the other side it vanishes. We argue that this physical picture describes the recently measured gap structure in shallow bands of iron pnictides and selenides.

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Recent discovery of superconductivity in iron-based materials is one of the most important developments in modern condensed matter physics[1–3]. In addition to high transition temperatures, these materials have several exciting features including the interplay of superconductivity with spin-density wave order, a possibility of electronic mechanism of pairing, and the formation of unconventional superconducting state[4,5]. The new physics is observed in a wide variety of materials, whose properties can be fine-tuned by doping.

A common feature of iron-based superconductors is the multiple-band electronic structure. Some of these bands are very shallow, with Fermi energies of several millielectronvolts, and may be depleted with doping or pressure[6–8]. Such a qualitative change of the Fermi-surface topology is known as the Lifshitz transition[9,10]. Superconducting properties of shallow bands have a number of interesting features. For example, if was recently demonstrated by ARPES technique that in the compounds $FeSe_{1-x}Te_x$[11,12] and $LiFe_{1-x}Co_xAs$[8] the minimum gap for the shallow band is realized at zero momentum, rather than at the Fermi surface, as expected in the standard BCS theory. Furthermore, in Refs.[8,12] the superconducting gap was observed on the side of the Lifshitz transition where the band would have been empty in the normal state. These observations were interpreted as a manifestation of the Bose-Einstein condensation of electron pairs formed as a result of strong electron-electron attraction[13].

The goal of this paper is to present an alternative physical scenario based on the notion that the superconductivity in the shallow band may be induced by deep bands via pair-hopping. In the case when superconducting pairing is dominated by the deep bands, the gap parameter in the shallow band is primarily determined by the properties of deep bands and may be understood in the mean-field approximation. Within our scenario the superconducting state in the shallow band is not a result of the Bose-Einstein condensation even though the gap may be larger than the Fermi energy. The influence of the shallow band on the transition temperature and other global properties is typically weak due to its small density of states[14]. However, its superconducting properties are very different from the conventional BCS state due to strong violation of the particle-hole symmetry.

It is interesting to note that superconductivity changes the nature of the Lifshitz transition. In particular, the carrier density in the shallow band remains nonzero on both sides of the transition. Finite density appears because the particle-hole mixing generates a finite density of states (DoS) in the energy range where normal-state DoS was zero leading to appearance of a long tail in superconducting-state DoS. The only qualitative change at the transition is modification of the excitation spectrum. At the critical value of the chemical potential the minimum energy of excitations moves to the band center, as observed experimentally[11]. This change is reflected in the shape of DoS which changes dramatically as a function of the chemical potential. While on one side of the transition DoS diverges at the gap energy as predicted by the BCS theory, on the other side it vanishes at the gap energy.

We consider a superconductor with M deep bands and one shallow band, as illustrated by the inset in Fig. 1. The starting point for our discussion of the superconductivity in the shallow band is the BCS Hamiltonian

$$H_0=\sum_{\mathbf{p},\sigma}\xi_{\mathbf{p}}a^{\dagger}_{\mathbf{p},\sigma}a_{\mathbf{p},\sigma}+\sum_{\mathbf{p}}\Delta_0\left(a^{\dagger}_{\mathbf{p},\uparrow}a^{\dagger}_{-\mathbf{p},\downarrow}+a_{-\mathbf{p},\downarrow}a_{\mathbf{p},\uparrow}\right), \quad (1)$$

Here the operator $a_{\mathbf{p},\sigma}$ destroys an electron in the shallow band with momentum $\mathbf{p}$ and spin σ, and

$$\xi_{\mathbf{p}}=p^2/(2m_0)-\mu, \quad (2)$$

where the chemical potential μ is measured from the bottom of the shallow band. For definiteness we assumed an isotropic electronlike shallow band, i.e., $m_0>0$. The point $\mu=0$ corresponds to the Lifshitz transition in the normal state at which this band becomes depleted, see inset in Fig. 1. The pairing amplitude Δ_0 is induced in the shallow band by Cooper pair exchange with the deep

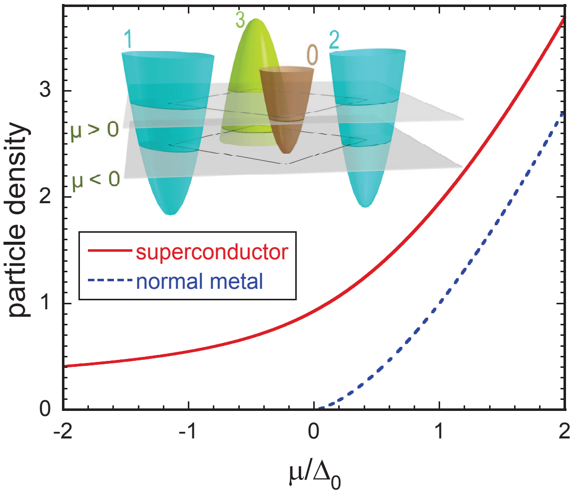

FIG. 1. The dependence of the particle density in shallow band on the chemical potential for normal metal and superconductor. The density unit is $n(\Delta_0)$. While in the normal state the density vanishes at the Lifshitz transition point, $\mu = 0$, in the superconducting state it remains finite for all μ. The inset illustrates electronic spectrum of a multiband metal with the shallow band.

bands. At zero temperature it is given by[15–17]

$$\Delta_0 = \sum_{j=1}^{M} V_{0,j}\nu_j\Delta_j \ln\frac{W}{\Delta_j}. \tag{3}$$

Here $V_{0,j}$ are the amplitudes of pair hopping between the shallow and deep bands, Δ_j and ν_j are the values of the gap and normal DoS in the deep bands. The value of the cut off parameter W depends on the mechanism of Cooper pairing; equation (3) only assumes that $W \gg \Delta_j$.

We emphasize that the validity of the mean-field equation (3) requires conditions that Δ_j are much smaller than the Fermi energies $E_{F,j}$ for the deep bands, while the relation between Δ_0 and $E_{F,0}\equiv\mu$ may be arbitrary. Note that the sum in the right hand side of Eq. (3) excludes the term $j=0$ corresponding to the contribution to pairing from the shallow band. In the limit $\mu\gg\Delta_0$ this term also has the mean-field form $V_{0,0}\nu_0\Delta_0\ln(\mu/\Delta_0)$. However, since we are interested in the regime when the bottom of the shallow band is close to the Fermi level, the density of states ν_0 is small, and such contribution is negligible compared to those of other bands[18]. Even though at $\mu\sim\Delta_0$ the shallow-band contribution can not be described by the mean-field approach, it remains small. As a result, all the gap parameters Δ_j, including Δ_0, can be assumed to be independent of μ.

Diagonalization of the Hamiltonian (1) with the Bogoliubov transformation gives the standard quasiparticle spectrum

$$E_p = \sqrt{\xi_p^2 + \Delta_0^2}. \tag{4}$$

The electron and hole contributions to the Bogoliubov wave function of quasiparticles are determined by the coherence factors

$$u_p^2 = \frac{1}{2}\left(1 + \frac{\xi_p}{E_p}\right),\ v_p^2 = \frac{1}{2}\left(1 - \frac{\xi_p}{E_p}\right).$$

We emphasize that in our case these standard mean-field results are valid for any relation between μ and Δ_0 including the region of empty band in the normal state, $\mu<0$.

The Lifshitz transition in the normal metal is characterized by non-analytic behavior of the particle density as a function of the chemical potential[9]. Indeed, the density of particles in the shallow band at zero temperature vanishes at $\mu < 0$,

$$n(\mu) = \frac{(2m_0\mu)^{3/2}}{3\pi^2}\,\theta(\mu). \tag{5}$$

Here $\theta(x)$ is the unit step function. To study the effect of superconductivity on the Lifshitz transition we evaluate the particle density as

$$n_s(\mu) = 2\int\frac{d^3p}{(2\pi)^3}\,v_p^2.$$

Introducing the natural scale $n(\Delta_0)$ for the density, we present $n_s(\mu)$ in the form

$$n_s(\mu) = n(\Delta_0)\ G\left(\mu/\Delta_0\right), \tag{6}$$

where the function $G\left(a\right)$ is defined as

$$G\left(a\right) = \frac{3}{4}\int_{-\mathrm{arcsinh}a}^{\infty} dx\exp(-x)\sqrt{a+\sinh x}.$$

It can be expressed in terms of the full elliptic integrals $K(x)$ and $E(x)$ as

$$G(a) = \frac{1}{2}\left(a^2+1\right)^{1/4}\left[\frac{K\left[r(a)\right]}{\sqrt{a^2+1}+a} + 2aE\left[r(a)\right]\right], \tag{7}$$

where $r(a) = \frac{1}{2}(\sqrt{a^2+1}+a)/\sqrt{a^2+1}$.

The dependences of particle densities on the chemical potential for normal and superconducting states are shown in Fig. 1. At $\mu \gg \Delta_0$ we use the asymptotic behavior $G(a) \simeq a^{3/2}$ at $a\to\infty$ and find that $n_s(\mu)$ approaches the normal-state density $n(\mu)$. In the opposite limit $-\mu\gg\Delta_0$ the particle density falls off gradually,

$$n_s(\mu) \approx \frac{\left(2m_0\right)^{3/2}\Delta_0^2}{16\pi\sqrt{|\mu|}}. \tag{8}$$

At $\mu = 0$, we find $n_s(0)/n(\Delta_0) = \frac{1}{2}K\left(\frac{1}{2}\right) \approx 0.927$.

Unlike the normal case, $n_s(\mu)$ does not vanish at $\mu = 0$. More importantly, one can see from Eq. (7) that the function $n_s(\mu)$ is analytic at all μ. This indicates that the Lifshitz transition at $\mu = 0$ is completely smeared by the superconductivity. Thus, in the thermodynamic sense, the change between the behaviors of the system at positive and negative values of the chemical potential should be classified as a crossover.

On the other hand, the spectrum of quasiparticles changes qualitatively at the normal-state Lifshitz transition point, $\mu = 0$, see insets in Fig. 2. For $\mu > 0$ the gap in the spectrum, $E_g = \Delta_0$ is realized at the Fermi momentum $p = p_F = \sqrt{2m_0\mu}$, whereas for $\mu < 0$ the spectral gap $E_g = \sqrt{\Delta_0^2 + \mu^2}$ is at the band center $p = 0$. This has dramatic consequences for the behavior of the density of states of the system.

The shallow band contribution to the DoS is given by

$$\nu_s(E) = \int \frac{d^3p}{(2\pi)^3} \frac{1}{2}\left(1 + \frac{\xi_p}{E}\right) \delta\left(|E| - E_p\right). \quad (9)$$

Here the electron and hole parts of DoS correspond to the energy regions $E > 0$ and $E < 0$, respectively. The momentum integral is determined by the roots of the equation $\left(p^2/2m_0 - \mu\right)^2 + \Delta_0^2 = E^2$. The resulting DoS has the form

$$\nu_s(E) = \frac{(2m_0)^{3/2}}{8\pi^2} \mathrm{Re}\left[\sum_{\delta=\pm1}\left(\frac{|E|}{\sqrt{E^2 - \Delta_0^2}} + \mathrm{sign}(E)\delta\right) \times \sqrt{\mu + \delta\sqrt{E^2 - \Delta_0^2}}\right]. \quad (10)$$

Note that the term with $\delta = -1$ contributes to Eq. (10) only if $\mu > 0$ and $|E| < \sqrt{\mu^2 + \Delta_0^2}$. At $\Delta_0 = 0$ our result (10) recovers the normal state DoS

$$\nu_n(E) = \frac{(2m_0)^{3/2}}{4\pi^2} \sqrt{E + \mu}\, \theta(E + \mu). \quad (11)$$

Representative DoSs for positive and negative μ are shown in Fig. 2.

Despite its simplicity, the result (10) has a number of interesting features. As expected, in the limit $\mu \gg \Delta_0$ the DoS approaches the standard symmetric BCS shape

$$\nu_s(E) \approx \nu_n(0)\frac{|E|}{\sqrt{E^2 - \Delta_0^2}} \text{ for } \Delta_0 < |E| \ll \mu.$$

The above result also describes the main diverging term for $E \to \pm\Delta_0$, meaning, in particular, that it remains symmetric for any positive μ. Nevertheless, in the region $\mu \sim \Delta_0$, due to the violation of the particle-hole symmetry, the overall DoS shape acquires significant asymmetry, see Fig. 2(a). In contrast to the normal-state DoS, which terminates at $E = -\mu$, the superconducting DoS remains finite at negative energies $E < -E_g$. In particular, at $-E \gg \sqrt{\mu^2 + \Delta_0^2}$ it has a power-law tail

$$\nu_s(E) \approx \frac{(2m_0)^{3/2}}{8\pi^2} \frac{\Delta_0^2}{2|E|^{3/2}}. \quad (12)$$

Another peculiar feature of the DoS at $\mu > 0$ is the square-root singularity at the energies $E = \pm\sqrt{\mu^2 + \Delta_0^2}$

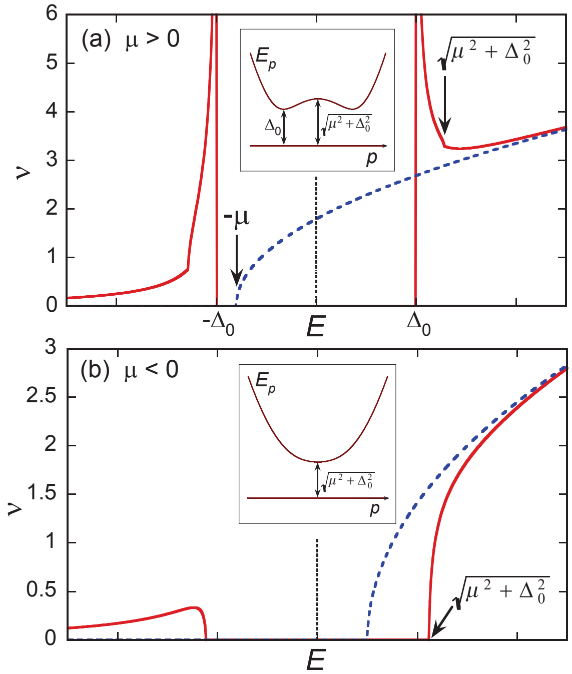

FIG. 2. Typical shapes of the DoS $\nu_s(E)$, Eq. (10), for the shallow band in superconducting state for (a) positive chemical potential, $\mu = 0.8\Delta_0$, and (b) negative chemical potential, $\mu = -0.5\Delta_0$. For comparison, the corresponding normal-state DoS $\nu_n(E)$, Eq. (11), is also shown by the dashed lines. The unit of DoS is $\nu_n(\Delta_0)$. The insets illustrate shapes of quasiparticle spectra.

marked in Fig. 2(a). This singularity appears due to the quasiparticle band edge at $p = 0$, see inset in Fig. 2(a).

The DoS exhibits a qualitatively different behavior at $\mu < 0$. In this regime it no longer diverges at the spectral gap energies $E = \pm E_g$, but approaches zero as $\sqrt{|E| - E_g}$, similar to behavior at the band edge in the normal state, see Fig. 2(b). More precisely, for $E \to \pm E_g$

$$\nu_s(E) \approx \frac{(2m_0)^{3/2}}{8\pi^2}\left(\frac{E_g}{|\mu|} \pm 1\right)\sqrt{\frac{E_g}{|\mu|}\left(|E| - E_g\right)}.$$

The qualitative difference in the behavior of the DoS at positive and negative μ is a direct consequence of the change in the excitation spectrum shown in the insets of Figs. 2(a) and 2(b). At $\mu > 0$ the square-root singularity of the DoS at $E \to \pm E_g$ is due to the fact that the lowest energy quasiparticle state has momentum $p \neq 0$. At $\mu < 0$ the minimum of the excitation spectrum is at $p = 0$, resulting in vanishing density of states at $E \to \pm E_g$. Thus, a careful measurement of the density of states at different values of the chemical potential should reveal a well-defined "crossover point" separating the regimes illustrated in the two panels of Fig. 2.

Our discussion of the superconductivity in the shallow band neglected the possible momentum dependence of the pair hopping amplitudes $V_{0,j}$ and the resulting dependence of the pairing amplitude $\Delta_0(p)$ in the Hamiltonian (1). Such dependence is indeed weak because the characteristic scale of the dependence $V_{0,j}(p)$ is of the order of the large Fermi momentum in the deep band j. It is easy to show that a weak dependence of Δ_0 on momentum will result in a shift of the "crossover point" separating the regimes of Fig. 2(a) and Fig. 2(b) away from $\mu = 0$[19].

Recent papers[8,11,12] studied the spectrum of excitations in the shallow band of iron-based superconductors and discovered that the minimum energy is achieved at $p = 0$. This observation is consistent with the scenario shown in the inset of Fig. 2(b). The authors of Refs.[8,11,12] interpreted this observation as a possible evidence of the Bose-Einstein condensation scenario of superconductivity. The latter assumes that two electrons in an otherwise empty shallow band form a bound state. In three dimensions such binding of electrons in pairs requires strong attractive interaction between them. In all other superconductors explored to date, the minimum of the excitation spectrum is achieved at $p \neq 0$, indicating that the interactions are weak, and electron pairing instead follows the conventional BCS scenario. Our work shows that the behavior shown in Fig. 2(b) may also be observed in multiband BCS superconductors due to pair hopping into the shallow band.

It was recently reported that in the compounds LiFeAs[20] and $\mathrm{LiFe}_{1-x}\mathrm{Co}_x\mathrm{As}$[8] the shallow band has the larger gap than the deep bands, which have conventional quasiparticle spectra, $|\Delta_0| > |\Delta_j|$. We point out that this does not contradict the scenario of induced superconductivity in the shallow band. For instance, in the case of just one deep band, one can easily obtain using Eq. (3) that $\Delta_0/\Delta_1 = V_{0,1}/V_{1,1}$. It is natural to expect that all paring amplitudes are of the same order of magnitude. Thus there is no reason why a situation with $|V_{0,1}| > V_{1,1}$ may not be realized, in which case $|\Delta_0|$ would exceed $|\Delta_1|$. Note that even in this regime the shallow band still gives a negligible contribution to superconducting pairing because $\nu_0 \ll \nu_1$. It is straightforward to generalize the above argument to the case of several deep bands. On the other hand, the predicted shapes of the DoS illustrated in Fig. 2 are most easily observed in materials where Δ_0 is the smallest gap. In this case, the singular behavior at energies near $\pm\Delta_0$ is not obscured by the nonvanishing contributions to the DoS from the deep bands.

To summarize, we showed that the Lifshitz transition in multiband metals with a shallow band is smeared by superconductivity. In particular, the particle density varies continuously as a function of the chemical potential, as shown in Fig. 1. The resulting crossover is nevertheless characterized by qualitatively different behaviors of the density of states above and below certain value of μ, as illustrated in the two panels of Fig. 2.

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