Gapless Fermi Surfaces of Anisotropic Multiband Superconductors in a Magnetic Field

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We propose that a new state with a fully gapless Fermi surface appears in quasi-2D multiband superconductors in magnetic field applied parallel to the plane. It is characterized by a paramagnetic moment caused by a finite density of states on the open Fermi surface. We calculate thermodynamic and magnetic properties of the gapless state for both s-wave and d-wave cases, and discuss the details of the first order metamagnetic phase transition that accompanies the appearance of the new phase in s-wave superconductors. We suggest possible experiments to detect this state both in the s-wave (2-H $NbSe_2$) and d-wave ($CeCoIn_5$) superconductors.

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In the original BCS theory of superconductivity (SC) excited states are separated from the ground state by an energy gap. SC does not necessarily lead to a fully gapped energy spectrum of quasiparticle excitations. It is well known that for unconventional SC, where the mechanism of SC is different from the BCS, nontrivial symmetry of the order parameter allows the existence of point or line nodes on the Fermi surface (FS) in momentum space [1–3]. For ordinary s-wave pairing gapless SC appears in the presence of paramagnetic impurities, when the time-reversal $t \to -t$ symmetry is broken [4]. Neglecting the orbital effects, for a SC placed in magnetic field one expects the realization of inhomogeneous Larkin-Ovchinnikov-Fulde-Ferrell (LOFF) state [5,6], in which the superconducting gap also passes through zeros this time at the points in real space.

A resurgence of interest to the new possibilities of gapless SC is related to the recent proposal of "interior gap superfluidity" of Liu and Wilczek [7], in which *whole regions of the Fermi surface* remain ungapped. Liu and Wilczek [7] have considered a situation often realized in atomic physics and high-energy physics [8], and the Bose-Einstein condensation, in which the superfluid pairing takes place for nonidentical fermions condensed by an optical trap. In this case [often called unbalanced (UB) pairing], due to both the difference in concentrations and bare masses, the two condensing components would have to form two FS with different Fermi momenta. For SC pairing between the two different Fermi surfaces it is energetically favorable to leave a part of momentum space near the larger FS in normal state. Ground states of this type have been studied for ordinary SC some time ago [9,10]. However, the tendency toward inhomogeneous LOFF state in ordinary s-wave SC always prevailed.

In this Letter we show that similar features in the energy spectrum should naturally appear in quasi-2D multiband SC, such as some organic SC or "115" heavy fermion materials, $CeMIn_5$ ($M =$ Co, Ir). Most recent experimental activity has been devoted to finding the LOFF state [11–15] in $CeCoIn_5$. The latter material is characterized by quasi-2D Fermi surfaces and a multiband energy spectrum. We consider a model of quasi-2D two-band SC of both s-wave and d-wave type in magnetic field applied parallel to the plane. Apart from the LOFF state in higher magnetic fields, for $\mu_B B \equiv I$ comparable with the smaller gap we observe whole regions of open FS, similar to the situation considered in Ref. [7]. For an s-wave SC we investigate analytically in detail this low-temperature and low-field region of the phase diagram.

We adopt the standard multiband interaction scheme (see, e.g., Ref. [16]). The matrix elements $U_{ik}(\boldsymbol{p}; \boldsymbol{p}')$ for the interaction enter the definitions of the gaps, $\Delta_i(\boldsymbol{p})$, for each Fermi surface (FS) as:

$$\Delta_i(\boldsymbol{p}) = -T \sum_{n,k,\boldsymbol{p}'} U_{ik}(\boldsymbol{p}, \boldsymbol{p}') F_k(i\omega_n, \boldsymbol{p}'), \tag{1}$$

where $F_k(i\omega_n, \boldsymbol{p})$ is the anomalous Gor'kov function, k, i are band indices, and U_{ik} is the interaction between bands i and k.

The type of the superconducting state below T_c depends on the choice of the pairing ansatz:

$$U_{ik}(\boldsymbol{p}; \boldsymbol{p}') = \chi(\varphi) U_{ik} \chi(\varphi'), \tag{2}$$

where $\chi(\varphi)$ is the appropriate irreducible representation; we take $\chi(\varphi)$ below as a const (1) for the s-wave pairing, or as $\cos(2\varphi)$ for the d-wave pairing. Solutions of the multiband Gor'kov equations [17,18] for the Green's functions in magnetic field $I = \mu_B B$ can be written as:

$$\hat{F}_k^{\dagger}(\omega_n, \boldsymbol{p}) = \frac{i\hat{\sigma}^y \Delta_k^*(\boldsymbol{p})}{(i\omega_n - I\hat{\sigma}^z)^2 - \xi_k(\boldsymbol{p})^2 - |\Delta_k(\boldsymbol{p})|^2} \tag{3}$$

$$\hat{G}_k(\omega_n, \boldsymbol{p}) = \frac{i\omega_n + \xi_k(\boldsymbol{p}) - I\hat{\sigma}^z}{(i\omega_n - I\hat{\sigma}^z)^2 - \xi_k(\boldsymbol{p})^2 - |\Delta_k(\boldsymbol{p})|^2}. \tag{4}$$

The energy spectrum of the system for excitations near each FS is given by the poles of the $\hat{G}_k(\omega_n, \boldsymbol{p})$:

$$\hat{E}_k(\boldsymbol{p}) = \sqrt{\xi_k(\boldsymbol{p})^2 + |\Delta_k(\boldsymbol{p})|^2} + I\sigma^z. \tag{5}$$

The bands with different k are coupled by the gap equation, Eq. (1). We consider below a model with 2 FS.

While the search for the LOFF state commonly starts from the side of higher fields, we study the effects in small magnetic fields of the order of the smaller gap, Δ_2. Our main interest lies in the field range where $\Delta_2 < I \ll \Delta_1$. Once the magnetic field $I = \mu_B B$ exceeds the smaller gap, then, according to Eq. (5), electron and hole pockets will open, forming an ungapped area near the second Fermi surface (FS2). In the s-wave case this process is accompanied by a weak 1st order phase transition. For a d-wave SC the energy gaps $\Delta_k(\boldsymbol{p})$ have line nodes and associated gapless states from the start. Nevertheless, depending on the strength of interactions, an irregular behavior of the gap amplitude as a function of magnetic field also occurs in some region of model parameters (see Fig. 2), which indicates a first order transition.

It is convenient [19] to express the solution of Eq. (1) in terms of dimensionless coupling constants, $\lambda_{ik} = U_{ik}\nu_k$, where ν_k is the density of states on the kth Fermi surface (FSk). The linearized gap equation Eq. (1) leads to the familiar [20] instability curve for T_c, which, we find, is independent of the number of FS involved:

$$\ln\frac{T_c}{T_{c0}} = \Psi\left(\frac{1}{2}\right) - \mathrm{Re}\left[\Psi\left(\frac{1}{2} + i\frac{I}{2\pi T_c}\right)\right]. \tag{6}$$

Here T_{c0} is the superconducting transition temperature without the magnetic field,

$$T_{c0} = \frac{2\Lambda\gamma}{\pi} e^{1/g} (g < 0) \tag{7}$$

$$g = 2\frac{\lambda_{11}\lambda_{22} - \lambda_{12}\lambda_{21}}{\lambda_{11} + \lambda_{22} + \sqrt{(\lambda_{11} - \lambda_{22})^2 + 4\lambda_{12}\lambda_{21}}}, \tag{8}$$

$\gamma \simeq 1.781$, and Λ is the upper cutoff for the interactions in Eq. (2). However, the total (T, B) phase diagram for two bands changes significantly, especially at lower temperatures and fields. Some main qualitative changes in the physics of multiband SC in this area can already be seen in a simplified model with Δ_1 as the primary gap, and $\Delta_2 \ll \Delta_1$ induced by the SC order on FS1 [21]. When I is close to the primary energy gap, Δ_1, an inhomogeneous LOFF state will appear [22,23]. For $\Delta_1 \simeq \Delta_2$ there could be significant modifications for the LOFF state and the boundaries of the LOFF state on the (T, B) phase diagram. We assume that two gaps differ enough for the LOFF state not to change significantly from the single-band model [22,23]. Below we consider in more detail the low-field region of the (T, B) plane.

In the weak coupling approach, $g \ll 1$, the ratio of $\Delta_2(T, B)$, the driven gap, and $\Delta_1(T, B)$, the primary gap, which we define as model parameter t, sets in at T_c and is temperature and magnetic field independent:

$$\frac{\Delta_2}{\Delta_1} \equiv t = \frac{2\lambda_{12}}{\lambda_{22} - \lambda_{11} + \sqrt{(\lambda_{11} - \lambda_{22})^2 + 4\lambda_{12}\lambda_{21}}}. \tag{9}$$

Equation (1) for the s-wave case can be easily solved analytically at $T = 0$. Introducing new parameters,

$$\alpha = t^2\nu_2(\nu_1 + \nu_2 t^2)^{-1}, \qquad \Delta_0 \equiv (\pi/\gamma)T_{c0}, \tag{10}$$

we find two different solutions for Eq. (1) for $I \le I_{\rm cr} = \Delta_0(1 + \sqrt{1 - t^2})^{-\alpha}$, and no solutions for $I > I_{\rm cr}$. The first solution is

$$\Delta_1 = \Delta_{10} = t^{-\alpha}\Delta_0, \qquad I < \Delta_{20}, \tag{11}$$

$$\frac{\Delta_1}{\Delta_0} = \left(\frac{\Delta_1}{I + \sqrt{I^2 - t^2\Delta_1^2}}\right)^{\alpha}, \qquad \Delta_{20} < I < I_{\rm cr}. \tag{12}$$

Here $\Delta_{i0} = \Delta_i(T = 0, B = 0)$, $i = 1, 2$. The second solution exists for magnetic fields $\Delta_0/2 < I < I_{\rm cr}$,

$$(I + \sqrt{I^2 - \Delta_1^2})^{1-\alpha}(I + \sqrt{I^2 - t^2\Delta_1^2})^{\alpha} = \Delta_0, \tag{13}$$

and is the familiar [5,18] unstable solution for the energy gap in high magnetic fields. The two solutions are plotted in Fig. 1. The reentrant behavior in magnetic fields $I \simeq \Delta_{20} = t\Delta_{10}$ clearly indicates the first order character of transition into the gapless state. At this transition an open Fermi surface is formed, according to the energy spectrum

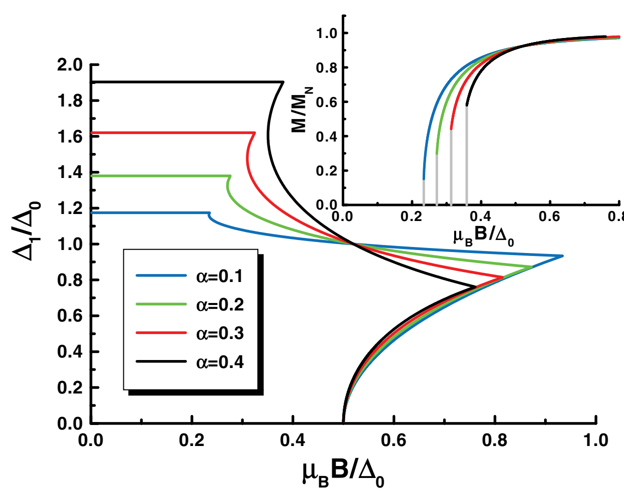

FIG. 1 (color). Magnetic field dependence of the primary energy gap Δ_1 for the s-wave case for $t = \Delta_2/\Delta_1 = 0.2$, and different values of parameter α, 0.1, 0.2, 0.3, and 0.4. The energy gap at $I = 0$ increases with growing α, see Eqs. (9)–(12). The inset shows the corresponding metamagnetic transition. The calculated paramagnetic moment is normalized to the full value of the normal moment from the second Fermi surface. The gray lines represent the positions of the first order phase transition.

given by Eq. (5). The position of the first order phase transition is found from the energy at $T = 0$, which for $I < \Delta_{20}$ has the usual form,

$$\Delta E \equiv E_S - E_{N0} = -(\nu_1 \Delta_1^2 + \nu_2 \Delta_2^2)/4. \quad (14)$$

For $I > \Delta_{20}$, we also find a contribution from the normal excitations:

$$\Delta E = -(\nu_1 \Delta_1^2 + \nu_2 \Delta_2^2 + 2\nu_2 I \sqrt{I^2 - \Delta_2^2})/4. \quad (15)$$

In Fig. 1 we also show the field dependence of the paramagnetic contribution to the total magnetization for the same values of the parameter α. There is a characteristic metamagnetic jump in the magnetization at $I = \Delta_{20}$. At $I > \Delta_{20}$ the finite density of states (DOS) arises on each new electron and hole FS that will result in the linear-in-T specific heat at low temperatures. The first order transition separating the two field regimes should be clearly seen in thermodynamic measurements.

We have obtained similar results for d-wave multiband superconductors, such as the 115 materials. The general theoretical formulas involve an average over the angular variable φ, and are more cumbersome than Eqs. (11)–(15) for the s-wave case. In Fig. 2 we show, for comparison, the dependence of the amplitude of the order parameter and the metamagnetic transition for the d-wave pairing. Because of the presence of line nodes in d-wave case, the energy spectrum is gapless already at $I = 0$. Nevertheless, similar processes take place near FS2 that

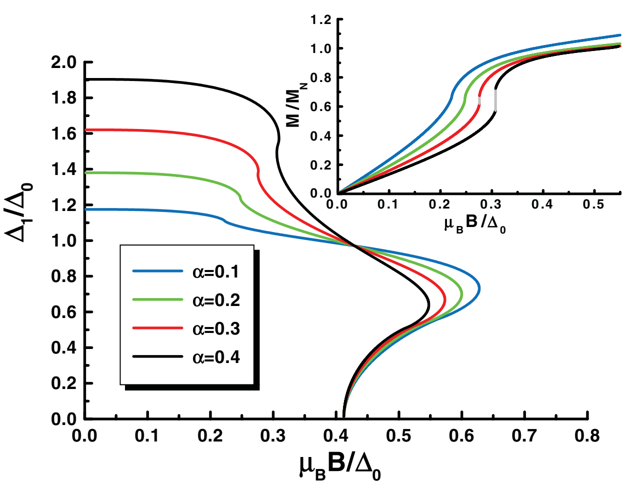

FIG. 2 (color). Magnetic field dependence of the primary energy gap amplitude, Δ_1, for the d-wave case for $t = \Delta_2/\Delta_1 = 0.2$, and different values of parameter α, 0.1, 0.2, 0.3, and 0.4. The energy gap at $I = 0$ increases with growing α. The plot is in reduced units of $\Delta_0 = 2\pi T_{c0}/\gamma\sqrt{e}$, the energy gap value corresponding to T_{c0} for a 1-band d-wave superconductor. The inset shows the corresponding metamagnetic transition, which only occurs at $\alpha > 0.24$. The calculated paramagnetic moment is normalized to the full value of the normal moment from the second Fermi surface. The gray lines represent the positions of the first order phase transition.

could lead to a first order metamagnetic transition for some values of the coupling constants. However, while for the s-wave case the first order transition is always present, for d-wave it turns into a smooth crossover for $\alpha \ll 1$.

The metamagnetic transition can be studied analytically for the s-wave case when the second gap and the parameter α are small [21], $\Delta_{20} \ll \Delta_{10}$, $\alpha \ll 1$. Introducing $\tau_I \equiv (I - \Delta_{20})/\Delta_{20}$ and $\tau_\Delta \equiv (\Delta_2 - \Delta_{20})/\Delta_{20}$, we find that in the vicinity of this transition Eq. (12) is considerably simplified,

$$\tau_I = (1/2)\tau_\Delta^2 \alpha^{-2} + \tau_\Delta. \quad (16)$$

Expanding the energy Eq. (15) in the vicinity of this transition, we find:

$$E_S - E_{N0} = E_0(1 - 2\tau_\Delta^2 - (4/3)\tau_\Delta^3 \alpha^{-2}), \quad (17)$$

where E_0 is the energy of superconducting state at $I = 0$. The cubic terms in the energy and the form of Eq. (16) clearly indicate a first order transition. After a simple calculation, we find that the first order transition occurs at $\tau_{Icr} = -3\alpha^2/8$. The energy gap τ_Δ changes abruptly from $\tau_\Delta = 0$ to $\tau_\Delta = -3\alpha^2/2$, which corresponds to a metamagnetic transition, with a paramagnetic jump in the magnetic moment $M = (3\alpha/2)\mu_B \nu_2 \Delta_{20}$ (or to a sudden appearance of the finite DOS). We find a simple expression for the magnetic moment for $I > I_{cr}$ in the vicinity of this transition:

$$M = \mu_B \nu_2 \Delta_{20}(\alpha + \sqrt{\alpha^2 + 2\tau_I}). \quad (18)$$

The paramagnetic moment in the s-wave case always appears at $I \gtrsim \Delta_{20}$ in a first order phase transition. Nevertheless, in case of the driven second gap, $\Delta_{20} \ll \Delta_{10}$, the first order transition is weak, and so is the corresponding change in the SC order parameter, $\Delta_2 = t\Delta_1$. In the first approximation this change can be neglected [21]. Then the temperature and field dependence of the magnetic moment is completely described by the standard [24] formulas that follow from the energy spectrum Eq. (5), where $\Delta_2 = \Delta_{20}$ is regarded as a constant. For example, a simple analytic expression for the magnetic moment in the s-wave case at $T = 0$ is

$$M = \mu_B \nu_2 \sqrt{I^2 - \Delta_2^2}, \qquad I > \Delta_2. \quad (19)$$

Note that $M = 0$ for $I < \Delta_2$. For a d-wave case, FS2 gives a contribution for I above and below Δ_2:

$$M_2 = \frac{2}{\pi}\mu_B \nu_2 \int_0^A d\varphi \sqrt{I^2 - \Delta_2^2 \sin^2\varphi}, \quad (20)$$

where the upper limit is $A = \pi/2$ for $I > \Delta_2$, or $A = \arcsin(I/\Delta_2)$ for $I < \Delta_2$. This is an elliptic integral of second kind. Note that in the d-wave case FS1 gives the usual nodal contribution, $M_1 = 0.5\mu_B \nu_1 I^2/\Delta_1$. The density of states for FS2 in the s-wave case is also given by a simple formula:

$$\nu_2(I) = \nu_2 I/\sqrt{I^2 - \Delta_2^2}. \quad (21)$$

In the d-wave case one has to introduce the appropriate angular averages of this result and add the familiar nodal contribution from the first Fermi surface [24].

In summary, we have shown that a gapless Fermi spectrum characterized by open Fermi surfaces is an inevitable feature for a quasi-2D multiband superconductor placed into a large enough field parallel to the plane. The new state is fully analogous to the one studied in Ref. [7] for the unbalanced pairing problem. Unlike Ref. [7], however, such a gapless state sets in as the first order transition in increased magnetic field. Measurements of the specific heat in applied field are the most direct way to observe the effect in s-wave superconductors, such as 2H-$NbSe_2$ [25,26]. The transition also leads to a metamagnetic jump in the magnetization. For a d-wave pairing, because of the nodes, gapless excitations are present even without external field. As the field is increased, the open Fermi surfaces develop gradually, although character of the process may depend on the interaction parameters. Applied fields should be low enough for these phenomena not to interact with the LOFF state. It is broadly believed [11,12,15] that the properties of $CeCoIn_5$ may be close enough to a two-dimensional model to display the inhomogeneous LOFF state [27]. If $CeCoIn_5$, indeed, belongs to the strongly quasi-2D class, the low-field properties studied above should manifest themselves as well. Then, if interactions in $CeCoIn_5$ were strong enough to result in a first order transition of Fig. 2, the latter could be observed best by calorimetric measurements, as for the s-wave pairing. If not, then one may rely on the NMR methods for the observation of a rather nonmonotonic field behavior for nonlinear susceptibility shown in the insert of Fig. 2 (we have not considered possible implications of the effect for thermal conductivity in the presence of a magnetic field). The above effects should be expected for other 2D organic compounds. An ideal realization of the scheme would be superconductivity localized at the surface [28].

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[1] G. E. Volovik and L. P. Gor'kov, Pis'ma Zh. Eksp. Teor. Fiz. **39**, 550 (1984) [JETP Lett. **39**, 674 (1984)]; Zh. Eksp. Teor. Fiz. **88**, 1412 (1985) [Sov. Phys. JETP **61**, 843 (1985)].

[2] L. P. Gor'kov, Soviet Scientific Reviews A **9**, 1 (1987).

[3] P. W. Anderson, Phys. Rev. B **30**, 4000 (1984).

[4] A. A. Abrikosov and L. P. Gor'kov, Zh. Eksp. Teor. Fiz. **39**, 1781 (1960) [Sov. Phys. JETP **12**, 1243 (1960)].

[5] A. I. Larkin and Yu. N. Ovchinnikov, Zh. Eksp. Teor. Fiz. **47**, 1136 (1964) [Sov. Phys. JETP **20**, 762 (1965)].

[6] P. Fulde and R. A. Ferrell, Phys. Rev. **135**, A550 (1964).

[7] W. V. Liu and F. Wilczek, Phys. Rev. Lett. **90**, 047002 (2003).

[8] E. Gubankova, E. G. Mishchenko, and F. Wilczek, Phys. Rev. Lett. **94**, 110402 (2005); E. Gubankova, W. V. Liu, and F. Wilczek, Phys. Rev. Lett. **91**, 032001 (2003).

[9] G. Sarma, J. Phys. Chem. Solids **24**, 1029 (1963).

[10] S. Takada and T. Izuyama, Prog. Theor. Phys. **41**, 635 (1969).

[11] Kun Yang, cond-mat/0603190.

[12] T. Mizushima, K. Machida, and M. Ichioka, Phys. Rev. Lett. **95**, 117003 (2005).

[13] K. Kakuyanagi *et al.*, Phys. Rev. Lett. **94**, 047602 (2005).

[14] V. F. Mitrovic *et al.*, Phys. Rev. Lett. **97**, 117002 (2006).

[15] C. Capan *et al.*, Phys. Rev. B **70**, 134513 (2004).

[16] D. F. Agterberg, V. Barzykin, and L. P. Gor'kov, Phys. Rev. B **60**, 14 868 (1999).

[17] A. A. Abrikosov, L. P. Gor'kov, and I. E. Dzyaloshinskii, *Methods of Quantum Field Theory in Statistical Physics* (Dover, New York, 1963).

[18] L. P. Gor'kov and A. I. Rusinov, Zh. Eksp. Teor. Fiz. **46**, 1363 (1964) [Sov. Phys. JETP **19**, 922 (1964)].

[19] M. E. Zhitomirsky and V.-H. Dao, Phys. Rev. B **69**, 054508 (2004).

[20] L. P. Gor'kov and T. T. Mnatsakanov, Zh. Eksp. Teor. Fiz. **63**, 684 (1972) [Sov. Phys. JETP **36**, 361 (1973)].

[21] V. Barzykin and L. P. Gor'kov, cond-mat/0606191.

[22] A. B. Vorontsov, J. A. Sauls, and M. J. Graf, Phys. Rev. B **72**, 184501 (2005).

[23] H. Burkhardt and D. Rainer, Ann. Phys. (Berlin) **3**, 181 (1994).

[24] V. P. Mineev and K. V. Samokhin, *Introduction to Unconventional Superconductivity* (Gordon and Breach, New York, 1999).

[25] T. Yokoya *et al.*, Science **294**, 2518 (2001).

[26] A. V. Sologubenko, I. L. Landau, H. R. Ott, A. Bilusic, A. Smontara, and H. Berger, Phys. Rev. Lett. **91**, 197005 (2003).

[27] In the real situation of a Q2D material the carriers "inside the plane," in addition to the external field, would, of course, experience a contribution from the inhomogeneous field of penetrating vortices.

[28] V. Barzykin and L. P. Gor'kov, Phys. Rev. Lett. **89**, 227002 (2002).