Fulde-Ferrell-Larkin-Ovchinnikov States in Two-Band Superconductors

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(Dated: May 17, 2013)

We examine possible phase diagram in an H-T plane for Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) states in a two-band Pauli-limiting superconductor. We here demonstrate that as a consequence of the competition of two different modulation length scales, the FFLO phase is divided into two phases via the first order transition: $Q_1$- and $Q_2$-FFLO phases at the higher and lower fields. The $Q_2$-FFLO phase is further subdivided by successive first order transitions into the infinite family of FFLO subphases with rational modulation vectors, forming a devil’s staircase structure for the field-dependence of the modulation vector and paramagnetic moment. The critical magnetic field above which the FFLO is stabilized gets lower than that in a single band superconductor, yet, tricritical Lifshitz point $L$ at $T_L$ is invariant under two-band parameter changes.

PACS numbers: 74.20.-z, 74.25.Dw, 74.81.-g

Introduction.— Owing to the fundamental significance for the coexistence of superconductivity and magnetism, Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) states have attracted a great deal of attention in the fields of condensed matter\cite{1}, cold atoms\cite{2–5}, and neutron stars \cite{6}, since the first proposals\cite{7,8}. Still FFLO is elusive in spite of extensive experimental and theoretical investigations in wide range fields. The emergence via the second-order transition is accompanied by the Jackiw-Rebbi soliton\cite{9} by which the Pauli paramagnetic moment is neatly accommodated\cite{10}. The soliton provides a generic key concept for commonly understanding the essential physics of the FFLO phase in a single-band superconductor, incommensurate structures\cite{11,12}, and fermionic excitations bound at topological defects of a superconductor through $\pi$-phase shift of the background fields\cite{13}.

Multi-band effects with multiple sheets of Fermi surfaces are observed in a variety of superconductors, such as MgB$_2$, Iron-based superconductors, and Sr$_2$RuO$_4$ to mention a few\cite{14,15}. It is now recognized that the multi-band superconductor is a rule rather than the exception. Nevertheless, in contrast to extensive studies in a single-band superconductor\cite{1}, the FFLO phases in multi-band systems have not been clarified so far other than a few exception\cite{10,17}.

In fact, several recent experiments collectively urge us to investigate the FFLO phase in multi-bands: The observations of strong Pauli effects in Iron-pnictides\cite{18–20} and of strange phase boundary line, $\frac{dT_{LO}}{dH} > 0$ ($T_{LO}$ is the BCS-FFLO transition line), in another multiband heavy fermion superconductor CeCoIn$_5$ for $H \parallel ab$\cite{21}, which is contrasted with a conventional phase diagram with $\frac{dT_{LO}}{dH} < 0$ (see the inset of Fig. 1 and Refs.\cite{1,22}).

In a single-band superconductor, the self-organized periodic structure of the FFLO state is a direct consequence of the cooperative effect between spin paramagnetism and superconductivity with the spontaneous breaking of the translational symmetry. The spatial modulation is characterized by a single length scale $Q^{-1}$, proportional to the Fermi velocity, $Q^{-1} \propto v_F$\cite{10}. Multi-band superconductivity is characterized by multi-component pair potentials. In the absence of the inter-band coupling, each band independently has their own favored modulation vector $Q_{\gamma_{i}}$, where $\gamma = 1, 2$ is the index of the electron bands. When the inter-band coupling becomes finite, however, two pair potentials are no longer independent, giving rise to the competition of multiple length scales of the FFLO modulation, $Q^{-1}_{\gamma}$. In general, the ordered phase under multiple competing length scales yields commensurate-incommensurate structures\cite{23,24} and type-1.5 superconductivity\cite{25} between type-I and II as a compromise.

In this Letter, we try to establish the essential features of FFLO characteristic to multi-band superconductors, which are absent in a single-band case\cite{10}, and exam-
ine the possible phase diagram for FFLO phases. The resulting phase diagram is summarized in Fig. 1 where our main outcome is threefold: (i) The FFLO phase is divided into two main phases via the first order transition, each having different modulation periodicity. The $Q_1$-FFLO phase stabilized in the higher field is understandable with the single-band picture with a single modulation vector $Q_1$ of the major band. The $Q_2$-FFLO phase in Fig. 2 is a consequence of the competing effect of two different length scales $Q_1^{-1} \neq Q_2^{-1}$ and peculiar to two-band superconductors. (ii) The $Q_2$-FFLO phase is further subdivided by first order transitions into the family of FFLO subphases with the sequence of rational modulation vectors $Q_2/(2n+1)$ ($n \in \mathbb{Z}$). This successive first-order phase transition exhibits a devil’s staircase structure for the modulation period and magnetization. (iii) The onset field to the FFLO phase is lower than the Lifshitz point $H_L$ due to the inter-band effect and the phase boundary indicates a positive slope $dH_{L2}(H)/dH > 0$.

Formulation. Here, we consider spin-1/2 fermions ($\sigma = \uparrow, \downarrow$) in two bands $\gamma = 1, 2$ under a magnetic field $H$, interacting through an attractive s-wave interaction $g_{\gamma'} \gamma' = g_{\gamma'} < 0$. We here deal with a quasi-one-dimensional (Q1D) system along the FFLO modulation vector, that is, the $z$-axis. This is a minimal extension of a single-band theory [10, 26]. The quasiparticles with the wave function $\varphi_{\nu, \gamma}(z + pL/2) = e^{i k_{\gamma} z} \varphi_{\nu, \gamma}(z)$, where $k_{\gamma} = 2 \pi n_{\gamma}$ is the Bloch vector and $\nu$ denotes the Bravais lattice vector which satisfies $k_{\gamma} = \pi pq/N_L$ with $p, q \in \mathbb{Z}$. Hence, we numerically solve the 1D BdG equation [11] coupled with the gap equation [22] in the interval $z \in [0, L/2]$. In this work, we deal with $L/\xi < 40$, where $\xi = v_F \tau_{D1,0}$ is the coherence length.

Sequence of FFLO states. Within the condition in Eq. 3, there exists the family of FFLO states as a consequence of interplay between two bands. To clarify this, we start with the Fourier expansion in FFLO states, $\Delta_0(z) = \sum_{m \in \mathbb{Z}} e^{i Q_m (2m+1) z} \Delta_0^m(z)$. Note that the symmetry requires $Q(2m+1) = q_1(2m+1) - q_2(2m+1)$. Then, $\Delta_{1,2}(z)$ is expanded with $Q = 2\pi m$ as

$$\Delta_{\gamma}(z) = \sum_{m \in \mathbb{Z}} e^{i Q(2m+1) z} \Delta_0^m(z).$$

In a single-band superconductor with $\Delta_2 = 0$, an isolated kink state is characterized by $\Delta_0^m = \frac{\Delta_{1,0}}{2|m| - 1}$, which is stabilized at the critical field $\mu_B H = \frac{\pi}{2} \Delta_{1,0}$. This is the one-soliton formation energy [10]. The higher Fourier components with $|m| \geq 2$ disappear as $H$ increases and the spatial modulation results in a sinusoidal form $\Delta_{1,2}(z) \propto \sin(Qz)$. The field dependence of $Q$ follows the relation, $Q \sim 2\mu_B H/v_F$ in the high field limit [10]. In the case of two-band superconductors, the modulation vector $Q_{\gamma}$ of $\Delta_{\gamma}(z)$ is determined as a consequence of the competition between two bands, where the $\gamma = 1$ ($\gamma = 2$) band favors the modulation vector $Q_1 \propto v_F^{-1} \propto \mu_1^{-1}$ ($Q_2 \propto v_F^{-1} \propto \mu_2^{-1}$) and $Q_1 < Q_2$ in our system.

Figure 2 shows the thermodynamic potential $\Omega = -\sum_{\gamma, \gamma'} g_{\gamma'} \langle \Phi_{\gamma}^2(z) \Phi_{\gamma'}^2(z) \rangle$ for a fixed FFLO period $L$, where $\langle \ldots \rangle$ denotes the spatial average over the system. The thermodynamic potential is evaluated with self-consistent solutions of Eqs. 11 and 22. It is seen from Fig. 2a) that $\Omega(L)$ has several local minima, $\frac{\partial \Omega}{\partial T} = 0$ and $\frac{\partial^2 \Omega}{\partial T^2} > 0$, in the lower temperature regime. The local minimum with the largest $Q (\xi Q \sim 0.8)$ corresponds to $Q_1 \xi$ which is favored
by the major band, and the other minima with small $Q$ follow $Q_{2}/(2n + 1)$ with $n \geq 1$. This is contrast to the higher temperature regime displayed in Fig. 2(b), where only a single minimum exists, which monotonically shifts towards the shorter $L$ as $H$ increases. The FFLO period $Q$ tends to $Q_{1} \sim \mu_{B}H/\nu_{F,1}$ in high fields, which is understandable with the single-band picture.

To clarify the distinction between the $Q_{1}$- and $Q_{2}$-FFLO states, we show $\Delta_{Q_{1}} = 0.546$ and $T = 0.075T_{c}$ in Figs. 3(a) and (b) which correspond to the local minimum with the largest and second largest $Q$, respectively. Figures 3(e-g) depict the Fourier components $\Delta_{Q_{k}}(n)$ in Eq. (4). It is seen from Figs. 3(a) and (e) that the local minimum state with $Q \xi = 0.76$ is characterized by a single peak at $m = 1$, corresponding to $Q = 2\pi/Q_{1}$. In that sense, we refer to this phase as the $Q_{1}$-FFLO phase. In the $Q_{1}$-FFLO phase, the Pauli paramagnetic moment is $M_{\gamma} = \langle m_{\gamma} \rangle = \sum_{\nu}(\langle |\psi_{\nu}|^{2} \rangle f(E_{\nu}) - \langle |\psi_{\nu}|^{2} \rangle f(-E_{\nu})\rangle$ in the $\gamma$-band accumulates in the FFLO node at which the mid-gap bound states with spin $\uparrow$ ($\downarrow$) are formed inside (outside) of the Fermi surface as the Jackiw-Rebbi soliton. Hence, the spatial modulation of $M_{\gamma} = 2\pi$ is characterized by single $Q$ as shown in Figs. 3(c) and (h), where the spatial uniform contribution of $M_{\gamma}$ with $n = 0$ is omitted. Here, $M_{\gamma}(z)$ is expanded with $Q = 2\pi$ as $M_{\gamma}(z) = \sum_{\nu}^{\text{even}} e^{i2\pi m_{\nu}} M_{\gamma}(m)\xi$.

In the low $T$ regime, the contributions from the minor band become competitive, giving rise to the appearance of several local minima in addition to the $Q_{1}$-FFLO state, as seen in Fig. 2(a). This competing effect is also reflected in the phase diagram shown in Fig. 4 where the critical field above which the $Q_{2}$-FFLO phase appears is much lower than $h_{\text{c1}} = \frac{2}{\pi}\Delta_{Q}$ in a single-band system [10]. To understand the structure of the $Q_{2}$-FFLO phase, in Figs. 3(b) and (g), we display the spatial profile of $\Delta_{1,2}(z)$ with $Q_{1} = 0.27$ at $\mu_{B}H/\Delta_{0} = 0.546$, corresponding to the local minimum labeled as $n = 2$ in Fig. 2(a). In the magnetic field regime around the critical field in two-band systems, $Q_{2}$ is comparable to the coherence length, $Q_{2} \sim \xi$, while one finds $Q_{1} = \xi$, since $\nu_{F,1} > \nu_{F,2}$. The FFLO phase with the single modulation vector $Q_{2}$ is not favorable because of the loss of the condensation energy, while the stability of the $Q_{1}$-FFLO phase requires the higher magnetic field. As shown in Eq. (4), however, it is possible to realize the family of $Q_{2}$, such as $Q_{2}/3, Q_{2}/5, \cdots$ in two-band systems. It is clearly seen from Figs. 3(b) and (g) that $\Delta_{1,2}(z)$ with $Q_{1} = 0.27$ is composed of multiple modulation vectors, $3Q_{2}/2\pi \sim 0.91\xi^{-1}$ ($m = 2$) and $5Q_{2}/2\pi \sim 1.4\xi^{-1}$ ($m = 3$) in addition to $Q_{2}/2\pi \sim 0.27\xi^{-1}$ ($m = 1$). While the own modulation vector favored in the minor band is estimated as $Q_{2} = 1.4\xi^{-1}$, the optimal wave number $Q_{1} = 0.27$ which determines the overall FFLO period corresponds to $Q \sim Q_{2}/5$, and the induced components, $3Q$ and $5Q$, are found to be $3Q_{2}/5$ and $Q_{2}$, respectively.

In the series of local minima labeled as $n = 1, 2, \cdots$ in Fig. 2(a), $\Delta_{1,2}(z)$ are composed of the overall modulation vector $Q \approx Q_{2}/(2n + 1)$ and the induced components $(2m - 1)Q_{2}/(2n + 1)$ with $m = 1, 2, \cdots$. This family of $Q_{2}/(2n + 1)$ is referred to as the $Q_{2}$-FFLO phase, which can be stabilized in the lower $H$ and $T$ regime in Fig. 4. The multiple-$Q$ modulated structure in the $Q_{2}$-FFLO phase is clearly reflected in the spatial profile of the Pauli paramagnetic moment displayed in Fig. 4(d) and the Fourier components in Figs. 3(i) and (j) have sharp peaks at $2Q_{2}$. It is also seen from Fig. 2(a) that the family of the $Q_{2}$-FFLO phase undergoes the first-order transition to the $Q_{1}$-FFLO phase as $H$ increases.

**Devil’s staircase structure.**— The appearance of the $Q_{2}$-FFLO phase is a consequence of the competition of two length scales $Q_{1}^{-1}$ and $Q_{2}^{-1}$, which is peculiar to
multi-band superconductors. We here discuss the thermodynamic stability of the $Q_1$ and $Q_2$ phases with respect to $H$. Figure 3(a) shows the quasiparticle dispersion in the minor band ($\gamma = 2$) of the $Q_1$-FFLO state with $Q\xi = 0.76$ and $n=1$ $Q_2$-FFLO state with $Q\xi = 0.45$ at $T = 0.075T_c$ and $\mu_B H = 0.546\Delta_{1,0}$. The band structure around $E_{k,\gamma} = -\mu_B H$ is interpreted as the lattice of the Jackiw-Rebbi solitons bound at the FFLO nodes, responsible for the paramagnetic moment.

The most distinct structure between the $Q_1$- and $Q_2$-FFLO phases is seen around $E_{k,\gamma} = 0$. In the $Q_1$-FFLO phase, the dispersion crosses $E_{k,\gamma} = 0$, giving rise to a large amount of the zero-energy density of states and paramagnetic moment as shown in Figs. 3(b) and 3(b). The density of states is defined as $N_{\gamma}(E) = \sum_{\nu}(|\langle u_{\nu,\gamma}|^2\delta(E - E_{\nu,\gamma}) + |\langle u_{\nu,\gamma}|^2\delta(E + E_{\nu,\gamma})|)$. In the case of the $Q_2$-FFLO phase with $n=1$, $\Delta_2(z)$ is mostly composed of two different Fourier components, $Q_2/3$ and $Q_2$, as seen in Fig. 3(f), while $\Delta_2(z)$ in the $Q_1$-FFLO phase is describable with a single $\gamma$. Hence, the original band in the $Q_2$-FFLO state with $Q = Q_2/3$ is fold back into a small reduced Brillouin zone, reflecting the mixed component with the larger modulation vector $3Q = Q_2$. Then, the band gap opens around the zero energy, which reduces $N_2(E = 0)$ but gains the condensation energy. Hence, the energetics of the FFLO phases is simply understandable as the competition between the $Q_1$-FFLO phase with zero-energy density of states and $Q_2$-FFLO phase with condensation energy.

Figure 5(a) summarizes the field-dependence of the modulation vector $Q \equiv 2\pi/L$ at $T = 0$, where the symbols (“$+$” and “$-$”) denote the metastable solutions. The ground state solution denoted by filled circles is determined by minimizing $\Omega(L)$. The field dependence of $Q_{1,2}$ in a single-band superconductor is plotted as a reference, where $Q_1$ and $Q_2$ are estimated with $(v_{F,1}, \Delta_{1,0})$ and $(v_{F,2}, \Delta_{2,0})$, respectively.

It is seen from Fig. 5(a) that the field-dependence of $Q$ is understandable with two competing modulation vectors, $Q_1$ and $Q_2$. The branch with the largest $Q$, called the $Q_1$-FFLO phase, follows the field-dependence of $Q_1$ which is dominated by the $\gamma = 1$ band with $v_{F,1}$ and $\Delta_{1,0}$, while the branches with the smaller $Q$’s are categorized to the family of the $Q_2$-FFLO phase with infinite rational vector $Q_2/(2n + 1)$ ($n=1, 2, \cdots, \infty$). Thus, as shown in Fig. 5 and $M$ in the ground state have a step structure, called the Devil’s staircase structure [23, 24]. At $\mu_B H = 0.552\Delta_{1,0}$, the $Q_2$-FFLO phase undergoes the first-order phase transition to the $Q_1$-FFLO phase with the shorter FFLO period.

Conclusions.— We have examined the multiband effects on FFLO phases and revealed generic and non-trivial features absent for a single-band case. Our calculation is based on a minimal model extended from a canonical 1D FFLO Hamiltonian [10]. We have demonstrated that the FFLO phase diagram in $H$ vs $T$ plane is divided into the two main sub-phases by the first order transition, where $Q_2$-FFLO phase in the lower $H$ regime is further subdivided, giving rise to a devil’s staircase in physical quantities. Yet, remarkably the tricritical Lifshitz point $L$ at $T_1/T_c = 0.561\ldots$, where the normal, FFLO, and uniform BCS phases meet [24, 30], is invariant even for the multiband case as shown in Fig. 5, independent of any parameters, $g_{12}/g_{11}$, $g_{22}/g_{11}$, and $\mu_1/\mu_2$ [31]. This is a generic feature observed in various systems [32, 33]. The present findings on the FFLO state is applicable not only to many multiband superconductors, but also to imbalanced superfluids with two

FIG. 4: (color online) (a) Dispersion in the reduced zone for the $\gamma = 2$ band of the $Q_1$-FFLO state with $Q\xi = 0.76$ and $n=1$ $Q_2$-FFLO state with $Q\xi = 0.45$. Density of states of $Q_1$-FFLO state with $Q\xi = 0.76$ (b) and $Q_2$-FFLO state with $Q\xi = 0.45$ (c) and $Q\xi = 0.27$ (d). The other parameters are same as those in Fig. 3.

FIG. 5: (color online) Field dependence of the FFLO modulation $Q(a)$ at $T = 0$. The symbols (“$+$” and “$-$”) indicate the metastable solutions in $\Omega(Q)$, where $\Omega$ in (+) is higher than that in the BCS phase. The shaded area denotes the $Q_2$-FFLO phase, where the transition between BCS and $Q_2$-FFLO phases takes place around $\mu_B H/\Delta_0 = 0.45$. It is seen from Fig. 5(a) that the field-dependence of $Q$ is understandable with two competing modulation vectors, $Q_1$ and $Q_2$. The branch with the largest $Q$, called the $Q_1$-FFLO phase, follows the field-dependence of $Q_1$ which is dominated by the $\gamma = 1$ band with $v_{F,1}$ and $\Delta_{1,0}$, while the branches with the smaller $Q$’s are categorized to the family of the $Q_2$-FFLO phase with infinite rational vector $Q_2/(2n + 1)$ ($n=1, 2, \cdots, \infty$). Thus, as shown in Fig. 5 and $M$ in the ground state have a step structure, called the Devil’s staircase structure [23, 24]. At $\mu_B H = 0.552\Delta_{1,0}$, the $Q_2$-FFLO phase undergoes the first-order phase transition to the $Q_1$-FFLO phase with the shorter FFLO period. Conclusions.— We have examined the multiband effects on FFLO phases and revealed generic and non-trivial features absent for a single-band case. Our calculation is based on a minimal model extended from a canonical 1D FFLO Hamiltonian [10]. We have demonstrated that the FFLO phase diagram in $H$ vs $T$ plane is divided into the two main sub-phases by the first order transition, where $Q_2$-FFLO phase in the lower $H$ regime is further subdivided, giving rise to a devil’s staircase in physical quantities. Yet, remarkably the tricritical Lifshitz point $L$ at $T_1/T_c = 0.561\ldots$, where the normal, FFLO, and uniform BCS phases meet [24, 30], is invariant even for the multiband case as shown in Fig. 5, independent of any parameters, $g_{12}/g_{11}$, $g_{22}/g_{11}$, and $\mu_1/\mu_2$ [31]. This is a generic feature observed in various systems [32, 33]. The present findings on the FFLO state is applicable not only to many multiband superconductors, but also to imbalanced superfluids with two
chains in ultracold atoms.
This work was supported by JSPS (Nos. 21340103 and 23840034) and MEXT KAKENHI (No. 22103005).

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