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Interplay between quantum confinement and Fulde–Ferrell–Larkin–Ovchinnikov phase in superconducting nanofilms

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HIGHLIGHTS

- Interplay between the quantum confinement and the FFLO state is studied in nanofilms.
- The FFLO stability region oscillates as a function of the nanofilm thickness.
- The shape resonant conditions are detrimental to the FFLO state.
- The FFLO stability region is divided into the subphases.
- Number of subphases is equal to the number of bands participated in the paired phase.

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ABSTRACT

In superconducting nanofilms the energy quantization induced by the confinement in the direction perpendicular to the film splits the band of single-electron states into series of subbands. The quantum size effect leads to the experimentally observed oscillations of the critical magnetic field with increasing nanofilm thickness. Here, we study the influence of the quantum confinement on the Fulde–Ferrell–Larkin–Ovchinnikov (FFLO) phase in superconducting nanofilms. We show that the range of the magnetic fields for which the FFLO phase is stable oscillates as a function of the film thickness with the phase shift equal to one half of the period corresponding to the critical magnetic field oscillations. Due to the multiband character of the system a division of the FFLO phase stability region appears leading to a phase diagram which is qualitatively different than the one corresponding to a single-band situation. The number of subregions created in such manner depends on the number of bands participating in the formation of the paired state.

1. Introduction

The Fulde–Ferrel–Larkin–Ovchinnikov (FFLO) phase is an unconventional superconducting state characterized by the nonzero total momentum of the Cooper pairs. According to the original concept, proposed by Fulde and Ferrel [1] as well as independently by Larkin and Ovchinnikov [2], such nonzero momentum pairing can be induced by the Zeeman spin splitting of the Fermi surface which appears in the external magnetic field. The Fermi wave vector mismatch caused by the Fermi surface splitting is detrimental to the pairing but can be compensated by the nonzero total momentum of the Cooper pairs. In spite of many theoretical studies regarding the FFLO state [3–6], the experimental signs of the nonzero momentum pairing have been reported only recently in the heavy fermion systems [7–10] and two dimensional organic superconductors [11–14]. The difficulties in experimental observation of the FFLO phase are caused by the stringent conditions for its appearance. First of all, the Pauli paramagnetic effect has to be strong relative to the orbital pair-breaking mechanism – the Maki parameter defined as $\alpha = \sqrt{2}H_{c2}^{orb}/H_{c2}^{P}$ should be higher than 1.8 [15]. Moreover, the system has to be ultra clean as the FFLO phase is easily destroyed by the impurities [16,17].

The ultra thin metallic nanofilms which can be fabricated due to the recent development of nanotechnology [18–24] may satisfy the conditions for the FFLO phase appearance. In the nanofilms subjected to the parallel magnetic field, the confinement in the direction perpendicular to the film reduces the orbital effect leading to a high value of the Maki parameter. However, if the width of the system becomes comparable to the electron wave length, the Fermi sphere splits into a set of discrete two-dimensional subbands, energies of which decreases with increasing the film thickness. As we show here, such multiband character of the

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system has a significant impact on the FFLO phase formation what has not been investigated in previous papers. It should be noted that the theoretical analysis of the FFLO phase stability in multiband models has been the subject of very few papers. Investigations regarding the non-zero momentum pairing in the multiband iron-based superconductors have been presented in Refs. [25,26]. Very recently we have suggested that the non-zero momentum paired phase can appear in the absence of the external magnetic field in $LaFeAsO_{1-x}F_x$ with a predominant interband pairing [27]. Furthermore, the multiband effects on the FFLO phase in a Pauli-limiting two-band superconductor have been theoretically studied in Refs. [28,29].

In the present paper we consider free-standing Pb(111) metallic nanofilms in the presence of the in-plane magnetic field and investigate the influence of the band splitting, caused by the quantum size effect, on the formation of the FFLO phase. In the considered system the number of the subbands induced by the confinement is determined by the nanofilm thickness. We have shown that the magnetic field range for which the FFLO state is stable oscillates as a function of the film thickness with the phase shift equal to one half of the period corresponding to the critical magnetic field oscillations. Moreover, the multiband effects lead to a division of the FFLO phase stability region into subregions number of which depends on the number of bands participating in the formation of the paired state. This results in a phase diagram which is qualitatively different from the one corresponding to the FFLO appearance in a single band model.

The paper is organized as follows: in Section 2 we introduce the basic concepts of the theoretical scheme based on the BCS theory. In Section 3 we present the results while the summary is included in Section 4.

2. Theoretical method

The first-principle calculations of the electronic structure for Pb nanofilms [30–32] demonstrated that the quantum size effect for Pb(111) can be well described by the quantum well states centered at the L-point of a two-dimensional Brillouin zone [30] and the energy dispersion calculated for Pb(111) nanofilms is nearly parabolic [30]. Based on these results, in our analysis we use the parabolic band approximation. The BCS Hamiltonian in the presence of external in-plane magnetic field $\mathbf{H}_{\parallel} = (H_{\parallel}, 0, 0)$ has the form

$$\hat{\mathcal{H}} = \sum_{\sigma} \int d^3r \hat{\Psi}^{\dagger}(\mathbf{r}, \sigma) \hat{H}_e^{\sigma} \hat{\Psi}(\mathbf{r}, \sigma) + \int d^3r \left[\Delta(\mathbf{r}) \hat{\Psi}^{\dagger}(\mathbf{r}, \uparrow) \hat{\Psi}^{\dagger}(\mathbf{r}, \downarrow) + H.c. \right] + \int d^3r \frac{|\Delta(\mathbf{r})|^2}{g}, \tag{1}$$

where σ corresponds to the spin state $(\uparrow, \downarrow)$, g is the phonon-mediated electron–electron coupling constant, while $\Delta(\mathbf{r})$ is the superconducting gap parameter in real space defined as

$$\Delta(\mathbf{r}) = -g \left\langle \hat{\Psi}(\mathbf{r}, \downarrow) \hat{\Psi}(\mathbf{r}, \uparrow) \right\rangle. \tag{2}$$

The single-electron Hamiltonian $\hat{H}_e^{\sigma}$ is given by

$$\hat{H}_e^{\sigma} = \frac{1}{2m} \left(-i\hbar\nabla + \frac{e}{c}\mathbf{A} \right)^2 + s\mu_B H_{\parallel} - \mu_F, \tag{3}$$

where $s = +1(-1)$ for $\sigma = \uparrow(\downarrow)$, m is the effective electron mass, μ_F is the chemical potential. We use the gauge for the vector potential as $\mathbf{A} = (0, -H_{\parallel}z, 0)$. Due to the confinement of electrons in the direction perpendicular to the film (z-axis) the quantization of the energy appears. Thus, the field operators in Eq. (1) have the form

$$\hat{\Psi}(\mathbf{r}, \sigma) = \sum_{\mathbf{k}n} \phi_{\mathbf{k}n}(\mathbf{r}) \hat{c}_{\mathbf{k}n\sigma}, \tag{4}$$

$$\hat{\Psi}^{\dagger}(\mathbf{r}, \sigma) = \sum_{\mathbf{k}n} \phi^{*}_{\mathbf{k}n}(\mathbf{r}) \hat{c}^{\dagger}_{\mathbf{k}n\sigma}, \tag{5}$$

where $\hat{c}_{\mathbf{k}n\sigma} (\hat{c}^{\dagger}_{\mathbf{k}n\sigma})$ is the annihilation (creation) operator for an electron with spin σ in a state characterized by the quantum numbers $(\mathbf{k}, n)$. The single-electron eigenfunctions $\phi_{\mathbf{k}n}(\mathbf{r})$ of the Hamiltonian $\hat{H}_e^{\sigma}$ are given below:

$$\phi_{\mathbf{k}n}(\mathbf{r}) = \frac{1}{2\pi} e^{ik_x x} e^{ik_y y} \varphi_{k_y n}(z), \tag{6}$$

where $\mathbf{k} = (k_x, k_y)$ is the electron wave vector, while n labels the discrete quantum states. We determine $\varphi_{k_y n}(z)$ by diagonalizing the Hamiltonian (3) in the basis of the quantum well states

$$\varphi_{k_y n}(z) = \sqrt{\frac{2}{d}} \sum_{l} c_{k_y l} \sin\left[\frac{\pi(l+1)z}{d} \right], \tag{7}$$

where d is the nanofilm thickness. We use the hard-wall potential as the boundary condition for the wave function in the z-direction.

In the FFLO phase, induced by the magnetic field, the Zeeman spin-splitting of the bands leads to the nonzero total momentum of the Cooper pairs, $(\mathbf{k}\, n \uparrow, -\mathbf{k} + \mathbf{q}\, n \downarrow)$. For such situation, the substitution of the expression for the gap parameter (2) and the field operators (5) into Eq. (1) gives the following form of the Hamiltonian in the second quantization representation:

$$\hat{\mathcal{H}} = \sum_{\mathbf{k}n} (\hat{c}^{\dagger}_{\mathbf{k}n\uparrow}\ \hat{c}_{-\mathbf{k}+\mathbf{q}n\downarrow}) \begin{pmatrix} \xi_{\mathbf{k}n} & \Delta_{\mathbf{q}n} \\ \Delta_{\mathbf{q}n} & -\xi_{-\mathbf{k}+\mathbf{q}n} \end{pmatrix} \begin{pmatrix} \hat{c}_{\mathbf{k}n\uparrow} \\ \hat{c}^{\dagger}_{-\mathbf{k}+\mathbf{q}n\downarrow} \end{pmatrix} + \sum_{\mathbf{k}n} \xi_{-\mathbf{k}+\mathbf{q}n} + \sum_{n} \frac{|\Delta_{\mathbf{q}n}|^2}{g}, \tag{8}$$

where $\mathbf{q}$ is the total momentum of the Cooper pairs in the (x,y) plane. Analogously as in the paper by Fulde and Ferrell [1] we have assumed that all the Cooper pairs have the same momentum $\mathbf{q}$. One should note that the direction of $\mathbf{q}$ is arbitrary for the case of s-wave pairing symmetry with parabolic dispersion relation. For simplicity we take on $\mathbf{q} = (q, 0)$. The energy gap in reciprocal space is defined as

$$\Delta_{\mathbf{q}n'} = \frac{g}{4\pi^2} \sum_{\mathbf{k}n} C_{\mathbf{k}n'n} \langle \hat{c}_{-\mathbf{k}+\mathbf{q}n\downarrow} \hat{c}_{\mathbf{k}n\uparrow} \rangle, \tag{9}$$

where

$$C_{\mathbf{k}n'n} = \int dz \varphi_{k_y n'}(z) \varphi_{-k_y n'}(z) \varphi_{k_y n}(z) \varphi_{-k_y n}(z). \tag{10}$$

Hamiltonian (8) can be reduced to the diagonal form by the Bogoliubov–de Gennes transformation $\hat{c}_{\mathbf{k}n\sigma} = u_{\mathbf{kq}n} \hat{\gamma}_{\mathbf{k}n\sigma} - s v_{\mathbf{kq}n} \hat{\gamma}^{\dagger}_{\mathbf{k}n\bar{\sigma}}$ [33], where $u_{\mathbf{kq}n}$, $v_{\mathbf{kq}n}$ are the Bogoliubov coherence factors. As a result, one obtains the following form of the quasiparticle energies:

$$E^{\pm}_{\mathbf{kq}n} = \frac{1}{2} \left(\xi_{\mathbf{k}n} - \xi_{-\mathbf{k}+\mathbf{q}n} \pm \sqrt{\alpha_{\mathbf{kq}n}} \right) + \mu_B H, \tag{11}$$

with

$$\alpha_{\mathbf{kq}n} = \left(\xi_{\mathbf{k}n} + \xi_{-\mathbf{k}+\mathbf{q}n} \right)^2 + 4\Delta^2_{\mathbf{q}n}. \tag{12}$$

The self-consistent equations for the superconducting gaps (for N bands we have N gap parameters) have the form

$$\Delta_{\mathbf{q}n'} = \frac{g}{4\pi^2} \sum_{\mathbf{k}n} C_{\mathbf{k}n'n} \frac{\Delta_{\mathbf{q}n}}{\sqrt{\alpha_{\mathbf{kq}n}}} \left[1 - f(E^{+}_{\mathbf{kq}n}) - f(E^{-}_{\mathbf{kq}n}) \right], \tag{13}$$