Fulde-Ferrell state induced by the orbital effect in the superconducting nanowire

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We demonstrate that the Fulde-Ferrell (FF) phase can be induced uniquely by the orbital effect in a cylindrical metallic nanowire. In the external magnetic field the two-fold degeneracy with respect to the orbital quantum number $m$ is lifted what leads to a Fermi wave vector mismatch between the subbands with opposite orbital momenta in the paired state. This mismatch can be compensated by the nonzero total momentum of the Cooper pairs created by electrons from split subbands what results in the formation of the FF phase. With increasing magnetic field a series of FF stability regions appear in between which the standard BCS superconducting phase is stable.

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Introduction.—According to the original concept by Fulde and Ferrell\cite{fulde64} (FF), as well as by Larkin and Ovchinnikov\cite{LarkinOv} (LO) a superconducting phase with nonzero center-of-mass momentum of the Cooper pairs 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. This allows for the superconducting phase to persist in magnetic fields higher than the second critical field $H_{c2}$. In order to make it possible for the non-zero momentum Cooper pairing to appear several requirements have to be met. First of all, the Maki parameter\cite{maki68} should be large meaning that the Pauli paramagnetic effect has to be strong relative to the orbital pair breaking mechanism. Moreover, the system has to be very clean as the FFLO phase is easily destroyed by the presence of impurities. Because of those rather stringent conditions there are not many examples for such nonzero-momentum pairing to occur. Until now, the experimental signs of the FFLO state have been suggested for the organic superconductors\cite{rotter99, rotter00, rotter01} and the heavy fermion compound CeCoIn$_5$\cite{yeshurun98, yeshurun99, yeshurun2003}. The quasi-two-dimensional structure of those systems leads to a strong reduction of the orbital pair breaking in the applied in-plane magnetic field, as well as to nesting properties of the quasi-2D Fermi surface. Both of these features are expected to stabilize the FFLO phase.

An indirect experimental evidence of nonzero-momentum pairing has been recently reported for a system consisting of ultracold $^6$Li atoms trapped in an array of one dimensional tubes\cite{Spin�허니}. One should also note the ongoing theoretical investigations regarding the appearance of the FFLO state in other systems such as heavy fermion superconductors with spin-dependent masses\cite{Zegrodnik2009, Zegrodnik2010} iron pnictides,\cite{Wang2011, Wang2012} ultracold fermionic atoms\cite{Kuvald10} as well as layered superconductors\cite{Zegrodnik2011}.

We consider the case of metallic cylindrical nanowire and demonstrate that the orbital effect, which so far has been regarded as detrimental to the FFLO phase formation, can in fact induce the nonzero momentum paired state. This situation is facilitated in a unique manner by the transfer of kinetic energy from the rotational to the translational degrees of freedom. Namely, the rotational degrees of freedom lead to the Fermi surface splitting since in the applied field the states with the magnetic quantum numbers $m$ and $-m$ have opposite magnetic moments what in turn results in opposite energy contributions. The Fermi wave-vector mismatch by the splitting is transferred to the nonzero total momentum of the Cooper pairs along the nanowire inducing the FF phase formation. We also provide an argument for a feasibility of such state observable.

Model.—We start with introducing the cylindrical coordinates $(r, \varphi, z)$ and choosing the gauge for the vector potential as $A = (0, e H_0|\varphi|/2, 0)$, where the magnetic field $H_0$ is parallel to the nanowire axis. The single-electron Hamiltonian in the cylindrical nanowire then has the following form

$$\hat{H}_0 = \frac{\hbar^2}{2m_e} \left[-\frac{1}{r} \frac{\partial}{\partial r} r \frac{\partial}{\partial r} + \left( -\frac{i}{r} \frac{\partial}{\partial \varphi} + \frac{e H_0 |\varphi|}{2\hbar} \right)^2 - \frac{\partial^2}{\partial z^2} \right],$$

where $m_e$ is the electron mass and $e$ is the electron charge. To underline the role of orbital degrees of freedom we have neglected the Zeeman term which complicates unnecessarily the analysis (the argument remains of the same type). Hamiltonian (1) is simplified further due to the negligible role of the diamagnetic term $\sim A^2$ which for nanowires is one order of magnitude lower than that of the order parameter. In the nanowire geometry the quantization of the single-electron energy into a series of subbands appears. These subbands are indexed by the orbital magnetic $m$ and radial $j$ quantum numbers what
leads to the dispersion relations
\[ \xi_{k,m,j} = \frac{\hbar^2 \gamma_{m,j}^2}{2 m_e R^2} + \frac{\hbar^2 k^2}{2 m_e} + m \mu_B H_{||} - \mu, \] (2)
where \( k \) is the particle momentum along the nanowire (\( z \) axis), \( \gamma_{m,j} \) is \( j \)-th zero of the \( m \)-th order Bessel function, \( R \) is the nanowire radius, and \( \mu \) is the chemical potential. The corresponding single electron wave functions have the form
\[ \phi_{kmj}(r, \varphi, z) = \frac{1}{2\pi} \hat{J}_{m} (r) e^{im\varphi} e^{ikz}, \] (3)
where \( \hat{J}_{m} (r) \) is defined as
\[ \hat{J}_{m} (r) = \frac{\sqrt{2}}{R J_{m+1}(\gamma_{m,j})} J_m \left( \frac{\gamma_{m,j}}{R} r \right), \] (4)
with \( J_m(r) \) being the \( m \)-th order Bessel function. One should note that \( \xi_{k,m,j} = \xi_{k,-m,j} \) for \( H_{||} = 0 \).

Next, we include the effective electron-electron attraction term in the model and perform the BCS approximation with the possibility of non-zero momentum pairing (with the momentum \( q \) along the \( z \)-axis). The BCS Hamiltonian is then of the form
\[ \hat{H} = \sum_{kmjq} \xi_{k,m,j} n_{k,m,j} + \sum_{mjq}' \left| \Delta_{mjq} \right|^2 \right|^{-1} + \sum_{mjq} (\Delta_{mjq} \hat{c}_{k,m,j} \hat{c}_{k+q,-m,j} + H.C.) \right|^{-1} \left( \xi_{k,m,j} + \xi_{k+q,-m,j} \right), \] (5)
where \( V \) is the coupling constant and \( \Delta_{mjq} \) is the superconducting (SC) gap defined by
\[ \Delta_{mjq} = \frac{V}{4\pi^2} \sum_{kmj'} C_{mjm'j'} \langle \hat{c}_{k+q,-m',j} \hat{c}_{k,m,j} \rangle, \] (6)
where
\[ C_{mjm'j'} = \int_0^R dr \hat{J}_{m}^2 (r) \hat{J}_{m'}^2 (r). \] (7)

The primed summation means that the \( m \) quantum number runs over the nonnegative values only. Additionally, for the summations over \( k \), the pairing appears only in the range \( [\mu - \hbar \omega_D, \mu + \hbar \omega_D] \), where \( \omega_D \) is the Debye frequency. From Eq. (5) one can see that for \( q = 0 \) the pairing appears within each subband labeled with the radial quantum number \( j \) between particles with opposite spins, momenta, and orbital momenta: \( \{k, m, j\uparrow; -k, -m, j\downarrow\}. \) So the pairing contains both the translational and the rotational degrees of freedom. In the applied field the degeneracy with respect to \( m \) is removed resulting in a shift between the subbands corresponding to \( m \) and \(-m \) [cf. Eq. (2)]. In such situation a Fermi-wave-vector mismatch appears. However, this mismatch can be transferred into the nonzero center-of-mass momentum of the Cooper pairs \( (q \neq 0) \) giving rise to the FF phase induced by the orbital effect. This process is represented in Fig. 1. For simplicity, we limit to the situation in which all the Cooper pairs have a single momentum \( q \) constituting the Fulde-Ferrell phase. Diagonalization of (5) leads to the quasiparticle energies
\[ E^{\pm}_{kmjq} = \frac{1}{2} (\xi_{k,m,j} - \xi_{k+q,-m,j}) \pm \sqrt{\frac{1}{4} (\xi_{k,m,j} + \xi_{k+q,-m,j})^2 + \Delta_{mjq}^2 + m \mu_B H_{||}}. \] (8)

The set of self-consistent equations for the SC gap parameter and the chemical potential have the form
\[ \Delta_{mjq} = \frac{V}{4\pi^2} \sum_{mjq}' C_{mjm'j'} \int_0^R dr \hat{J}_{m}^2 (r) \hat{J}_{m'}^2 (r) \times \frac{\Delta_{mjq} \left[ 1 - f(E^{+}_{kmjq}) - f(E^{-}_{kmjq}) \right]}{\sqrt{(\xi_{m,j,k} + \xi_{k+q,-m,j})^2 + 4 \Delta_{mjq}^2}}. \] (9)

\[ n_e = \frac{1}{\pi^2 R^2} \int_0^\infty dk \sum_{mjq}' \int_0^R dr \left| \tau_{kmjq}(r) \right|^2 f(E_{kmjq}) \] (10)
\[ + \left| \nu_{kmjq}(r) \right|^2 \left[ 1 - f(E_{kmjq}) \right], \]
where \( n_e \) is the electron concentration and \( f(E) \) is the Fermi-Dirac distribution. One should note that Eqs. (9) and (10) correspond to the SC gap in reciprocal space. The confinement in the radial directions of the nanowire leads to the \( r \) dependence of the SC gap determined by
\[ \Delta_q(r) = \frac{V}{4\pi^2} \int_0^R \left| \tau_{kmjq}(r) \right|^2 u_{kmjq}(r) \times \left[ 1 - f(E^{+}_{kmjq}) - f(E^{-}_{kmjq}) \right], \] (11)
where \( u_{kmjq}(r) = U_{kmjq} \tilde{T}_{mjq}(r) \) and \( v_{kmjq}(r) = V_{kmjq} \tilde{T}_{mjq}(r) \), with \( U_{kmjq}, V_{kmjq} \) being the Bogoliubov coherence factors which in turn are elements of the diagonalization matrix of \( \tilde{H} \).

The SC gaps \( \Delta_{mjq} \) and the chemical potential are obtained by solving Eqs. (9) and (10) numerically, whereas the wave-vector \( q \) is determined by minimizing the free energy of the system.\(^{25}\) Additionally, by using Eq. (11) the spatial dependence of the gap can be determined explicitly.

Results.—Calculations have been carried out for the following values of the parameters: \( \hbar \omega_D = 32.31 \) meV, \( gN(0) = 0.18 \), where \( N(0) = \frac{\text{meV}}{\text{eV}} \) is the bulk density of states at the Fermi level, \( \Delta_{\text{bulk}} = 0.25 \) meV and \( \mu_{\text{bulk}} = 0.9 \) eV which corresponds to the electron density \( n_e = 3.88 \times 10^{18} \) cm\(^{-3} \). The selected parameter values correspond to Al superconductor.\(^{26}\) To determine the values of \( R \) which are appropriate for the analysis of the proposed unconventional paired phase, we have calculated the nanowire radius dependence of the critical temperature in zero magnetic field. The \( T_c \) oscillations seen in Fig. 2 have identical form as those presented in Ref. 24 and result from the electrons energy quantization due to the confinement effect. Maximum of the \( T_c \) appears each time an electron subband passes through the energy window \( [\mu_F - \hbar \omega_D, \mu_F + \hbar \omega_D] \). In what follows, the possibility of non-zero momentum pairing due to the orbital effect is analyzed for the values of the nanowire radius which correspond to the maxima (shape resonances) labeled by I-IV in Fig. 2. The magnetic field dependence of the averaged superconducting gap

\[
\bar{\Delta} = \frac{1}{R} \int_0^R \Delta(r) \, dr, \tag{12}
\]

for the value of \( R \) corresponding to \( T_c \) maximum labeled by II is shown in Fig. 3. As one can see from Eq. (2), the orbital pair breaking mechanism caused by the Fermi surface splitting has different magnitude for bands corresponding to different values of \( |m| \). As a result, the zero temperature superconducting-to-normal metal transition driven by the magnetic field occurs as a cascade of jumps in the order parameter as displayed in Fig. 3(a). It has been reported in Ref. 27 that each jump corresponds to Cooper pair breaking in a subsequent subband. Here, we show that the Fermi wave vector mismatch, which appears in individual bands due to the orbital effect, can be compensated by nonzero center-of-mass momentum of the Cooper pairs leading to the FF phase appearance. It is shown in Fig. 3(a) that the stability of the FF phase appears for certain ranges of \( H || \) in between which the BCS phase is stable. In Fig. 3(c) we show the minimum in the \( q \)-dependence of the system energy for the selected value of external magnetic field which corresponds to the stability of the FF state.

![FIG. 2. Superconducting critical temperature \( T_c/T_{c,\text{bulk}} \) as a function of nanowire radius \( R \). The analysis of the unconventional paired phase proposed in this work is carried out for \( R \) corresponding to the maxima labeled by I, II, III, and IV. Note that the same results have been obtained in Ref. 24 (cf. Fig. 1). The \( T_c \) enhancement is very strong.](Image)

![FIG. 3. (a) Magnetic field dependence of the averaged superconducting gap; (b) total Cooper pair momentum which minimizes the energy vs. \( H || \); (c) Cooper pair momentum dependence of the energy in the paired and normal states for selected value of the field. The energy minimum visible in (c) corresponds to the stability of FF phase. Results are for \( R = 0.97 \) nm labeled by II in Fig. 2.](Image)
appears only if the dominant quasi-particle branch has the orbital quantum number lower than the other superconducting branches excluding those with $m = 0$. The number of FF stability regions is equal to the number of the subbands which fulfill this criterion. From Fig. 4 one can see that for $R = 0.97$ nm there are two subbands $(1, 0)$ and $(2, 0)$ (subbands with $m = 0$ are excluded) with a larger quantum number than the dominant subband $(0, 1)$. This results in two FF stability regions shown in Fig. 3(a) with different slopes of $q(H_{11})$, (Fig. 3(b)) depending on the orbital quantum number $|m|$ corresponding to branches responsible for the $q \neq 0$ paired phase. As one can see in Fig. 5 the FF stability does not al-

\[ \Delta_{0,1} \]

that controls the superconducting gap enhancement. The dominant contribution to the SC state, which comes solely from single branch is a characteristic feature of each resonant radius. The critical field, $H_{||,c}$ at which the transition SC-normal metal appears, is mainly determined by such dominant energy gap. The remaining quasiparticle branches are responsible for the appearance of the FF-state stability ranges seen in Fig. 3(a). Their influence on the formation of the FF phase can be explained as follows. As already mentioned, the impact of the applied magnetic field on different subbands is dependent on the orbital quantum number $|m| \neq 0$. The larger $|m|$, the faster the Fermi wave vector mismatch rises with increasing $H_{||}$. Close to $H_{||}$, the Fermi wave vector mismatch between the paired electrons $|(k, m, j, \uparrow), (-k, -m, j, \downarrow)|$ is compensated by the non-zero total momentum of the Cooper pairs leading to the stable FF phase. However, upon further increase of the field it is not possible to adjust the vector $q$ so as to sustain the pairing in such subband and the Cooper pairs in this subband break up leading to a decrease of the energy gap and standard BCS pairing reentrance. This allows to formulate the conditions for the appearance of the FF stability regimes induced by the orbital effect in nanowires. Namely, the FF phase ways appear with increasing field. Such situation takes place when the dominant band corresponds to large value of $|m|$ and the depairing in this band appears before in other quasiparticle branches. The quasiparticle dispersion relations in such case ($R = 1.13$ nm, (III)) are shown in Fig. 4 together with the corresponding $r$ dependence of the averaged gap parameter and the contributions to the pairing coming from particular subbands. As one can see, for $R = 1.13$ nm the largest contribution to the pairing originates from the subband with $m = 3$ and $j = 0$. Due to relatively large value of $m$, the corresponding quasiparticle branch reaches zero energy before any other and as a result, the FF state induced by the less important branches does not appear.

Summary.—The orbital effect in cylindrical superconducting nanowires results in the Fermi wave vector mismatch which can be transferred to the nonzero total momentum of the Cooper pairs. By solving the Bogoliubov-de Gennes equations numerically we have shown that this effect leads to stability of the FF phase in certain ranges of the external magnetic field oriented parallel to the nanowire. The nonzero total momentum of the Cooper pairs is induced to sustain the pairing in the corresponding subbands what leads to the structure of the FF and BCS stability ranges as shown in Figs. 3 and 4. To present the proposed idea and to expose the role of orbital effect we have analyzed nanowires with uniform cross section. The effect of nonuniform cross section of

\[ \text{FIG. 4.} \text{ Quasi-particle subbands labeled by} (m, j) \text{ participating in SC state; (b,e) } r\text{-dependence of the SC gap } \Delta(r); (e,e) \text{ contributions to the paired phase coming from different subbands. Results are for } R = 0.97 \text{ nm (II - left panels) and } R = 1.13 \text{ nm (III - right panels), both for } H_{11} = 0. \]

\[ \text{FIG. 5. Magnetic field dependences of the averaged SC gap for four nanowire radii corresponding to resonances I-IV, respectively.} \]
the samples can make the experimental observation of the proposed state difficult as the energy gain coming from the nonzero momentum pairing is rather small [cf. Fig. 3(c)]. Given the circumstances, a strong enhancement of the $T_c$ value with respect to that for a bulk sample should make the effect observable for uniform wires in the clean limit.

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