Phase diagram of a surface superconductor in parallel magnetic field

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Universal phase diagram of 2D surface superconductor with generic Rashba interaction in a parallel magnetic field is found. In addition to uniform BCS state we find two inhomogeneous superconducting states, the stripe phase with $\Delta(r) \propto \cos(Qr)$ at high magnetic fields, and a new "helical" phase with $\Delta(r) \propto \exp(iQr)$ which intervenes between BCS state and stripe phase at intermediate magnetic field and temperature. We prove that the ground state for helical phase carries no current.

Many efforts both theoretical and experimental have been spent in search of exotic nonhomogeneous superconducting states beginning with a pioneering papers by Larkin-Ovchinnikov and Fulde-Ferrel (LOFF) predicting the stripe state in superconductors with competing ferromagnet interaction. Nevertheless no convincing experimental evidence for existence of such a state was found till now, partially due to rather narrow existence range of the LOFF state. Recently Barzykin and Gor’kov did find a system where such inhomogeneous superconducting phase could be prominent. It is a two-dimensional surface superconductor with spin-orbital Rashba interaction. One of possible realization of such a system probably was reported in very interesting experiments, where various signatures of surface superconductivity with $T_c \approx 90K$ were detected in the insulating WO3 doped by small amount of Na. Surface spin-orbit superconductivity is unusual one due to the absence of inversion symmetry: this results in the presence of the the spin-orbital Rashba term and the chiral subband splitting of free electron spectrum at the surface. In such a superconductor condensate wave-function is a mixture of both singlet and triplet states, therefore Pauli susceptibility is not vanishing at $T \to 0$; paramagnetic breakdown of superconductivity in a parallel magnetic field is shifted towards much higher field values due to the formation of LOFF state. The line of transition from normal to (any of) superconductive state $T_c(h)$ was determined in; however, the nature of the phase intervening between uniform BCS and stripe LOFF state was not studied. This question is important because phenomenological theory predicts the possibility for a new helical state distinct from both BCS and stripe LOFF states.

In this Letter we provide a detailed phase diagram of a surface superconductor in a parallel magnetic field $h$. The phase diagram turns out to be universal after normalization of the temperature and the Zeeman energy by the critical temperature in zero magnetic field $T_c(h)$ for two models of high (I) and low (II) electron density. The model I assumes a normal 2D metal with Fermi energy being much greater than chiral splitting. The model II is suited for an electron gas in field effect heterostructures where electrons fill only the bottom of one of chiral bands. We demonstrate the existence of a helical state with order parameter $\Delta \propto \exp(iQr)$ (where $Q \perp h$) and $Q \sim \mu_B h/\nu_F$ in a considerable part of the phase diagram, which is summarized in Fig.1. The line $LT$ is the second-order transition line separating helical state from the homogeneous superconductor. Below the $T$ point first-order transition between BCS and inhomogeneous state takes place. The line $ST$ is the line of small instability of the helical state (see below). The point $S$ in the $T_c(h)$ line is special in that here the order parameter symmetry is $U(2)$ instead of usual $U(1)$. Full details of our theory will be presented in a separate publication.

Near the surface of a crystal the translational symmetry is reduced and the inversion symmetry is broken even if it is present in the bulk. As a result a transverse electric field appears at interface and gives rise to the relativistic spin-orbit interaction known as the Rashba term: $H_{so} = \alpha \vec{r} \times \vec{p} \cdot \vec{n}$, where $\alpha > 0$ is the spin-orbit coupling constant, $\vec{n}$ is a unit vector perpendicular to the surface, $\vec{p} = (\vec{\alpha}^\sigma, \vec{\alpha}^s, \vec{\alpha}^r)$ are spin Pauli matrices. Spin operator does not commute with the Rashba term, thus spin projection is not a good quantum number. On the other hand the chirality operator: $\vec{\alpha}^\sigma \sin \varphi_p - \vec{\alpha}^s \cos \varphi_p$, does commute with the Hamiltonian, where $\varphi_p$ is the angle between the momentum of the electron and the $x$-axis. Its eigenvalue: $\lambda = \pm 1$ is a quantum number of an electron state ($\vec{p}, \lambda$). The Rashba term preserves the Kramers degeneracy with states ($\vec{p}, \lambda$) and ($-\vec{p}, \lambda$) belonging to the same energy.

In this Letter we consider the simplest model of surface superconductor: Gor’kov model for two-dimensional metal with the Rashba term being included, in the limit $\alpha h/\nu_F \gg T_c$. The Hamiltonian written in the coordinate representation reads

$$\hat{H} = \int \left[ \frac{\hat{p}^2}{2m} - g \mu_B \vec{h} \cdot \hat{\sigma}_{\alpha\beta}/2 \right] \psi_\beta^\dagger(\vec{r}) \psi_\beta(\vec{r}) d^2r - \frac{U}{2} \int \psi_\alpha^\dagger(\vec{r}) \psi_\beta^\dagger(\vec{r}) \psi_\beta(\vec{r}) \psi_\alpha(\vec{r}) d^2r,$$

where $m$ is the electron mass and $\alpha, \beta$ are spin indices, $\hat{p} = -i\vec{\nabla} + \frac{\alpha}{2} \vec{A}(\vec{r})$ is the momentum operator in the presence of infinitesimal in-plane vector-potential $\vec{A} = \vec{A}(\vec{r})$. Zeeman interaction with a uniform external magnetic field $\vec{h}$ parallel to the interface and in the $x$-direction

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is included. The vector-potential of such a field can be chosen to have only z-component, therefore it decouples from the 2D kinetic energy term. $\mu_B$ is Bohr magneton and $q$ is the Lande factor. Hereafter we use a notation $H = gq\mu_B h/2$.

The electron operator can be expanded in the basis of plane waves $\hat{\psi}_\alpha(\vec{r}) = \sum_\vec{p} e^{i\vec{p}\cdot\vec{r}}\hat{c}_{\alpha\vec{p}}$. The one-particle part of the Hamiltonian (1) in the momentum representation:

$$\hat{H}_0 = \sum_{\vec{p}} \hat{c}_{\alpha\vec{p}}^\dagger \left( \frac{p^2}{2m} + \alpha [\hat{\sigma}_{\alpha\beta} \times \hat{p}] \cdot \mathbf{n} - \hat{H} \cdot \hat{\sigma}_{\alpha\beta} \right) \hat{c}_{\beta\vec{p}}$$

(2)

can be diagonalized by the transformation $\hat{c}_{\alpha\vec{p}} = \eta_{\lambda\alpha}(\vec{p})\hat{a}_\lambda$ with the two-component spinor $\eta_{\lambda}(\vec{p}) = (1, i\lambda \exp(i\varphi_{\alpha\vec{p}}))/\sqrt{2}$. Eigenvalues of the Hamiltonian corresponding to the chiralities $\lambda = \pm 1$ are

$$\epsilon_{\lambda}(\vec{p}) = p^2/2m - \lambda \sqrt{\alpha^2 p^2 - 2\alpha p_H H^2 + H^4}.$$ (3)

In the case of high electron density and respectively chemical potential $\mu \gg ma^2$ (model I) both chiral-ity branches are filled and the equal momentum electron states are split by $2\alpha p_H$. Fermi circles with different chiral-ities are split with the radii $p_H = \sqrt{2m\mu + m^2\alpha^2 \pm ma}$. Densities of states on the two Fermi circles are almost the same, $\nu_\pm = \frac{2\pi}{2\alpha} \left( 1 \pm \frac{\omega}{v_F} \right)$; in this paper we neglect the difference $\nu_+ - \nu_-$. In the case of the low electron density (model II): $-ma^2/2 < \mu < 0$, the electrons fill the bottom of only one chiral branch $\lambda = 1$, i.e. a ring. The two Fermi circles of the ring in zero magnetic field have radii $p_H = ma + l \sqrt{2m\mu + m^2\alpha^2}$, where $l = \pm 1$ is the number specifying the inner and the outer part of the ring and is analogous to chirality. Density of states on the outer and inner part of the Fermi ring ($l = \pm 1$) is almost the same $\nu_\pm = \frac{2\pi}{2\alpha} \left( 1 \pm \frac{\omega}{v_F} \right)$ in the case of narrow ring: $v_F \ll \alpha$. If magnetic field is applied, the two Fermi circles are displaced in opposite $y$-directions by a momentum $Q = \pm H/v_F$, where $v_F = \sqrt{2m\mu + m^2\alpha^2}$ is the Fermi velocity in the I model, or half width of the ring divided by $m$ in the II model. The pairing interaction (the last term in Eq. (1)) can be factorized in the chiral plane waves $\hat{\psi}_\alpha = \sum_\lambda e^{i\vec{p}\cdot\vec{r}}\hat{a}_\lambda$, where the pair annihilation operator $\hat{A}(\vec{q}) = \sum_{\alpha\beta} \hat{\psi}_{\alpha\vec{q}}^\dagger \hat{\psi}_{\beta-\vec{q}}$, with $p_\pm = p \pm q/2$.

To calculate thermodynamic potential $\Omega = -T \ln Z$, we employ imaginary-time functional integration technique with Grassmanian electron fields $\alpha_{\lambda\vec{p}}, \bar{\alpha}_{\lambda\vec{p}}$, and introduce auxiliary complex field $\Delta(\vec{r}, \tau)$ to decouple pairing term $H_{int}$, cf.10. The resulting effective Lagrangian is of the form:

$$L[\alpha, \bar{\alpha}, \Delta, \Delta^*] = \sum_{\vec{p}} \bar{\alpha}_{\lambda\vec{p}} (-\partial_\tau - \epsilon_{\lambda}(\vec{p})) \alpha_{\lambda\vec{p}} +$$

$$\sum_{\vec{q}} \left[ -\frac{[\Delta\vec{q}]^2}{U} + \sum_{\lambda\mu} \left( \Delta_{\lambda\mu} e^{-i\vec{q}\cdot\vec{r}} \bar{\alpha}_{\lambda\vec{p}} \alpha_{\mu, -\vec{p}} + \Delta_{\lambda\mu}^* e^{i\vec{q}\cdot\vec{r}} \bar{\alpha}_{\mu, -\vec{p}} \alpha_{\lambda, \vec{p}} \right) \right].$$ (4)

Below we will work within the mean-field approximation which is controlled by the small Ginzburg number $G \sim T_c/E_F$. It is equivalent to the saddle-point approximation for the functional integral over $\Delta$ and $\Delta^*$, thus we will be studying minima of the functional $\Omega[\Delta, \Delta^*]$ appearing after Gaussian integration over Grassmanian fields.

Near the normal-superconducting phase transition the order parameter $\Delta(\vec{r})$ is small and $\Omega$ may be expanded in powers of $\Delta(\vec{r})$ and its gradients. We consider the order parameter as a superposition of the finite number of harmonics, $\Delta(\vec{r}) = \sum_i \Delta_{\lambda_i}(\vec{r}) \exp(i\vec{Q}\cdot\vec{r})$, where $\Delta_{\lambda_i}(\vec{r})$ are slowly varying in 2D space functions, and derive the corresponding Ginzburg-Landau functional:

$$\Omega = \int \left[ \sum_i \alpha_i |\Delta_{\lambda_i}|^2 + \sum_{ijkl} \beta_{ijkl} \Delta_{\lambda_i} \Delta_{\lambda_j}^* \Delta_{\lambda_k} \Delta_{\lambda_l} \right] d^2r$$

(5)

The coefficient $\alpha(\vec{Q})$ includes Cooper loop diagram with transferred momentum $Q$:

$$\alpha(\vec{Q}) = \frac{1}{\mathcal{U} - \mathcal{T} \sum_{\omega,\vec{k},\vec{p}} G_{\chi}^\dagger(\omega, \vec{p}) G_{\chi}^\dagger(\omega, \vec{p} - \vec{Q}) G_{\chi}^\dagger(\omega, -\vec{p}) G_{\chi}^\dagger(\omega, -\vec{p} - \vec{Q})}$$ (6)

where in the I model the normal-state Green function in in-plane magnetic field $H < \alpha \mu_F$ is $G_{\chi}^\dagger(\omega, \vec{p}) = (i\omega - \xi - \lambda H \sin \varphi_{\vec{p}})^{-1}$, and $\xi = p^2/2m - \lambda H \mu - \mu$ is assumed to be small compared to $\alpha \mu_F$, whereas in the II model $H < ma^2$ and $\xi\ell = v_F(l\pi - m\mu_F)$ is assumed to be small compared to $ma^2$ ($\pi$ is related to the center of the ring). Hereafter we present results for high density (I model), but results for low density are identical. The condition $\min Q \alpha(\vec{Q}) = 0$ determines the second-order transition line (if $\beta > 0$) between the normal metal and the superconductor:

$$\frac{1}{\mathcal{U}} = \max_Q \sum_{\omega,\vec{p}} \frac{\pi \nu T}{\sqrt{\omega^2 + H_x^2}}.$$ (7)

hereafter $H_x = \lambda H + v_F Q/2$. Depending upon $H$, the maximum in Eq. (4) is attained either at $Q = 0$ or at nonzero $\pm Q$. $T_c(H)$ line is shown on Fig.1 where both $T_c$ and $H$ are normalized by the critical temperature at zero magnetic field $T_{\alpha} = 2\omega_D \exp(-1/3\mathcal{U} + C)/\pi$, where $C = 0.5777$ is the Euler constant. Near $L$ point $v_F Q(H) \sim \sqrt{H^2 - H_x^2}$. In the limit $H/T_{\alpha} \to \infty$ we recover the asymptotics of $T_c(H)$ line, and find $v_F Q(H)$:

$2H - \frac{\pi^2}{12} H_x$. Note that $Q = 2H/v_F$ is the momentum splitting of two $\lambda = \pm 1$ Fermi surfaces in parallel magnetic field. Lifshitz point $L$ separates $Q = 0$ and $Q \neq 0$ solutions on the $T_c(H)$ line; it is the end point of the second order phase transition between the two superconducting phases. $H > H_L$ inhomogeneous superconductive phase is formed below $T_c(H)$ line. No more than two harmonics contribute to $\Delta(\vec{r})$ just below $T_c(H)$ line.
is defined through the Jacoby complete elliptic integrals of the first and the second kind,

$$f(H_{\lambda}) = \frac{1}{H_{\lambda}} \left( (\omega^2 + H_{\lambda}^2 + \Delta^2) \frac{K(k)}{r(H_{\lambda}, \omega)} - r(H_{\lambda}, \omega) E(k) \right).$$

We prove by direct microscopic calculation that \( \bar{J}_s = \frac{2e}{h} \partial \Omega / \partial Q \), therefore the equilibrium state carries no supercurrent.

Minimum of the thermodynamic potential \( \Omega \) over \( \Delta \) can be expanded in series of small \( Q \):

$$\Omega_{\text{hel}}(Q) = \Omega_{\text{hel}}(0) + \frac{1}{2} n_s^q y^2 Q^2 + b Q^4 + c Q^6, \quad c > 0.$$  

The condition \( n_s^q y = 0 \) determines the second order Lifshitz transition line \( LT \), which ends at the point \( T_c \), where coefficient \( b = 0 \) changes sign. We compute the coordinates of \( T_c \) point using Eqs. (9,10). At lower temperatures \( b < 0 \) and first-order transition out of BCS state occurs.

The domain of helical state local stability was determined via consideration of the thermodynamic potential variations due to weak static modulation of the form \( \delta \Delta(iQy) = v_{-q} \exp(-iqy) + v_{+q+2Q} \exp(i(q + 2Q)y) \) (the presence of two Fourier harmonics in the perturbation is due to inhomogeneity of the background helical state):

$$\delta \Omega_{\text{hel}} = \bar{v}^* \bar{A}(q) \bar{v},$$

where \( \bar{v} = (\bar{v}_{-q}, \bar{v}_{q+2Q}) \) and

$$\bar{A}(q) = \frac{1}{U} - \sum_{\omega,0,\lambda,p} \begin{pmatrix} G_{\lambda p} - G_{\lambda p - } & F_{\lambda p} - F_{\lambda p - } \\ F_{\lambda p - }^* - F_{\lambda p}^* & G_{\lambda p - } + q G_{\lambda p - } + Q \end{pmatrix}.$$  

The matrix \( A \) has two eigenvalues \( \epsilon_1(q) > \epsilon_2(q) \). We define the helical state metastability line \( ST' \) as a collection of points where one mode \( \delta \nu \) becomes energetically favorable: \( \min_{\nu} \epsilon_1(q) = 0 \). We solve numerically four equations simultaneously: two gap equations (10) that determine equilibrium \( \Delta \) and \( Q \), together with the two equations \( \partial_\nu \epsilon_1(q) = 0 \) and \( \epsilon_2(q) = 0 \). By means of expansion of the Ginzburg-Landau functional up to the terms of order \( |\Delta|^6 \), we checked that the next-order "anisotropic" term in the expansion (8) is of the form \( \epsilon (|\Delta|^2 - |\Delta_\perp|^2)^4 \), with \( \varepsilon > 0 \). This fact ensures that the phase transition out of the helical state is of the second order (at least, near the \( T_c(H) \) line).

We calculated electromagnetic response function \( \delta j_{\alpha} / \delta A_\beta = -\frac{e}{mc} n_s^{\alpha \beta} \) for helical state using standard diagram methods and found that \( n_s^{xy} = 4 \frac{m}{h} \frac{c^3}{\Omega_{\text{hel}}} \). Thus on the Lifshitz line \( LT \) there is no linear supercurrent in the direction perpendicular to the magnetic field. The component \( n_s^{xy} \) does not vanish anywhere in helical state region and is of the order of \( n_s \) of the BCS state. This is in contrast with the classical LOFF problem, where \( n_s \) was shown to vanish in the whole helical state; the difference is probably due to the fact that in our problem the direction of \( Q \) is fixed by an applied field \( h \), while for the case of ferromagnetic superconductor it is arbitrary. The obtained behaviour of \( n_s^{xy} \) tensor indicates strongly anisotropic electromagnetic response of surface superconductor near the Lifshitz line \( LT \).

So far we discussed the clean case; below we demon-
strate that sufficiently high concentration of nonmagnetic impurities suppress both helical and stripe states. Consider impurities with weak short-range potential, characterized by to elastic scattering time \( \tau \). By means of diagram technique, we calculate the coefficient \( \alpha(Q) \) in the Ginzburg-Landau expansion which is the electron-electron vertex in the Cooper channel in the presence of nonmagnetic impurities. It is given by a sum of ladder diagrams which are an alternating sequence of blocks of two normal metal Green functions \( G_\lambda = (i\omega - \xi - \lambda H \sin \varphi_p + \frac{1}{\tilde{H}} \text{sgn} \omega)^{-1} \) and an impurity line. In every block momenta on the upper and lower lines are opposite whereas the chiralities are the same. \( T_c(H) \) line is found from \( \min_Q \alpha(Q) = 0 \), where

\[
K(\omega, H, \tau, Q) = 4\pi \frac{I_{\alpha}^2 [1 - I_{\alpha}^2]}{(1 - I_{\alpha}^2) [1 - I_{\alpha}^2] - (I_{\alpha}^2)^2},
\]

where \( I_{\alpha,\beta} = I_0^\alpha + \frac{2}{\alpha} \) are functions of \( (T, H, \tau, Q) \), \( I_0^\alpha = (\alpha^2 + \lambda H^2)^{-1/2} / 4\alpha \), \( I_1^\alpha = i(\omega I_0^\alpha - \frac{1}{\tilde{H}})/H\lambda \), \( I_2^\alpha = \alpha I_0^\alpha / H\lambda \), \( \omega = \omega + \frac{1}{\tilde{H}} \). At \( H = 0 \) time-reversal symmetry is recovered and Eq. (13) simplifies to \( K = 2/\omega \) independently on disorder, in agreement with Anderson theorem. We evaluate numerically \( \alpha'' = \partial^2 \alpha(Q)/\partial Q^2 \) along the the transition line \( \alpha(T, H, Q) = 0 \). At \( \tau T_0 / \hbar \leq 0.11 \) we found \( \alpha'' > 0 \) at any \( H \), i.e. both stripe and helical state disappear from the phase diagram at \( \tau \leq \hbar / 9T_0 \). Similar condition for usual LOFF state is more stringent, cf. [13]. In the dirty limit \( \tau T_0 \ll 1 \) the kernel \( K \) simplifies to \( K = 2/(\omega + 2H^2\tau + v_F^2Q^2\tau/4) \). From this form of \( K \) one easily concludes that the paramagnetic critical field \( \alpha'' \) grows with increase of disorder as \( H_p = \sqrt{\pi T_0 / 4\tau C} \), cf. similar result in [14].

The phase diagram Fig. was obtained neglecting small parity-breaking term of the order \( \alpha/v_F \ll 1 \) in the thermodynamic potential: \( \delta \Omega = \eta Q \) with \( \eta = -\alpha/2 \sum f(H, \omega) \), where function \( f \) is defined for the clean case in Eq. (11). Taking this term into account while minimizing \( \Omega \), one finds that uniform BCS state transforms into a weakly helical state (predicted phenomenologically in [15]) with small wave-vector \( \tilde{Q} \approx \frac{2\alpha H}{v_F} \) and without supercurrent (homogeneous state would carry supercurrent, as was found in [15], but it is not the ground-state). The line of 2nd order transition \( LT \) broadens then into a sharp cross-over region between two helical states with small and large values of \( Q \). Within this crossover region, the superfluid density tensor is strongly anisotropic, with \( \eta_{yy}/\eta_{xx} \sim (\alpha/v_F)^{2/3} \). In the dirty limit long-wavelength helical modulation is present everywhere in superconducting state; near the transition line its wave-vector \( \tilde{Q} = \frac{2\alpha H}{v_F} \)

We have calculated \( T_c(H) \) line within mean-field approximation (MFA), those accuracy is usually of order \( T_c/\epsilon_F \) for clean 2D superconductor: actual transition is of Berezinsky-Kosterlitz-Thouless vortex depairing type, and is shifted downwards in temperature by about \( T_c/\epsilon_F \). In our system fluctuations are enhanced strongly around \( L \) and \( S \) points. Near the \( L \) point it is due to smallness of \( \eta_{yy} \), and the enhancement factor is of the order of \( \sqrt{\eta_{yy}/\eta_{xx}} \sim (\alpha/v_F)^{-1/3} \). In the vicinity of the point \( S \) fluctuations are enhanced due to extended \( U(2) \) symmetry of the order parameter; 2D renormalization group calculation shows that \( U(2) \) fluctuation modes shift actual \( T_c \) by \( \Delta T_c \approx 4(T_c/\epsilon_F) \log \beta_x/\beta_y \) downwards at \( \beta_x \ll \beta_y \). In result, phase transition line \( T_c(H) \) is deformed in the vicinities of \( L \) and \( S \) points, as shown on Fig. 1.

In conclusions, we have demonstrated an existence of three different superconductive states (two helical states and stripe state) in clean surface superconductor in parallel magnetic field, and have located transition lines between them. Strong disorder eliminates short-wavelength helical and stripe states, whereas long-wavelength helical state survives. We thank P. M. Ostrovsky and M. A. Skvortsov for many useful discussions. This research was supported by SCOPES grant, RFBR grant 01-02-17759, Russian ministry of science and Program "Quantum macrophysics" of RAS. O. V. Dimitrova is grateful to Dynasty Foundation for financial support.

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