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FERMION ZERO MODES ON VORTICES IN CHIRAL SUPERCONDUCTORS.

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The energy levels of the fermions bound to the vortex core are considered for the general case of chiral superconductors. There are two classes of chiral superconductivity: in the superconducting state of class I the axisymmetric singly quantized vortex has the same energy spectrum of bound states as in s-wave superconductor: $E = (n + 1/2)\omega_0$ with integral n. In the class II the corresponding spectrum is $E = n\omega_0$ and thus contains the state with exactly zero energy. The effect of a single impurity on the spectrum of bound state is also considered. For the class I the spectrum acquires the double period $\Delta E = 2\omega_0$ and consists of two equidistant sets of levels in accordance with Larkin and Ovchinnikov in Phys. Rev. **B57**, 5457 (1998) [1]. The spectrum is not influenced by a single impurity if the same approximation is applied for the class II states.

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Introduction. The low-energy fermions bound to the vortex core play the main role in the thermodynamics and dynamics of the vortex state in superconductors and Fermi-superfluids. The spectrum of the low-energy bound states in the core of the axisymmetric vortex with winding number $m = \pm 1$ in the isotropic model of s-wave superconductor was obtained in microscopic theory by Caroli, de Gennes and Matricon [2]:

$$E_n = \omega_0 \left(n + \frac{1}{2}\right) . \quad (1)$$

This spectrum is two-fold degenerate due to spin degrees of freedom. The integral quantum number n is related to the angular momentum of the fermions $n = -mL_z$. The level spacing is small compared to the energy gap of the quasiparticles outside the core, $\omega_0 \sim \Delta^2/E_F \ll \Delta$. So, in many physical cases the discreteness of n can be neglected and one can apply the quasiclassical approach to calculate the energy spectrum. Using this simplified approach one obtaines that the spectrum crosses zero energy as a function of continuous angular momentum L_z. So, one has the fermion zero modes. The fermions in this 1D "Fermi liquid" are chiral: the positive energy fermions have a definite sign of the angular momentum L_z. In general case of arbitrary winding number m, the number of fermion zero modes, i.e. the number of branches crossing zero level, equals $-2m$ (see Ref.[3]). This represents an analogue of the index theorem known in the relativistic quantum field theory.

At low temperature $T \sim \omega_0$ the discrete nature of the spectrum becomes important. The quantization of the zero modes was obtained within the quasiclassical approach using the Bohr–Sommerfeld scheme [4]. However the term 1/2 in Eq.(1), which came from the phase shift, was missing in this approach and was restored only after using the general symmetry arguments in Ref.[5]. Here we extend the quasiclassical approach and obtain an exact quantization rule. We find that with respect to the phase shift the superconducting/superfluid states can be divided into 2 classes: In the states of class I the spectrum of bound states in the $m = \pm 1$ vortices is the same as in Eq.(1). In the states of class II the corresponding spectrum is:

$$E_n = \omega_0 n \ , \tag{2}$$

it contains the state with $n = 0$, which has exactly zero energy. The repesentatives of this class are the superfluid ^{3}He-A, where the existence of the zero-energy bound state was first calculated by Kopnin and Salomaa in a microscopic theory [6], and possibly the layered superconductor Sr_2RuO_4, where the chiral p-wave superconductivity is suggested [7].

Using the quasiclassical approach we also consider how the spectrum changes under the influence of a single impurity in the vicinity of the vortex core. We find that the Larkin – Ovchinnikov result obtained for s-wave vortex [1, 8] is valid only for the class I of superconducting states.

Quasiclassical approach to bound states in the vortex core. In this approach developed in [3, 9, 4], the fast radial motion of the fermions in the vortex core is integrated out and one obtains only the slow motion corresponding to the fermion zero modes. Since many properties of the fermion zero modes do not depend on the exact structure of the order parameter and vortex core, we consider for simplicity the following pairing states

$$\text{spin singlet}: \ \ \mathbf{\Delta} = \Delta(\mathbf{r})(\hat{p}_x + i\hat{p}_y)^N \hat{p}_z^{l-|N|} \ , \ \text{odd } l \ , \tag{3}$$

$$\text{spin triplet}: \ \ \mathbf{\Delta} = \sigma_z \Delta(\mathbf{r})(\hat{p}_x + i\hat{p}_y)^N \hat{p}_z^{l-|N|} \ , \ \text{even } l. \tag{4}$$

Here $\hat{\mathbf{p}}$ is the direction of the quasiparticle momentum; N and $l \geq |N|$ are integers; σ_z is the Pauli matrix for conventional spin. The chiral superconductors are characterized by the nonzero value of the index N, which in our simple case represents the projection of the orbital angular momentum l of Cooper pair along the axis z. For example, the s-wave superconductor has numbers $N = l = 0$ in Eq.(3), while the triplet p-wave ($l = 1$) superconductor with the order parameter of the ^{3}He-A type is specified by the numbers $|N| = l = 1$ in Eq.(4). The index N is also the topological invariant in the momentum space, which is responsible for the Chern – Simons terms in the 2D superfluids/superconductors (see Refs.[10 – 12], that is why it is well determined even in the case, when the momentum l and its projection are not determined.

We assume the following structure of the order parameter in the core:

$$\Delta(\mathbf{r}) = \Delta(r)e^{im\phi} \ , \tag{5}$$

where z, r, ϕ are the coordinates of the cylindrical system with the axis z along the vortex line.

The Bogoliubov – Nambu Hamiltonian for quasiparticles is given by

$$\mathcal{H}_{\mathbf{p}} = \begin{pmatrix} \frac{p^2-p_F^2}{2m_e} & \mathbf{\Delta} \\ \mathbf{\Delta}^* & -\frac{p^2-p_F^2}{2m_e} \end{pmatrix} . \tag{6}$$

In the quasiclassical approach it is assumed that the characteristic size ξ of the vortex core is much larger than the wave length: $\xi p_F \gg 1$. In this quasiclassical limit the description in terms of trajectories is most relevant. The trajectories are almost the straight lines. The low energy trajectories are characterized by the momentum $\mathbf{q}$ of the incident quasiparticle on the Fermi surface, i.e. with $|\mathbf{q}| = p_F$, and the impact parameter b. Let us consider for simplicity the 2D or layered superconductors, so that $\mathbf{q} = p_F(\hat{\mathbf{x}}\cos\theta + +\hat{\mathbf{y}}\sin\theta)$. Then substituting $\Psi \to e^{i\mathbf{q}\cdot\mathbf{r}}\Psi$ and $\mathbf{p} \to \mathbf{q} - i\nabla$, and expanding in small ∇, one obtains the quasiclassical Hamiltonian for the fixed trajectory $\mathbf{q}, b$:

$$\mathcal{H} = -i\tau_3\mathbf{v}_F\cdot\nabla + \Delta(r)\left(\tau_1\cos(N\theta + m\phi) - \tau_2\sin(N\theta + m\phi)\right) \ , \ \mathbf{v}_F = \frac{\mathbf{q}}{m_e} \ . \quad (7)$$

We omitted spin indices, since they are not important for the spectrum in superconducting states under consideration.

Since the spatial derivative is along the trajectory it is convinient to choose the coordinate system: $s = r\cos(\phi - \theta)$ – the coordinate along the trajectory, and $b = r\sin(\phi - \theta)$ (see e.g. [6]). In this system the Hamiltonian is

$$\mathcal{H} = -iv_F\tau_3\partial_s + \tau_1\Delta(r)\cos\left(m\tilde{\phi} + (m+N)\theta\right) - \\ -\tau_2\Delta(r)\sin\left(m\tilde{\phi} + (m+N)\theta\right) \ , \quad \tilde{\phi} = \phi - \theta \ . \quad (8)$$

The dependence of the Hamiltonian on the direction θ of the trajectory can be removed by the following transformation:

$$\Psi = e^{i(m+N)\tau_3\theta/2}\tilde{\Psi}, \quad (9)$$

$$\tilde{\mathcal{H}} = e^{-i(m+N)\tau_3\theta/2}\mathcal{H}e^{i(m+N)\tau_3\theta/2} = -iv_F\tau_3\partial_s + \\ +\Delta(\sqrt{s^2+b^2})\left(\tau_1\cos m\tilde{\phi} - \tau_2\sin m\tilde{\phi}\right), \quad (10)$$

$$\tan\tilde{\phi} = \frac{b}{s}. \quad (11)$$

Now θ enters only the boundary condition for the wave function, which according to Eq.(9) is

$$\tilde{\Psi}(\theta + 2\pi) = (-1)^{m+N}\tilde{\Psi}(\theta) \quad (12)$$

With respect to this boundary condition, there are two classes of vortices: with odd and even $m + N$. The quantum spectrum of fermions in the core is essentially determined by this condition. Let us consider vortices with $m = \pm 1$.

The quasiclassical Hamiltonian in Eq.(11) is the same as for the s-wave vortex and thus can be treated in the same manner as in Ref.[3]. The state with the lowest energy corresponds to trajectories, which cross the center of the vortex, i.e. with $b = 0$. Along this trajectory one has $\sin\tilde{\phi} = 0$ and $\cos\tilde{\phi} = \text{sign}\ s$. So that the Eq.(11)

$$\tilde{\mathcal{H}} = -iv_F\tau_3\partial_s + \tau_1\Delta(|s|)\text{sign}\ s \quad (13)$$

becomes supersymmetric and thus contains the eigenstate with zero energy. Let us write the corresponding eigen function including all the transformations:

$$\Psi_0(s,\theta,b=0) = e^{ip_F s} e^{i(m+N)\tau_3\theta/2} \begin{pmatrix} 1 \\ -i \end{pmatrix} \psi_0(s) \ ,$$

$$\psi_0(s) = \exp\left(-\int^s ds' \mathrm{sign}\ s' \frac{\Delta(|s'|)}{v_F}\right) . \tag{14}$$

When b is small the third term in Eq.(11) can be considered as perturbation and this gives the energy levels in terms of b and thus in terms of the angular momentum $L_z = p_F b$:

$$E(L_z,\theta) = -mL_z\omega_0 \ , \ \omega_0 = \frac{\int_{-\infty}^{\infty} ds |\psi_0(s)|^2 \frac{\Delta(|s|)}{p_F|s|}}{\int_{-\infty}^{\infty} ds |\psi_0(s)|^2} \tag{15}$$

The next step is the quantization of motion in the θ, L_z plane. Since the angle and momentum are canonically conjugated variable, the quantized energy levels are obtained from the quasiclassical energy in Eq.(15), if L_z is considered as an operator. The Hamiltonian

$$H(\theta) = im\omega_0\partial_\theta \tag{16}$$

has the eigenfunctions $e^{-iE\theta/m\omega_0}$. The boundary condition, the Eq.(12), gives the following quantization of the energy levels for $m = \pm 1$ vortices

$$E_n = n\omega_0, \ \text{odd} \ N; \ E_n = \left(n + \frac{1}{2}\right)\omega_0, \ \text{even} \ N. \tag{17}$$

Effect of single impurity. As distinct from the Andreev scattering in the vortex core, which leads to the bound states, the microscopic impurity leads to the conventional elastic scattering in which the momentum $\mathbf{q}$ of quasiparticle changes and thus the transition between different trajectories occurs. In the limit of low energy of the quasiparticle the impact parameter b of the scattered particle is close to zero and thus is smaller than the distance R from impurity to the center of the vortex, which is of order ξ. If we assume the atomic size of impurity, then the scattering of the low-energy quasiparticle occurs only between two trajectories which cross simultaneously the vortex center and impurity. Thus we are interested in the matrix element between the states with $\theta = \theta_{imp}$ and $\theta = \pi + \theta_{imp}$ [8]. In the general case this coupling has a form

$$\mathcal{H}_{imp} = 2\lambda e^{i\gamma}\psi(\pi + \theta_{imp})\psi^*(\theta_{imp}) + 2\lambda e^{-i\gamma}\psi^*(\pi + \theta_{imp})\psi(\theta_{imp}) \ . \tag{18}$$

Together with free Hamiltonian in Eq.(16) this gives the following Schrödinger equation for the motion in θ-space:

$$im\omega_0\frac{\partial\psi}{\partial\theta} + 2\lambda e^{i\gamma}\delta(\theta - \theta_{imp})\psi(\pi + \theta_{imp}) +$$

$$+ 2\lambda e^{-i\gamma}\delta(\theta - \pi - \theta_{imp})\psi(\theta_{imp}) = E\psi(\theta) \ , \tag{19}$$

with boundary condition

$$\psi(\theta + 2\pi) = \pm\psi(\theta) \ . \tag{20}$$

Here the sign $-$ and $+$ is for the $|m| = 1$ vortex in class I and class II superconducting states correspondigly. The solution of these equations give the energy eigenvalues:

$$\cos\frac{\pi E}{\omega_0} = \frac{2\omega_0\lambda}{\omega_0^2+\lambda^2}\sin(m\gamma) \quad , \quad |m|=1 \quad , \quad \text{class I} \; , \tag{21}$$

$$\sin\frac{\pi E}{\omega_0} = \frac{2\omega_0\lambda}{\omega_0^2+\lambda^2}\cos\gamma \quad , \quad |m|=1 \quad , \quad \text{class II} \; . \tag{22}$$

For the class I of superconducting states the Eq.(21) is similar to Eq.(2.10) of Ref.[8] obtained for the s-wave case: the spectrum in the presence of impurity has the double period $\Delta E = 2\omega_0$ and consists of two equdistant sets of levels. These two sets transform to each other under symmetry transformation $E \to -E$, which is the analogue of CPT-symmetry.

For the class I of states the Eq.(22) also gives two sets of levels with the alternating shift. But the two sets are not mutually symmetric with respect to $E = 0$. This contradicts to the CPT-symmetry of the system. The only way to reconcile the Eq.(22) with this symmetry is to assume that because of the CPT-symmetry either (i) there is no coupling between the two trajectories; or (ii) the phase of the coupling is fixed, $\gamma = \pi/2$. Then the energy levels are $E_n = n\omega_0$, i.e. the same as without impurities. Thus the same CPT-symmetry, which is responsible for the eigenstate with $E = 0$, provides the rigidity of the spectrum.

Now we shall show that in the simplest model of the impurity potential $H_{imp} = U\tau_3\delta(\mathbf{r}-\mathbf{R})$ the coupling between the opposite trajectories does disappear for the superconducting states of class II. Let us consider the lowest energy trajectories; they cross the center of the vortex, as a result $\delta(\mathbf{r}-\mathbf{R}) = \delta(s-R)\delta(\theta-\theta_{imp})/R$. The matrix element between two wave functions in Eq.(14) corresponding to the opposite trajectories, i.e. which angles θ differ by π, is proportional to

$$\lambda e^{i\gamma} \sim \frac{U}{R\xi} e^{2ip_F R} \exp\left(-\frac{2}{v_F}\int_0^R dr\Delta(r)\right)\begin{pmatrix}1 & i\end{pmatrix}\left[\tau_3 e^{i(m+N)\tau_3\pi/2}\right]\begin{pmatrix}1\\ -i\end{pmatrix} \; . \tag{23}$$

From the spinor structure it follows that the impurity scattering between the opposite trajectories disappears, $\lambda = 0$, for vortices with even $m+N$. Thus in the superconducting states of class II the spectrum of fermions in the $m = \pm 1$ vortices is not influenced by the single impurity.

Conclusion. The phase $(m+N)\tau_3\theta/2$ in Eq.(9) plays the part of Berry phase. It shows how the wave function of quasiparticle changes, when the trajectory is rotating by angle θ. This Berry phase is instrumental for the Bohr–Sommerfeld quantization of the energy levels in the vortex core. It chooses between the two possible quantizations consistent with the CPT-symmetry of states in superconductors: $E_n = n\omega_0$ and $E_n = (n+1/2)\omega_0$.

The same phase is also important for the effect of single impurity on the spectrum of bound states. We found that if in a pure superconductor the spectrum is $E_n = (n+1/2)\omega_0$, the impurity splits it into two series according to the Larkin–Ovchinnikov prescription [1, 8]. However if the initial spectrum is $E_n = n\omega_0$ (an example is $m = \pm 1$ vortex in the chiral p-wave superconductor, where $N = 1$) then the impurity does not change this spectrum. This rigidity of the spectrum must be taken into account when the effect of randomness due to many impurities is considered and new level statistics for the fermionic spectrum in the core is introduced [13]. The existence of the level with exactly zero energy can essentially change the estimation [14] of the fractional charge carried by the vortex core in chiral superconductors.

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