Flat band in the core of topological defects: bulk-vortex correspondence in topological superfluids with Fermi points

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We consider the dimensional crossover in the topological matter, which involves the transformation of different types of topologically protected zeroes in the fermionic spectrum. In the considered case, the multiple Dirac (Fermi) point in quasi 2-dimensional system evolves into the flat band on the surface of the 3-dimensional system when the number of atomic layers increases. This is accompanied by formation of the spiral nodal lines in the bulk. We also discuss the topological quantum phase transition at which the surface flat band shrinks and changes its chirality, while the nodal spiral changes its helicity.

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1. INTRODUCTION

When the fermion zero modes localized on the surface or on the topological defects are studied in topological media, the investigation is mainly concentrated on the fully gapped topological media, such as topological insulators and superfluids/superconductors of the ³He-B type [1, 2, 3]. However, the gapless topological media may also have fermion zero modes with interesting properties, in particular they may have the dispersionless branch of spectrum with zero energy – the flat band [4, 5].

The dispersionless bands, where the energy vanishes in a finite region of the momentum space, have been discussed in different systems. Originally the flat band has been discussed in the fermionic condensate – the Khodel state [6, 7, 8, 9], and for fermion zero modes localized in the core of vortices in superfluid ³He-A [10, 11, 12]. The flat band has also been discussed on the surface of the multi-layered graphene (see [13, 14] and references therein). In particle physics, the Fermi band (called the Fermi ball) appears in a 2+1 dimensional nonrelativistic quantum field theory which is dual to a gravitational theory in the anti-de Sitter background with a charged black hole [15].

Recently it was realized that the flat band can be topologically protected in gapless topological matter. It appears in the 3D systems which contain the nodal lines in the form of closed loops [4] or in the form of spirals [5]. In these systems the surface flat band emerges on the surface of topological matter. The boundary of the surface flat band is bounded by the projection of the nodal loop or nodal spiral onto the corresponding surface. Here we extend this bulk-surface correspondence to the bulk-vortex correspondence, which relates the flat band of fermion zero modes in the vortex core to the topology of the point nodes (Dirac or Fermi points) in the bulk 3D topological superfluids.

2. VORTEX-DISGYRATION

As generic example we consider topological defect in 3D spinless chiral superfluid/superconductor of the ³He-A type, which contains two Fermi points (Dirac points). Fermions in this chiral superfluid are described by Hamiltonian

$$H = \tau_3 \epsilon(p) + c \left(\tau_1 \mathbf{p} \cdot \mathbf{e}_1 + \tau_2 \mathbf{p} \cdot \mathbf{e}_2\right) \quad , \quad \epsilon(p) = \frac{p^2 - p_F^2}{2m},$$
(1)

where $\tau_{1,2,3}$ are Pauli matrices in the Bogoliubov-Nambu space, and in bulk liquid the vectors \mathbf{e}_1 and \mathbf{e}_2 are unit orthogonal vectors. There is only one topologically stable defect in such superfluid/superconductor, since the homotopy group $\pi_1(G/H) = \pi_1(SO_3) = Z_2$. We choose the following order parameter in the topologically non-trivial configuration (in cylindrical coordinates $\mathbf{r} = (\rho, \phi, z)$):

$$\mathbf{e}_1(\mathbf{r}) = f_1(\rho)\hat{\boldsymbol{\phi}} , \ \mathbf{e}_2(\mathbf{r}) = \hat{\mathbf{z}}\sin\lambda - f_2(\rho)\hat{\boldsymbol{\rho}}\cos\lambda , \ (2)$$

with $f_{1,2}(0) = 0$, $f_{1,2}(\infty) = 1$. The unit vector $\hat{\mathbf{l}}$, which shows the direction of the Dirac points in momentum space, $\mathbf{p}_{\pm} = \pm p_F \hat{\mathbf{l}}$, is

$$\hat{\mathbf{l}}(\mathbf{r}) = \frac{\mathbf{e}_1 \times \mathbf{e}_2}{|\mathbf{e}_1 \times \mathbf{e}_2|} = \frac{f_2(\rho)\hat{\mathbf{z}}\cos\lambda + \hat{\rho}\sin\lambda}{\sqrt{f_2^2(\rho)\cos^2\lambda + \sin^2\lambda}}.$$
 (3)

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Asymptotically at large distance from the vortex core one has

$$\mathbf{e}_{1}(\rho = \infty) = \boldsymbol{\phi} \quad , \quad \mathbf{e}_{2}(\rho = \infty) = \hat{\mathbf{z}}\sin\lambda - \hat{\boldsymbol{\rho}}\cos\lambda \, , \\ \hat{\mathbf{l}}(\rho = \infty) = \hat{\mathbf{z}}\cos\lambda + \hat{\boldsymbol{\rho}}\sin\lambda \, , \tag{4}$$

which means that changing the parameter λ one makes the continuous deformation of the pure phase vortex at $\lambda = 0$ to the disgyration in the $\hat{\mathbf{l}}$ vector without vorticity at $\lambda = \pi/2$, and then to the pure vortex with opposite circulation at $\lambda = \pi$ (circulation of the superfluid velocity around the vortex core is $\oint d\mathbf{s} \cdot \mathbf{v}_{s} = \kappa \cos \lambda$, where $\kappa = \pi \hbar/m$). We consider how the flat band in the core of the defect evolves when this parameter λ changes. In bulk, i.e. far from the vortex core, the Dirac points are at

$$\mathbf{p}_{\pm} = \pm p_F \hat{\mathbf{l}}(\rho = \infty) = \pm p_F \left(\hat{\mathbf{z}} \cos \lambda + \hat{\boldsymbol{\rho}} \sin \lambda\right) \,. \tag{5}$$

Due to the bulk-vortex correspondence, which we shall discuss in the next section, the projection of these two points on the vortex axis gives the boundary of the flat band in the core of the topological defect:

$$E(p_z) = 0$$
 , $p_z^2 < p_F^2 \cos^2 \lambda$. (6)

This is the central result of the paper: in general the boundaries of the flat band in the core of the linear topological defect (a vortex) are determined by the projections on the vortex axis of the topologically protected point nodes in bulk. In the next section we consider the topological origin of the flat band and geometrical derivation of its boundaries. In Sec. 4, the boundaries of the flat band (6) are obtained analytically.

3. BULK-VORTEX CORRESPONDENCE

Let us first give the topological arguments, which support the existence of the flat band inside the vortexdisgyration line. Let us consider the Hamiltonian (1) in bulk (i.e. far from the vortex core) treating the projection p_z as parameter of the 2D system. At each p_z except for two values $p_z = \pm p_F \cos \lambda$ corresponding to two Fermi points (see Fig. 1), the Hamiltonian has fully gapped spectrum and thus describes the effective 2D insulator. One can check that this 2D insulator is topological for $|p_z| < p_F |\cos \lambda|$ and is topologically trivial for $|p_z| > p_F |\cos \lambda|$. For that one considers the following invariant describing the 2D topological insulators or fully gapped 2D supefluids [16]:

$$\tilde{N}_{3}(p_{z}) = \frac{1}{4\pi^{2}} \operatorname{tr} \left[\int dp_{x} dp_{y} d\omega \ G \partial_{p_{x}} G^{-1} G \partial_{p_{y}} G^{-1} G \partial_{\omega} G^{-1} \right],$$
(7)

where G is the Green's function matrix, which for noninteracting case has the form $G^{-1} = i\omega - H$. This invariant, which is applicable both to interacting and non-interacting systems, gives

$$\tilde{N}_3(p_z) = 1$$
 , $|p_z| < p_F |\cos \lambda|$, (8)

$$N_3(p_z) = 0$$
 , $|p_z| > p_F |\cos \lambda|$. (9)



Projections of Dirac (Fermi) points on Fig. 1. the direction of the vortex axis (the z-axis) determine the boundaries of the flat band in the vortex core. Fermi point in 3D systems represents the hedgehog (monopole) in momentum space [16]. For each plane $p_z = \text{const}$ one has the effective 2D system with the fully gapped energy spectrum $E_{p_z}(p_x, p_y)$, except for the planes with $p_{z\pm} = \pm p_F \cos \lambda$, where the energy $E_{p_z}(p_x, p_y)$ has a node due to the presence of the hedgehogs in these planes. Topological invariant $\tilde{N}_3(p_z)$ in (7) is non-zero for $|p_z| < p_F |\cos \lambda|$, which means that for any value of the parameter p_z in this interval the system behaves as a 2D topological insulator or 2D fully gapped topological superfluid. Point vortex in such 2D superfluids has fermionic state with exactly zero energy. For the vortex line in the original 3D system with Fermi points this corresponds to the dispersionless spectrum of fermion zero modes in the whole interval $|p_z| < p_F |\cos \lambda|$ (thick line).

At $p_z = \pm p_F |\cos \lambda|$, there is the topological quantum phase transition between the topological 2D "insulator" and the non-topological one. The difference of 2D topological charges on two sides of the transition, $\tilde{N}_3(p_z = p_F \cos \lambda + 0) - \tilde{N}_3(p_z = p_F \cos \lambda - 0) = N_3$, represents the topological charge of the Dirac point in the 3D system – hedgehog in momentum space [16]. As we know, the topological quantum phase transitions are accompanied by reconstruction of the spectrum of fermions bound to the topological defect: fermion zero modes appear or disappear after topological transition in bulk [2, 17, 18, 19]. For the pure vortex, i.e. at $\lambda = 0$ or $\lambda = \pi$, we know from [10] that the vortex contains the fermionic level with exactly zero energy for any p_z in the region $|p_z| < p_F$, i.e. in the region of parameters where the 2D medium has non-trivial topological charge, $\tilde{N}_3 = 1$. On the other hand no such levels are present after the topological transition to the state of matter with $\tilde{N}_3 = 0$.

The similar reconstruction of the spectrum at the topological quantum phase transition takes place for any parameter $\lambda \neq \pi/2$ of the considered defect. This can be understood using the topology in the mixed real and momentum space [20, 21]. To study fermions with zero energy (Majorana fermions) in the core of a point vortex in a 2D topological superconductor, the Pontryagin invariant for mixed space has been exploited in Ref. [1]. The Pontryagin invariant describes classes of mappings $S^2 \times S^1 \to S^2$. Here the mixed space $S^2 \times S^1$ is the space (p_x, p_y, ϕ) , where ϕ is the coordinate around the vortex-disgyration far from the vortex core. This space is mapped to the sphere S^2 of unit vector $\hat{\mathbf{g}}(p_x, p_y, \phi) = \mathbf{g}(p_x, p_y, \phi) / |\mathbf{g}(p_x, p_y, \phi)|$ describing the 2D Hamiltonian. In our case it is the Hamiltonian (1)outside the vortex core:

$$H_{p_{z},\lambda}(p_{x}, p_{y}, \phi) = \tau_{i}g^{i}(p_{x}, p_{y}, \phi; p_{z}, \lambda), \quad (10)$$

$$g^{3} = \frac{p_{x}^{2} + p_{y}^{2}}{2m} - \mu(p_{z}) , \quad \mu(p_{z}) = \frac{p_{F}^{2} - p_{z}^{2}}{2m}, \quad g^{1} = c(p_{y}\cos\phi - p_{x}\sin\phi), \quad g^{2} = c(p_{z}\sin\lambda - \cos\lambda(p_{x}\cos\phi + p_{y}\sin\phi)), \quad (11)$$

with p_z and λ being the parameters of this effective 2D Hamiltonian. The Pontryagin Z_2 invariant is non-trivial and thus the zero energy state exists in the core of the defect the effective 2D superconductor, if the parameters p_z and λ of the 2D Hamiltonian (10) satisfy condition $|p_z| < p_F |\cos \lambda|$.

For the considered linear topological defect (vortexdisgyration) in the 3D system this implies that the core of this defect contains the dispersionless band in the interval of momentum $|p_z| < p_F |\cos \lambda|$, i.e. one obtains equation (6).

4. FLAT BAND FROM QUASI-CLASSICAL APPROACH

Let us now support the above topological arguments by explicit calculation of the fermionic flat band in the vortex-disgyration, which is described by the order parameter (2). The Bogoliubov-de Gennes Hamiltonian for fermions localized on the defect line is obtained from (1) by substitution of the classical transverse momentum by the quantum-mechanical operator,

$$\mathbf{p}_{\perp} \to \left(-i\nabla_x, -i\nabla_y\right),\tag{12}$$

while p_z remains the good quantum umber which serves as parameter of the effective 2D system. The zero energy states in this 2D system can be studied using the quasiclassical approximation, see details in Chapter 23 of the book [16]. For our purposes it is sufficient to consider the Hamiltonian on the trajectory *s* which crosses the center of the vortex. The modification of quasiclassical Hamiltonian in Eq.(23.16) in [16] for the considered vortex-disgyration is

$$H_{qcl}(p_z) = -i\frac{q}{m}\tau_3\partial_s + U(s)\tau_2,$$

$$U(s) = cp_z \sin\lambda - cqf_2(|s|)\mathrm{sign}(s)\cos\lambda, \qquad (13)$$

$$q = \sqrt{p_F^2 - p_z^2}.$$

The Hamiltonian $H_{qcl}(p_z)$ is super-symmetric if the asymptotes of the potential U(s) have different sign for $s = -\infty$ and $s = +\infty$. The latter takes place if

$$|p_z|\sin\lambda < q|\cos\lambda|. \tag{14}$$

The super-symmetric Hamiltonian $H_{qcl}(p_z)$ has the state with zero energy, $E_{qcl}(p_z) = 0$, for any p_z in the interval (14). For vortices in chiral superfluids it is known [16] that the zero energy state of the quasiclassical Hamiltonian, $E_{qcl} = 0$, automatically results in the true zero energy state, E = 0, obtained in the exact quantum-mechanical problem using the Bogoliubov-de Gennes Hamiltonian. This proves the existence of the flat band in the range of momentum (14), which coincides with equation (6) and is in agreement with the topological analysis in previous section.

5. DISCUSSION

We discussed the 3D matter with topologically protected Fermi points. Topological defects (vortices and vortex disgyrations) in such matter contain the dispersionless fermionic band with zero energy – the flat band. The boundaries of the flat band are determined by projections of the Fermi points on the axis of the topological defect. This bulk-vortex correspondence for flat band is similar to the bulk-surface correspondence discussed in the media with topologically protected lines of zeroes [5, 4]. In the latter case the flat band is formed on the surface of the system, and its boundary is determined by projection of the nodal line (closed loop [4] or spiral [5]) on the corresponding surface.

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