Bogoliubov-Fermi surfaces in non-centrosymmetric multi-component superconductors

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We show that when the time reversal symmetry is broken in a multi-component superconducting condensate without inversion symmetry the resulting Bogoliubov quasiparticles generically exhibit mini Bogoliubov-Fermi (BF) surfaces, for small superconducting order parameter. The absence of inversion symmetry makes the BF surfaces stable with respect to weak perturbations. With sufficient increase of the order parameter, however, the Bogoliubov Fermi surface may disappear through a Lifshitz transition, and the spectrum this way become fully gapped. Our demonstration is based on the computation of the effective Hamiltonian for the bands near the normal Fermi surface by the integration over high-energy states. Exceptions to the rule, and experimental consequences are briefly discussed.

The appearance of the gap in the quasiparticle spectrum of an s-wave superconductor has been one of the defining features of the superconducting state of matter since the conception of the theory of Bardeen, Cooper, and Schrieffer [1]. Many unconventional superconductors of today do not feature a full gap, but still reduce the density of quasiparticle states near the Fermi energy by leaving only lines or points in the momentum space where the gap vanishes. These, however, are not the only possibilities [2–4], and Fermi surfaces of Bogoliubov excitations in the superconducting state are possible as well [5–7]. These arise in superconductors with more than one band participating in pairing, and when the condensate breaks time reversal (TR) symmetry while preserving inversion, which is present in both normal and superconducting phases. The presence of inversion symmetry has been deemed crucial for the appearance and particularly the stability of a Bogoliubov-Fermi (BF) surface, which then comes out topologically protected. The existence of a surface of gapless quasiparticle excitations leads to a finite residual density of states, and has many consequences for the low temperature properties of the superconducting phase. It should be detectable in the temperature dependence of the penetration depth, heat conductivity, and heat capacity at low temperatures, for example [8].

It has been recently found in an example of TR-symmetry-breaking superconducting ground state in a topologically nontrivial (Rarita-Schwinger-Weyl) four-band system that the BF surfaces can form despite the complete lack of inversion symmetry in the superconducting states [9]. Other instances of the same phenomenon have also been considered [10, 11]. The generality of the emergence of the BF-surfaces in materials with no inversion symmetry has not been clear, however, and its possible relevance to the large number of known non-centrosymmetric superconductors [12] is an open issue.

In this paper we show that in a multi-band system without inversion symmetry the spontaneous breaking of TR in the superconducting state generically leads to the formation of a BF surface, at least right below the critical temperature, if the superconducting phase transition is continuous. With an increase of the order parameter the BF surface may eventually shrink to a point and then be replaced by a gap. The latter phenomenon would typically require a strong coupling. Central to our demonstration is the derivation of the effective low-energy Hamiltonian, which may be thought of as a result of iteratively integrating out the energy bands far away from the Fermi energy. It provides more than just a useful approximate picture of the spectrum of Bogoliubov quasiparticles, as we show that the location of the zero modes of the effective Hamiltonian in the momentum space coincides with the location of the BF surface of the original Bogoliubov-de Gennes (BdG) quasiparticle Hamiltonian of arbitrary size. The absence (or presence) of the TR symmetry in the superconducting state governs the algebra behind the computation of the effective Hamiltonian, and dictates the low-energy spectrum. The breaking of the TR symmetry leads to mini BF-surfaces, while the preservation of the TR symmetry leads generically to gapless lines of Bogoliubov quasiparticles, similarly as in inversion-symmetric systems [13].

Bogoliubov-de Gennes Hamiltonian. Consider the quantum-mechanical action for the Bogoliubov quasiparticles in the superconducting state:

\[ S = k_B T \sum_{\omega_n, \mathbf{p}} \Psi^\dagger(\omega_n, \mathbf{p}) \left[ -i \omega_n + H_{\text{BdG}}(\mathbf{p}) \right] \Psi(\omega_n, \mathbf{p}), \]

where the Nambu spinor is

\[ \Psi(\omega_n, \mathbf{p}) = (\psi(\omega_n, \mathbf{p}), T \psi^\dagger(\omega_n, \mathbf{p}))^T, \]

\[ \mathbf{p} \text{ is the momentum, } \omega_n = (2n + 1)\pi k_B T \text{ is the Matsubara frequency, and } T \text{ is the temperature.} \]

\[ \psi = (\psi_1, \ldots, \psi_N) \text{ is a } N \text{-component Grassmann number describing } N \text{ energy bands, and its time reversed counterpart is } T \psi(\omega_n, \mathbf{p}) = U \psi^*(-\omega_n, -\mathbf{p}), \text{ where } U \text{ is the unitary time-reversal operator, and } U \text{ its unitary part.} \]

This way the BdG Hamiltonian becomes:

\[ H_{\text{BdG}}(\mathbf{p}) = \begin{pmatrix} H(\mathbf{p}) - \mu & \Gamma \\ \Gamma^\dagger & -[H(\mathbf{p}) - \mu] \end{pmatrix}. \]

We assume that the N-dimensional Hamiltonian \( H(\mathbf{p}) \) is only TR-symmetric, so that \( U^\dagger H(\mathbf{p}) U = H^*(-\mathbf{p}) \). Recalling that it is also Hermitian and \( H^*(\mathbf{p}) = H^T(\mathbf{p}) \), the action in Eq. (1) would assume its textbook form.
For simplicity we also assume that the $N$-dimensional pairing matrix $\Gamma$ is constant, so that the pairing term is local in real space, $\sim \bar{\Psi}^\dagger(x,\tau)\Gamma\Psi(x,\tau)$. The matrix $\Gamma$ can then be expanded as $\Gamma = \sum_a \Delta_a M_a$, where $\Delta_a = \Delta_n + i\Delta_n$ are complex order parameters, and $M_a$ Hermitian matrices that form a basis. It is easy to check that the fermionic statistics then implies that all $M_a$ need to be even under TR when $\langle T \rangle^2 = -1$ [13, 14]. In the case of pairing of the (fictitious) spinless fermions for which $\langle T \rangle^2 = +1$, the matrices $M_a$ would need to be TR-odd [11]. Our method will work for both cases, and can also be easily generalized to momentum-dependent pairing.

The BdG Hamiltonian in Eq. (2) can thus also be written as

$$H_{\text{BdG}} = \sigma_3 \otimes [H(p) - \mu] + \sum_a (\Delta_a \sigma_1 \otimes M_a - \Delta_2 \sigma_2 \otimes M_a),$$

where $\sigma_i$, $i = 1, 2, 3$ are the usual Pauli matrices. The phase common to all $\Delta_n$ is assumed to have been gauged away. If $M_a$ is TR-even, $H_{\text{BdG}}$ is even under the time-reversal operator $\mathbb{1}_{2 \times 2} \otimes T$ only when all $\Delta_2 = 0$. If some $\Delta_2 \neq 0$, and consequently $\Gamma \neq \Gamma^\dagger$, TR is broken in the superconducting phase. For completeness, let us also consider the case when $\langle T \rangle^2 = +1$ when $M_a$ are odd: $H_{\text{BdG}}$ will then be even under $\mathbb{1}_{2 \times 2} \otimes T$ when all $\Delta_1 = 0$. One can then still gauge away the overall phase of $\pi/2$ to have the pairing matrix $\Gamma$ Hermitian. For either type of the TR symmetry, non-Hermiticity of the pairing matrix $\Gamma$ is thus tantamount to breaking of the TR symmetry in the superconducting state.

**Effective Hamiltonian.** Let us define the eigenvalues (bands) and the eigenstates of the normal state Hamiltonian $H(p)$, as $E_i(p)$ and $\phi_i(p)$, $i = 1, \ldots, N$. Take that for every $p$ at the normal state’s Fermi surface there is only one eigenvalue equal to the chemical potential $\mu$, i.e., that the normal Fermi surface is non-degenerate. There could be more than one connected Fermi surface, but without inversion there is no double degeneracy of the Fermi surface at any momentum $p$; the TR alone implies only that if a momentum $p$ belongs to the Fermi surface, the opposite momentum $-p$ does as well. We may call the eigenstate with its energy arbitrarily close to the Fermi surface $\phi_1(p)$ “light”, and the remaining $N-1$ eigenstates “heavy”. This separation may depend on the Fermi surface point under consideration.

The spectrum of the Bogoliubov quasiparticles at a momentum $p$ is given by the solution of the equation for the real frequency $\omega$

$$\det(H_{\text{BdG}}(p) - \omega) = 0.$$  

(4)

With the separation into light and heavy states at a given momentum near the normal Fermi surface one can write the BdG Hamiltonian in the basis $\{\phi_1(p), 0\}^T, (0, \phi_i(p))^T\}, \ i = 1, \ldots, N$ as

$$H_{\text{BdG}}(p) = \begin{pmatrix} H_{\text{f}}(p) & H_{\text{h}}(p) \\ H_{\text{h}}^\dagger(p) & H_{\text{h}}^\dagger(p) \end{pmatrix}.$$  

(5)

The block for the light particle and hole states $H_{\text{f}}(p)$ is a two-dimensional matrix. The heavy modes are described by the $(2(N-1))$-dimensional matrix $H_{\text{h}}(p)$, and the coupling between the light and heavy states $H_{\text{h}}(p)$ is a $2 \times 2(N-1)$ matrix. The above determinant can now be rewritten as

$$\det(H_{\text{BdG}}(p) - \omega) = \det(H_{\text{h}}(p) - \omega) \det L_{\text{ef}}(\omega, p),$$  

(6)

where the effective Lagrangian $L_{\text{ef}}$ is the Schur complement [15] of the block matrix for the heavy modes:

$$L_{\text{ef}}(\omega, p) = H_{\text{f}}(p) - \omega - H_{\text{h}}(p)(H_{\text{h}}(p) - \omega)^{-1}H_{\text{h}}^\dagger(p).$$  

(7)

The first factor in Eq. (6) may be understood as the fermionic partition function at a fixed frequency for the heavy modes, and the second factor is therefore the residual partition function (at fixed frequency) for the light modes, which are modified by the integration over the heavy modes (see Supplementary material). $L_{\text{ef}}(\omega, p)$ is defined whenever the heavy block is invertible, which is the case if $|\omega| < |E_i(p) - \mu|$ for $i \neq 1$. Under this condition the eigenvalue equation in Eq. (4) reduces to

$$\det L_{\text{ef}}(\omega, p) = 0.$$  

(8)

Although $L_{\text{ef}}(\omega, p)$ is only a two-dimensional matrix, its computation involves an inversion of the $2(N-1)$-dimensional matrix, so for a general $\omega$ there is no obvious gain. $\omega = 0$, however, is a solution only when

$$\det H_{\text{ef}}(p) = 0,$$

(9)

with $H_{\text{ef}}(p) = L_{\text{ef}}(0, p)$, and which may be called the effective Hamiltonian. We emphasize that only the solutions for zero modes of $H_{\text{ef}}(p)$ are exactly the same as those for the original $H_{\text{BdG}}(p)$; the rest of their spectra differs. This is, however, all that is needed to understand the emergence of the BF surface, as we show next.

**Bogoliubov-Fermi surface.** The effective Hamiltonian is two-dimensional and thus may be expanded in the Pauli basis

$$H_{\text{ef}} = \sum_{\alpha=0}^3 f_{\alpha}(p) \sigma_{\alpha},$$  

(10)

with $\sigma_0 = \mathbb{1}_{2 \times 2}$. The Eq. (9) can now be written as

$$f_{\alpha}^2(p) - \sum_{i=1}^3 f_i^2(p) = 0.$$  

(11)

We will show that if in some direction in the momentum space the last equation is solved by two different magnitudes $p = p_1$ and $p = p_2$, the emergence of a BF surface follows from continuity:

varying the direction smoothly changes the solutions $p_1$ and $p_2$, until they merge and that way close a surface.

In the normal phase when $\Delta_n = 0$ all the states are decoupled, and there is of course the normal Fermi surface
at which \( f_3(p) = E_i(p) - \mu \) changes sign, and \( f_3(p) \equiv 0 \), for \( \beta = 0, 1, 2 \) (See Fig. 1).

We will show that in the TR-symmetry-breaking superconducting phase \( f_0 = O(\Delta^2) \), \( f_0(p) - (E_1(p) - \mu) = O(\Delta^2) \), whereas \( f_{1,2} = O(\Delta) + O(\Delta^3) \). More explicitly: a finite value of \( f_0 \) introduces a shift of the order \( O(\Delta^2) \) in the energy of the bands of the light particle and hole states, \( f_3(p) - (E_1(p) - \mu) \) introduces a shift in the momentum direction of the energy bands of the light states also of the order \( O(\Delta^2) \), and \( f_{1,2} \) open a gap between the light particle and light hole state of the order \( O(\Delta) + O(\Delta^3) \). Whenever the leading \( O(\Delta) \) contributions to \( f_{1,2} \) vanish somewhere on the normal Fermi surface, there will be two different points at \( p_1 \) and \( p_2 \) where the energy of the quasiparticles is equal to the chemical potential and the BF surface will be nucleated in the superconducting phase provided \( \Delta \) is small enough. The vanishing of the leading order contribution to \( f_{1,2} \) yields two conditions on two polar angles, so the BF surface in form of an inflated point node will in general emerge around particular points near the normal Fermi surface. If the two conditions on the polar angles happen to be the same, the form of the BF surface will be an inflated line node. The principle behind the emergence of the BF surface is depicted in Fig. 1.

When the TR is preserved in the superconducting state, on the other hand, we will find that \( f_i(p) = 0 \) for \( i = 0, 2 \); there is no shift in the energy of the light particle and light hole mode induced by \( f_0 \), but only a shift in the momentum. This implies \( p_1 = p_2 \). Zero-energy solutions are then given by \( f_i(p) = 0 \) for \( i = 1, 3 \), which provides two conditions on three variables, and generally leads to a line of gapless points [10].

**Iterative procedure.** To see how this comes about let us write the BdG Hamiltonian for \( N \) bands in Eq. (5) once again as

\[
H^{(0)}_{\text{BdG},N} = \begin{pmatrix}
H^{(0)}_{1,1} & H^{(0)}_{1,2} & \ldots & H^{(0)}_{1,N} \\
H^{(0)*}_{1,2} & H^{(0)*}_{2,2} & \ldots & H^{(0)*}_{2,N} \\
\vdots & \vdots & \ddots & \vdots \\
H^{(0)*}_{1,N} & H^{(0)*}_{2,N} & \ldots & H^{(0)*}_{N,N}
\end{pmatrix},
\]

(12)

with the two-dimensional blocks as

\[
H_{k,m}^{(0)} = \delta_{k,m} [E_k(p) - \mu] \sigma_3 + \sum_a (\phi^*_a \chi_{\alpha} \phi_m)(\Delta_\alpha \sigma_1 - \Delta_\alpha \sigma_2).
\]

(13)

Note that the diagonal blocks are Hermitian matrices whereas the off-diagonal blocks in general are not.

Using the Schur decomposition [15] again,

\[
det H^{(0)}_{\text{BdG},N} = det H^{(0)}_{N,N} det H^{(1)}_{\text{BdG},N-1},
\]

(14)

where \( H^{(1)}_{\text{BdG},N-1} \) is the Schur complement of the last block on the diagonal \( H^{(0)}_{N,N} \),

\[
H^{(0)}_{\text{BdG},N-1} - H^{(1)}_{\text{BdG},N-1} = \begin{pmatrix}
H^{(0)}_{1,1} \\
H^{(0)*}_{1,2} \\
\vdots \\
H^{(0)*}_{N,N}
\end{pmatrix} \cdot \left( H^{(0)}_{N,N} \right)^{-1} \cdot \begin{pmatrix}
H^{(0)*}_{1,1} \\
H^{(0)*}_{2,2} \\
\vdots \\
H^{(0)*}_{N-1,N}
\end{pmatrix}.
\]

(15)
and as a matrix it consists of \((N - 1) \times (N - 1)\) two-dimensional blocks. One can think of it as the effective Hamiltonian for the \(N-1\) bands after only the \(N\)-th band has been integrated out. This step can be now iterated so that

\[
\det H_{\text{BdG},N}^{(0)} = \det H_{N,N}^{(0)} \det H_{N-1,N-1}^{(1)} \det H_{N-2,N-2}^{(2)} \ldots \det H_{1,1}^{(N-1)},
\]

where each matrix \(H_{N-k,N-k}^{(k)}\) is a two-dimensional “heavy” diagonal block of the effective BdG Hamiltonian at the (intermediate) \(k\)-th stage of the iteration, and the requisite effective Hamiltonian \(H_{\text{ef}}\) for the light states is simply the final \(H_{1,1}^{(N-1)}\). This way no inversion of anything larger than a two-dimensional matrix is ever required, but the price is the tracking of the evolution of the parameters appearing in the effective Hamiltonians of the reduced size.

**Results.** What is the result of this procedure? To answer this question, let us first consider the superconducting state where TR is preserved before we turn to the case where TR is broken.

If the TR is preserved and \(M_e\) is TR-even one can set \(\Delta_{2\alpha} = 0\). Eq. \((15)\) implies that at each iteration one multiplies three matrices which are linear combinations of only \(\sigma_1\) and \(\sigma_3\). Such a multiplication can yield only another linear combination of the same \(\sigma_1\) and \(\sigma_3\), since \(\text{Tr}(\sigma_\mu \sigma_\nu \sigma_\alpha) \equiv 0\) if \(\mu, \nu, \alpha = 1, 3\) and \(\mu = 0, 2\). All the blocks \(H_{N-k,N-k}^{(k)}\) are thus real and traceless, and therefore in the final effective Hamiltonian \(f_\alpha(p) \equiv 0\) for \(\alpha = 0, 2\) at every momentum \(p\) as well. The solution of two equations \(f_\beta(p) = 0\), for \(\beta = 1, 3\) will then in general lead to lines of gapless points in the momentum space.

When TR is broken in the superconductor, the functions \(f_\alpha(p)\) for both \(\alpha = 0\) and \(\alpha = 2\) in general become finite. The result becomes particularly transparent when the superconducting order parameter is small. The leading-order correction to \(H_{1,1}^{(0)}\) in the \(H_{\text{ef}}\) is of second order in the superconducting order parameter, and comes from neglecting all off-diagonal elements in \(H_k\), i.e. ignoring all couplings between only heavy modes. This way one finds

\[
H_{\text{ef}} = H_{1,1}^{(0)} \sum_{k=2}^{N} H_{1,k}^{(0)} (H_{k,k_\Delta_{=0}}^{(0)})^{-1} H_{1,k}^{(0)\dagger} + \mathcal{O}(\Delta^3),
\]

and therefore

\[
f_1(p) - if_2(p) = \phi_1(p) \Gamma \phi_1(p) + \mathcal{O}(\Delta^3),
\]

\[
f_3(p) = E_1(p) - \mu - \sum_{k=2}^{N} \frac{\left|\phi_1(p) \Gamma \phi_k(p)\right|^2 + \left|\phi_1(p) \Gamma \phi_k(p)\right|^2}{2[E_k(p) - \mu]}.
\]
topology. The details of this approach will be presented in a separate publication.

Examples of non-centrosymmetric superconductors with broken TR are believed to include LaNiC$_2$ [12–21], LaNiGa$_2$ [22], La$_7$Ir$_3$ [23], and Ro$_6$Zr [24]. All four materials are also commonly assumed to be fully gapped, however. It would be interesting to identify a non-centrosymmetric material that breaks TR but displays $\sim T^3$ behavior in the specific heat over a range of temperatures, for example. Instead of extending all the way to zero we would predict this behavior crossing over to $\sim T$ at the lowest temperatures, provided the superconductor is weakly coupled and that the BF surface survives. Similar crossovers that would reflect a finite residual density of states in the superconducting phase should be observable in the penetration depth and thermal conductivity as well.

We are grateful to I. Boettcher and C. Timm for many useful discussions and comments. JML is supported by the DFG grant No. LI 3628/1-1, and IFH by the NSERC of Canada.

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I. SUPPLEMENTARY MATERIAL

An alternative to the standard way [15] of arriving at Eqs. (6) and (7) is the (Gaussian) integration over the heavy modes in the partition function for a fixed frequency. Let us write such a partition function defined by the Hamiltonian in Eq. (5):
Changing the Grassmann integration variables in the second integral as

\[ \tilde{\psi}_h = \psi_h + (H_h - \omega)^{-1} H_{lh}^\dagger \psi_l, \]

we thus readily find

\[ Z(\omega) = Z_{\text{eff}}(\omega) \int_{\tilde{\psi}_h} e^{-\tilde{\psi}_h^\dagger (H_h - \omega) \tilde{\psi}_h}, \]

with the effective partition function of the light fermions

\[ Z_{\text{eff}}(\omega) = \int_{\psi_l} e^{-\psi_l^\dagger L_{\text{ef}}(\omega, p) \psi_l}, \]

and with the \( L_{\text{ef}}(\omega, p) \) as defined by Eq. (7). The result in Eq. (6) follows.