Instability of $j = 3/2$ Bogoliubov Fermi-surfaces

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Exotic quantum phases including topological states and non-Fermi liquids may be realized by quantum states with total angular momentum $j = 3/2$, as manifested in HgTe and pyrochlore iridates. Recently, an exotic superconducting state with non-zero density of states of zero energy Bogoliubov quasiparticles, Bogoliubov Fermi-surface (BG-FS), was also proposed in a centrosymmetric $j = 3/2$ system, protected by a $Z_2$ topological invariant. Here, we consider interaction effects of a centrosymmetric BG-FS and demonstrate its instability by using mean-field and renormalization group analysis. The Bardeen-Cooper-Schrieffer (BCS) type logarithmical enhancement is shown in fluctuation channels associated with inversion symmetry. Thus, we claim that the inversion symmetry instability is an intrinsic characteristic of an interacting BG-FS. In drastic contrast to the conventional BCS superconductivity, a Fermi surface may survive under the instability depending on higher order fluctuations. We propose the experimental setup, a second harmonic generation experiment with a strain gradient, to detect the instability. Possible applications to iron based superconductors and heavy fermion systems including FeSe are also discussed.

Introduction: Electrons on a lattice may form quantum states with a total angular momentum $j = 3/2$, especially with strong spin-orbit coupling [1]. Cubic and time reversal symmetries may protect degeneracy of the the four states as in GaAs and HgTe. A minimal model of the $j = 3/2$ band structures were provided by Luttinger, so-called Luttinger Hamiltonian, [2, 3] and its low energy properties have been thoroughly understood, being a backbone of semiconductor physics [4].

Recent advances in topology and correlation research unveil unconventional phases associated with the Luttinger Hamiltonian. Topological insulators may be realized by breaking cubic symmetry, for example applying uniaxial pressure, [5, 6] and Weyl semi-metals may be formed by breaking time reversal symmetry, for example the onset of all-in-all-out order parameter in pyrochlore iridates [7, 8]. In the presence of the long range Coulomb interaction, either non-Fermi liquid or topological states with broken symmetries may be realized with renormalized physical quantities [9], and significant advances in experiments have been reported recently [10–13]. Furthermore, quantum phase transitions between the unconventional phases have been investigated finding new universality classes [14–18].

Exotic superconducting states with $j = 3/2$ states were also proposed [19–26]. In the presence of inversion symmetry, it was proved that a non-interacting Bogoliubov Hamiltonian may host a Fermi surface of Bogoliubov quasiparticles in drastic contrast to conventional nodeless, point node, and line node gap structures, named Bogoliubov Fermi surface (BG-FS). It is characterized by a $Z_2$ topological invariant of the Hamiltonian [19], and several heavy fermion systems such as $\text{URu}_2\text{Si}_2$ and $\text{UB}_1\text{B}_3$ are suggested as candidate material though its presence has not been reported yet [27–30]. It is highly desired to uncover characteristics of a BG-FS for its discovery.

In this work, we propose enhanced fluctuations of an inversion symmetry order parameter as a key property of a centrosymmetric BG-FS. It is shown that a centrosymmetric BG-FS becomes unstable at zero temperature under infinitesimally weak interaction between Bogoliubov quasi-particles. Our results indicate that an inversion order parameter must be included in a phenomenological Ginzburg-Landau functional of a centrosymmetric BG-FS, and we also propose second harmonic generation experiments with strain gradient to identify enhanced fluctuations of an inversion symmetry order parameter.

One Bogoliubov pair problem: Let us consider a generic BG-FS with inversion symmetry. Two Bogoliubov quasi-particles with momentums $\pm \vec{k}$ and additional quantum numbers $\alpha$, for example angular momentum, $(|+\vec{k}, \alpha\rangle, |-\vec{k}, \alpha\rangle)$ are inversion partners. With the inversion symmetry unitary operator $U_{\text{inv}}$, the single particle Hamiltonian with the superscript (1) is characterized by

$$H_B^{(1)}|\vec{k}, \alpha\rangle = \epsilon_k|\vec{k}, \alpha\rangle, \quad U_{\text{inv}}|+\vec{k}, \alpha\rangle = |-\vec{k}, \alpha\rangle.$$ 

The inversion symmetry of the BG-FS, $[H_B^{(1)}, U_{\text{inv}}] = 0$, guarantees $\epsilon_{+\vec{k}}(\alpha) = \epsilon_{-\vec{k}}(\alpha)$.

We define one Bogoliubov pair problem of the inversion partners as a bound state quantum mechanics problem

$$H_B^{(1)}|\vec{k}, \alpha\rangle = \epsilon_k|\vec{k}, \alpha\rangle, \quad U_{\text{inv}}|\vec{k}, \alpha\rangle = |\vec{k}, \alpha\rangle.$$ 

The interaction between the Bogoliubov quasi-particles is negligible. Our results indicate that a centrosymmetric BG-FS becomes unstable at zero temperature under infinitesimally weak interaction between Bogoliubov quasi-particles.
between the partners,
\[(H_{B,1}^{(1)} + H_{B,2}^{(1)} + V)\Psi^{(2)} = E\Psi^{(2)}\]
where an interaction between pairs, \(V\), is introduced. The superscript \((2)\) is to specify a two-body problem. Solving the quantum mechanical problem is standard. With a gap function, \(\Gamma(\vec{k},\alpha,\beta) = (E - \epsilon_{\vec{k}}(\alpha) - \epsilon_{-\vec{k}}(\beta)) \times \langle (\vec{k},-\vec{k});\alpha,\beta|\Psi^{(2)} \rangle\), we have the integral equation,
\[\Gamma(\vec{k},\alpha,\beta) = \sum_{\vec{k}',\gamma,\delta} \frac{V_{\alpha\beta\gamma\delta}(\vec{k},\vec{k}')}{E - \epsilon_{\vec{k}'}(\gamma) - \epsilon_{\vec{k}'}(\delta)} \Gamma(\vec{k}',\gamma,\delta) .\]
with \(V_{\alpha\beta\gamma\delta}(\vec{k},\vec{k}') \equiv \langle (\vec{k},-\vec{k});\alpha,\beta|V|(\vec{k}',-\vec{k}');\gamma,\delta \rangle\). The two particle states, \((\vec{k},-\vec{k});\alpha,\beta\), whose quantum numbers are \((\vec{k},\alpha)\) and \((-\vec{k},\beta)\), is introduced.

The inversion symmetry restricts a form of a gap function of the Bogoliubov pair in a sense that only odd-parity functions are allowed. Moreover, we are interested in the pairing potential, \(\epsilon_{\vec{k}}(\alpha) - \epsilon_{-\vec{k}}(\beta)\) with a lower symmetry than SO(3) and a generic pairing.

Thus, a bound state exists on a BG-FS for a negative integral equation gives the BCS logarithmic dependence. It is easy to show that the theorem \([31]\) except the fact that the inversion symmetry prohibits even parity channels. As a proof of concept, we consider a pairing potential, \(V_{\alpha\beta\gamma\delta}(\vec{k},\vec{k}') = \sum_{\text{odd},m} \lambda_{\alpha\gamma}^{(l)} u_{\vec{k},\alpha}^{m} u_{\vec{k}',\gamma}^{m} Y_{l}^{m}(\vec{k}) Y_{l}^{m}(\vec{k}')^{*}\) assuming a SO(3) symmetry in energy spectrum. The structure of the integral equation is similar to the original Cooper pair problem \([31]\) except the fact that the inversion symmetry prohibits even parity channels. It is easy to show that the integral equation gives the BCS logarithmic dependence.

Thus, a bound state exists on a BG-FS for a negative interaction channel \((\lambda_{\alpha\gamma} < 0)\).

Our discussions can be easily generalized into a system with a lower symmetry than SO(3) and a generic pairing potential form (see SI). The former may be achieved by replacing the quantum numbers \((l,m)\) with a generic representation index, and the latter can be shown by relying on the Kohn-Luttinger effect \([32]\). The essential part of a pair formation is the presence of a BG-FS as in a Cooper pair on a Fermi liquid \([31]\). Thus, a pair of Bogoliubov quasi-particles forms a bound state in the presence of a BG-FS.

**Model Hamiltonian**: We now consider many Bogoliubov pair problems to investigate instability of a BG-FS. Let us consider a Luttinger Hamiltonian in a cubic system as a normal Hamiltonian,
\[H_{0}(\vec{k}) = \left( c_{0}\vec{k}^{2} - \mu \right)\gamma^{0} + \sum_{a=1}^{3} c_{a} d_{a}(\vec{k})\gamma^{a} + \sum_{a=4}^{5} c_{2} d_{a}(\vec{k})\gamma^{a}.\]
The \(4 \times 4\) identity matrix \(\gamma^{0}\) is used, and \(\gamma^{a}\) are five Clifford gamma matrices, and a four component transposed spinor \(\xi^{T}_{\vec{k}} = (\xi^{+}_{\vec{k}},\xi^{-}_{\vec{k}},\xi^{+}_{-\vec{k}},\xi^{-}_{-\vec{k}})\) is implicitly used. The four parameters of the Luttinger Hamiltonian are chemical potential \(\mu\) and \(c_{0},c_{1},c_{2}\) for particle-hole and cubic anisotropies. The five functions \(d_{1}(\vec{k}) = \sqrt{3}k_{z}k_{y},\)
\(d_{2}(\vec{k}) = \sqrt{3}k_{x}k_{z},\)
\(d_{3}(\vec{k}) = \sqrt{3}k_{x}k_{y},\)
\(d_{4}(\vec{k}) = \frac{\sqrt{2}}{2} \left( k_{x}^{2} - k_{y}^{2} \right),\)
and \(d_{5}(\vec{k}) = \frac{1}{2} \left( 2k_{x}^{2} - k_{z}^{2} - k_{y}^{2} \right)\) are used. The Hamiltonian is asymptotically exact near the gamma point \((\vec{k} = 0)\) which may be supplemented by higher order terms away from the gamma point.

For a BG-FS, a superconducting pairing is considered. Introducing a Nambu spinor \(\chi^{T}_{\vec{k}} = (\xi_{\vec{k}},\xi^{+}_{-\vec{k}})\), we have the Hamiltonian of a BG-FS,
\[H_{0}^{0}(\vec{k}) = \left( H_{0}(\vec{k}) \Delta(\vec{k}) \Delta^{\dagger}(\vec{k}) \right).\]
The Bogoliubov Hamiltonian enjoys the particle-hole symmetry due to its superconducting origin. We introduce an anti-unitary operator \(U_{C} = (\tau^{x} \otimes \gamma^{0})K\) with a Pauli matrix in the particle-hole spinor space, \(\tau^{x}\), and the complex conjugation operator, \(K\). It is easy to show that \(U_{C}H_{0}^{0}U_{C}^{\dagger} = -H_{0}^{0}\). The inversion operator \((U_{P})\) acts as an identity except the momentum inversion \(\vec{k} \rightarrow -\vec{k}\), giving \(U_{P}H_{0}^{0}U_{P}^{\dagger} = H_{0}^{0}\). The inversion symmetry imposes the conditions, \(H_{0}(\vec{k}) = H_{0}(-\vec{k})\) and \(\Delta(\vec{k}) = \Delta(-\vec{k})\). For example, one may choose the chiral pairing channel in the literature \([19]\), \(\Delta(\vec{k}) = \Delta_{0}(\gamma^{3} + i\gamma^{2})\gamma^{1}\) with a SO(3) symmetric band structure \((c_{1} = c_{2})\) and a constant pairing \(\Delta_{0} \neq 0\). In Fig. 1(a), the contour of zero-energy states is illustrated.

The zero energy states are degenerate at each momentum because of the particle-hole symmetry, and we construct an effective low energy Hamiltonian of a centrosymmetric BG-FS, \(H_{\text{eff}}^{0} = E_{0}(\vec{k})\tau^{x}\), with a two-component spinor \(\Psi_{\vec{k}}^{0}\) and a positive semi-definite dispersion relation, \(E_{0}(\vec{k}) \geq 0\) (see SI for the explicit expression of \(E_{0}(\vec{k})\) of Eq. (2)). Hereafter, a generic BG-FS energy spectrum is considered for the effective Hamiltonian. We stress that the spinor at each momentum is rotated properly and the Hamiltonian respects the particle-hole symmetry with \(U_{c} = \tau^{x}K\). Next, we couple an inversion symmetry order parameter, \(\phi\). A generic Hamiltonian is
\[H_{\text{eff}}^{0}(\phi) = H_{\text{eff}}^{0,0} + \phi \sum_{\mu = 0, x, y, z} \rho_{\mu}(\vec{k}) \tau_{\mu}\]
due to the Hermitian property. The inversion symmetry imposes the odd parity conditions, \((\rho_{\mu}(\vec{k}) = -\rho_{\mu}(-\vec{k}))\), and the particle-hole symmetry transformation gives \(U_{c}H_{\text{eff}}^{0}(\phi)U_{c}^{\dagger} = -H_{\text{eff}}^{0}(\phi) + 2\phi \rho_{z}(\vec{k})\tau^{z}\). Thus one of the inversion-odd terms is disallowed, \(\rho_{z}(\vec{k}) = 0\). The energy spectrum of the non-interacting Hamiltonian is easily obtained, \(E_{\pm}(\vec{k},\phi) = \phi \rho_{0}(\vec{k}) \pm \sqrt{E_{0}(\vec{k})^{2} + \phi^{2}(\rho_{x}(\vec{k})^{2} + \rho_{y}(\vec{k})^{2})}\), giving the condition of gapping a BG-FS, \(|\rho_{0}| < \sqrt{\rho_{x}^{2} + \rho_{y}^{2}}\) at each \(\vec{k}\) on a Fermi surface.

Next, let us consider a Hamiltonian with a generic
short-range interaction of a centrosymmetric BG-FS,
\[ H = H_0^G - \frac{1}{2} \sum_{\mu, \nu; \vec{k}, \vec{k}'} g_{\mu \nu} V_{\mu \nu}(\vec{k}, \vec{k}') (\Psi_{\vec{k}}^\dagger \tau_\mu \Psi_{\vec{k}'}^\dagger \tau_\nu \Psi_{\vec{k}'}) \]
with a two component spinor \( \Psi_{\vec{k}} \) and \( H_0^{\text{eff}} = \sum_{\vec{k}} \Psi_{\vec{k}}^\dagger (H_{0,0}^{\text{eff}}) \Psi_{\vec{k}}. \) For simplicity, we consider a separable interaction \( V_{\mu \nu}(\vec{k}, \vec{k}') = \rho_{\mu}(\vec{k}) \rho_{\nu}(\vec{k}') \) and later we argue its generalization. The particle-hole symmetry imposes the conditions \( g_{x0} = g_{xx} = g_{yy} = 0. \) On the other hand, the mixing terms \( (g_{z0}, g_{y0}, g_{xy}) \) are generically non-zero unless an extra constraint is imposed.

**Mean-field analysis**: The standard mean-field analysis gives the mean-field Hamiltonian,
\[ H_{\text{MF}} = H_0^{\text{eff}} - \sum_{\mu, \vec{k}} \phi_{\mu} \rho_{\mu}(\vec{k}) (\Psi_{\vec{k}}^\dagger \tau_\mu \Psi_{\vec{k}} + \frac{1}{2} \sum_{\nu} \phi_{\mu} g_{\mu \nu}^{-1} \phi_{\nu}) \]
with \( \phi_{\mu} = \sum_{\nu, \vec{k}} g_{\mu \nu} \rho_{\nu}(\vec{k}) (\Psi_{\vec{k}}^\dagger \tau_\nu \Psi_{\vec{k}}). \) For convenience, we introduce a vector notation \( \phi_{\mu} \) because symmetries other than inversion may play a role. The inverse matrix of \( g_{\mu \nu} (g_{\mu \nu} g_{\nu \sigma} = \delta_{\mu \nu}) \) is introduced whose determinant is generically non-zero. A mean-field phase diagram is obtained by minimizing the mean-field free energy, \( F_{\text{MF}} = -T \log(\text{Tr}(e^{-H_{\text{MF}}/T})) \). In Fig. 2, we illustrate a case with three coupling constants, \( (g_{xx}, g_{x0}, g_{00}) \) for simplicity. The ground state mean-field energy is
\[ E_{\text{MF}}^{G} = - \sum_{\vec{k}} \sqrt{E_0(\vec{k})^2 + \phi_{x0}^2 \rho_{x}(\vec{k})^2 + \frac{1}{2} \sum_{\mu, \nu} \phi_{\mu} g_{\mu \nu}^{-1} \phi_{\nu}}. \]

We stress that the \( \rho_{0}(\vec{k}) \) does not appear in the ground state energy, which is an artifact of our mean field analysis.

Main results of our mean field calculations are as follows. First, a centrosymmetric BG-FS is absent at zero temperature \( T = 0 \). The inversion symmetry is always broken at \( T = 0 \), indicating that the inversion symmetry breaking is instability of a BG-FS. Second, a centrosymmetric BG-FS survives at non-zero temperature whose regime diminishes at lower temperatures. Third, the original Fermi surface is transformed by the inversion symmetry breaking, and the presence of a Fermi surface is determined by higher order fluctuations. As mentioned above, the mean field ground state energy suffers from the artifact, and to cure it, we implement a generic symmetry-allowed terms to the free energy and consider a phenomenological ground state energy,
\[ E_{\text{MF}}^h = E_{\text{MF}}^{G} + \Delta E \]
where
\[ \Delta E = \sum_{\vec{k}} -u_0 \rho_{0}(\vec{k}) \rho_{x}(\vec{k}) + \frac{u_2}{2} \rho_{0}(\vec{k})^2 + \frac{v_2}{2} \rho_{x}(\vec{k})^2 + \cdots. \]
Non-zero coupling constants \( u_n, v_m \) are introduced phenomenologically, and higher order terms of \( \{\rho_{\mu}\} \) are omitted with \( \cdots \). Keeping the lowest order terms with \((u_0, u_2, v_2)\), it is obvious that the same channel condition \( (\rho_{x}(\vec{k}) \propto \rho_{0}(\vec{k})) \) is satisfied. Thus, the Fermi surface may be gapped. On the other hand, if higher order fluctuations are considered, the same channel condition is not satisfied, inducing a Fermi surface.

Note that there is no theorem to prohibit a Lifshitz transition between a BG-FS and a conventional superconductor without a Fermi-surface because the Luttinger theorem of the volume conservation does not hold in superconductors.

To go beyond the mean-field analysis, we perform the standard renormalization group analysis. For simplicity, we illustrate the case with the three coupling constants, and the generic cases with six coupling constants are discussed in SI. Introducing dimensionless coupling constants, \( g_{\mu \nu} \) which are averaged quantities over a Fermi-surface weighted by \( \rho_{\mu}(\vec{k}) \), we find
\[ \frac{d \tilde{g}_{xx}}{dl} = \tilde{g}_{xx}^2, \quad \frac{d \tilde{g}_{x0}}{dl} = \tilde{g}_{x0} \tilde{g}_{xx}, \quad \frac{d \tilde{g}_{00}}{dl} = \tilde{g}_{20}^2, \]
with the conventional scale variable \( l \) of renormalization group analysis. The long wavelength limit is \( l \rightarrow \infty \). In the \( \tilde{g}_{xx} \) channel, the BCS type logarithmic dependence manifests. It is obvious that the first two equations have the positive eigenvalues, and the right-hand-side of the third one is always positive. Thus, the original BG-FS is unstable at \( T = 0 \), which is consistent with the mean-field results.

**Ginzburg-Landau Theory**: The above instability cal-
Calculations indicate that the inversion symmetry order parameter should be included in a phenomenological Ginzburg-Landau theory of Bogoliubov Fermi-surfaces from the beginning. The Ginzburg-Landau functional is
\[
F[\Delta, \phi] = r_\Delta \text{Tr}[\Delta^\dagger \Delta] + r_\phi \phi^2 + \cdots, \tag{5}
\]
which can be obtained by integrating out fermions at a non-zero temperature. A BG-FS may be considered by the condition \( r_\Delta < 0 \), and our instability calculation indicates \( r_\phi = r_\phi^0 - \langle O \rangle_{FS} \log(\frac{T}{T_c}) \) with a positive-definite quantity averaged over a BG-FS, \( \langle O \rangle_{FS} \). The explicit form of \( \langle O \rangle_{FS} \) is obtained in SI.

Let us consider a schematic phase diagram of the Ginzburg-Landau functional. Adjusting the parameters \((r_\Delta, r_\phi)\), we may set \( O = (0,0) \), the multi-critical point. Possible four phases are

- (A) \((r_\Delta > 0, r_\phi > 0)\) : centrosymmetric metal,
- (B) \((r_\Delta < 0, r_\phi > 0)\) : centrosymmetric BG-FS,
- (C) \((r_\Delta > 0, r_\phi < 0)\) : polar metal,
- (D) \((r_\Delta < 0, r_\phi < 0)\) : non-centrosymmetric SC.

Note that an intermediate phase between (A) and (B) may be present. For example, a time reversal symmetric superconductor may appear if \( (A) \) is a time reversal symmetric metal. Our instability calculations indicate that the phase (D) always appear at low temperature. In (D), the inversion partners of Bogoliubov quasi-particles have different energy. Without higher order fluctuations, the BG-FS may be gapped as discussed above, but the fluctuations induce non-centrosymmetric BG-FSs similar to the ones in literature [20, 33, 34].

Discussion and Conclusion: In the seminal work by Kohn and Luttinger [32], it was shown that a Fermi liquid is always susceptible to a superconducting instability, which may be interpreted as one of the main characteristics of a Fermi-liquid. Along the same line, we propose enhanced fluctuations of an inversion order parameter is a key property of a centrosymmetric BG-FS. In Fig. 3, we illustrate a schematic phase diagram with a tuning parameter of quantum fluctuations of an inversion order parameter. Our results indicate that a weakly interacting centrosymmetric BG-FS is unstable, and the phase X is absent. On the other hand, it is an interesting question whether strongly interacting Bogoliubov quasi-particles stabilize a centrosymmetric BG-FS because our above calculations are based on the assumption of well-defined Bogoliubov quasi-particles. The recent work of a pairing instability in a non-Fermi liquid [35] suggests that a stable BG-FS may be possible down to zero temperature if its excitations lose quasi-particle nature.

Enhanced fluctuations of an inversion order parameter may be captured by inversion susceptibility. An external field of the order parameter is required to measure the susceptibility. Motivated by recent advances in flexoelectricity, we note that a strain gradient on a sample breaks inversion symmetry and plays a role of an external field of an inversion order parameter. Moreover, it is well known that second harmonic generation (SHG) experiment is a probe to identify an inversion order parameter [36]. In other words, SHG provides information of the onset of an inversion order parameter, for example, \( \phi \sim (T_c - T)^\beta \), with the critical temperature of inversion symmetry breaking \( T_c \). Combining the two methods, we propose a second harmonic generation experiment with a strain gradient to measure inversion susceptibility and expect to obtain information of the susceptibility, \( \chi_\phi \sim |T_c - T|^{-\gamma} \). Note that the susceptibility has a non-trivial signatures even at higher temperatures, \( T > T_c \) in sharp contrast to the absence of an order parameter at higher temperatures. We believe the SHG with a strain gradient may be applied in both superconducting and normal states with enhanced inversion fluctuations since inversion symmetry acts in the same way. It is desired to test the experiment in the candidate heavy fermion materials including URu2Si2 and UBe13. Recently, FeSe is also proposed to be a candidate system of a BG-FS [37], and we believe that inversion order parameter fluctuations may be enhanced in FeSe.

In conclusion, we investigate interaction effects of a centrosymmetric BG-FS and find its instability in the inversion symmetry channel. Condensation of Bogoliubov pairs induces the instability, similar to the BCS instability of Fermi liquids where Cooper pairs condense and break \( U(1) \) symmetry. On the other hand, in contrast to the conventional BCS superconductivity, a Fermi surface may or may not survive depending on higher order fluctuations. The instability enforces a phenomenological Ginzburg-Landau functional to include an inversion order parameter from the beginning. Future works including disorder effects and strong quantum fluctuations...
are highly desired, and microscopic calculations of SHG with a strain gradient would be also useful.

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[1] W. Witczak-Krempa, G. Chen, Y. B. Kim, and L. Balents, Annual Review of Condensed Matter Physics 5, 57 (2014).
[2] J. M. Luttinger, Phys. Rev. 102, 1030 (1956).
[3] S. Murakami, N. Nagosa, and S.-C. Zhang, Phys. Rev. B 69, 235206 (2004).
[4] P. YU and M. Cardona, Fundamentals of Semiconductors: Physics and Materials Properties, Advanced texts in physics No. v. 3 (Springer Berlin Heidelberg, 2005).
[5] L. Fu and C. L. Kane, Phys. Rev. B 76, 045302 (2007).
[6] M. Z. Hasan and C. L. Kane, Rev. Mod. Phys. 82, 3045 (2010).
[7] X. Wan, A. M. Turner, A. Vishwanath, and S. Y. Savrasov, Phys. Rev. B 83, 205101 (2011).
[8] N. P. Armitage, E. J. Mele, and A. Vishwanath, Rev. Mod. Phys. 90, 015001 (2018).
[9] E.-G. Moon, C. Xu, Y. B. Kim, and L. Balents, Phys. Rev. Lett. 111, 206401 (2013).
[10] Y. Tokiwa, J. J. Ishikawa, S. Nakatsuji, and P. Gegenwart, Nature Materials 13, 356 EP (2014).
[11] T. Kondo, M. Nakayama, R. Chen, J. J. Ishikawa, E.-G. Moon, T. Yamamoto, Y. Ota, W. Malaeb, H. Kanai, Y. Nakashima, Y. Ishida, R. Yoshida, H. Yamamoto, M. Matsunami, S. Kimura, N. Inami, K. Ono, H. Kugimashira, S. Nakatsuji, L. Balents, and S. Shin, Nature Communications 6, 10042 EP (2015), article.
[12] Z. Tian, Y. Kohama, T. Tomita, H. Ishizuka, T. H. Hsieh, J. J. Ishikawa, K. Kindo, L. Balents, and S. Nakatsuji, Nature Physics 12, 134 EP (2015).
[13] K. Ueda, R. Kaneko, H. Ishizuka, J. Fujioka, N. Nagaoasa, and Y. Tokura, Nature Communications 9, 3032 (2018).
[14] I. F. Herbut and L. Janssen, Phys. Rev. Lett. 113, 106401 (2014).
[15] B. Roy, Phys. Rev. B 96, 041113 (2017).
[16] L. Savary, E.-G. Moon, and L. Balents, Phys. Rev. X 4, 041027 (2014).
[17] S. Han, C. Lee, E.-G. Moon, and H. Min, Phys. Rev. Lett. 122, 187601 (2019).
[18] H. Oh, S. Lee, Y. B. Kim, and E.-G. Moon, Phys. Rev. Lett. 122, 167201 (2019).
[19] D. F. Agterberg, P. M. R. Brydon, and C. Timm, Phys. Rev. Lett. 118, 127001 (2017).
[20] C. Timm, A. P. Schnyder, D. F. Agterberg, and P. M. R. Brydon, Phys. Rev. B 96, 094526 (2017).
[21] J. W. F. Venderbos, L. Savary, J. Ruhman, P. A. Lee, and L. Fu, Phys. Rev. X 8, 011029 (2018).
[22] B. Roy, S. A. A. Ghorashi, M. S. Foster, and A. H. Nevidomskyy, Phys. Rev. B 99, 054505 (2019).
[23] Y. Nakajima, R. Hu, K. Kirshenbaum, A. Hughes, P. Syers, X. Wang, K. Wang, R. Wang, S. R. Saha, D. Pratt, J. W. Lynn, and J. Paglione, Science Advances 1, e1500242 (2015).
[24] H. Kim, K. Wang, Y. Nakajima, R. Hu, S. Ziemak, P. Syers, L. Wang, H. Hodovanets, J. D. Denlinger, P. M. R. Brydon, D. F. Agterberg, M. A. Tanatar, R. Prozorov, and J. Paglione, Science Advances 4 (2018), 10.1126/sciadv.aao4513.
[25] I. Boettcher and I. F. Herbut, Phys. Rev. Lett. 120, 057002 (2018).
[26] G. Sim, A. Mishra, M. J. Park, Y. B. Kim, G. Y. Cho, and S. Lee, Phys. Rev. B 100, 064509 (2019).
[27] E. R. Schenum, R. E. Baumbach, P. H. Tobash, F. Ronning, E. D. Bauer, and A. Kapitulnik, Phys. Rev. B 91, 140506 (2015).
[28] Y. Kasahara, T. Iwasawa, H. Shishido, T. Shibauchi, K. Behnia, Y. Haga, T. D. Matsuda, Y. Onuki, M. Sigrist, and Y. Matsuda, Phys. Rev. Lett. 99, 116402 (2007).
[29] R. H. Heffner, J. L. Smith, J. O. Willis, P. Birrer, C. Baines, F. N. Gygax, B. Hitti, E. Lippelt, H. R. Ott, A. Schenck, E. A. Knetsch, J. A. Mydosh, and D. E. MacLaughlin, Phys. Rev. Lett. 65, 2816 (1990).
[30] R. J. Zieve, R. Duke, and J. L. Smith, Phys. Rev. B 69, 144503 (2004).
[31] L. N. Cooper, Phys. Rev. 104, 1189 (1956).
[32] W. Kohn and J. M. Luttinger, Phys. Rev. Lett. 15, 524 (1965).
[33] P. M. R. Brydon, L. Wang, M. Weinert, and D. F. Agterberg, Phys. Rev. Lett. 116, 177001 (2016).
[34] G. Sim, M. J. Park, and S. Lee, arXiv preprint arXiv:1909.04015 (2019).
[35] M. A. Metlitski, D. F. Mross, S. Sachdev, and T. Senthil, Phys. Rev. B 91, 115111 (2015).
[36] R. W. Boyd, Nonlinear optics (Elsevier, 2003).
[37] C. Setty, S. Bhattacharyya, A. Kreisel, and P. Hirschfeld, arXiv preprint arXiv:1903.00481 (2019).
Supplementary Information for “Instability of $j = 3/2$ Bogoliubov Fermi-surfaces”

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ONE BOGOLIUBOV PAIR PROBLEM

Let us consider two states which are inversion partners ($| + \vec{k}, \alpha \rangle, | - \vec{k}, \alpha \rangle$) in a centrosymmetric Bogoliubov Fermi surface (BG-FS). The two eigenstates of a single-particle Hamiltonian are related by an inversion symmetry unitary operator $U_{\text{inv}}$,

$$U_{\text{inv}}| + \vec{k}, \alpha \rangle = | - \vec{k}, \alpha \rangle, \quad H_B^{(1)}| \vec{k}, \alpha \rangle = \epsilon_k| \vec{k}, \alpha \rangle.$$ 

The superscript (1) specifies an one-particle Hamiltonian, and inversion symmetry indicates $\epsilon_{\vec{k}, \alpha} = \epsilon_{-\vec{k}, \alpha}$. The parameter $\alpha$ is for an additional quantum number such as a spin degree of freedom.

We define one Bogoliubov pair problem as a quantum mechanics bound state problem of a two-particle state $| \Psi^{(2)} \rangle$, which is specified by the superscript (2). The Schrödinger equation of the two particles is

$$\left( H_B^{(1)} + H_B^{(1)} + V \right)| \Psi^{(2)} \rangle = E| \Psi^{(2)} \rangle,$$

and the gap integral equation is

$$\Gamma(\vec{k}, \alpha, \beta) = \sum_{\vec{k}, \gamma, \delta} \frac{V_{\alpha \gamma \delta}(\vec{k}, \vec{k}')}{E - \epsilon_{\vec{k}}(\alpha) - \epsilon_{\vec{k}'}(\beta)} \Gamma(\vec{k}', \gamma, \delta),$$

(S1) with the gap function,

$$\Gamma(\vec{k}, \alpha, \beta) \equiv (E - \epsilon_{\vec{k}}(\alpha) - \epsilon_{-\vec{k}}(\beta)) \langle (\vec{k}, -\vec{k}); \alpha, \beta | \Psi^{(2)} \rangle.$$ (S2)

A pairing matrix element between the two-particle states ($| (\vec{k}, -\vec{k}); \alpha, \beta \rangle, | (\vec{k}', -\vec{k}'); \gamma, \delta \rangle$) is introduced, $V_{\alpha \gamma \delta}(\vec{k}, \vec{k}') \equiv \langle (\vec{k}, -\vec{k}); \alpha, \beta | V | (\vec{k}', -\vec{k}'); \gamma, \delta \rangle$. The structure of the integral equation is similar to that of an original Cooper pair problem, which are compared in TABLE S1.

We consider a system with SO(3) symmetry whose kinetic energy is isotropic, $\epsilon_{\vec{k}}(\alpha) \equiv \epsilon_k(\alpha)$. The wave functions and interaction potentials are decomposed by the angular momentum quantum numbers ($l, m$) of SO(3) group. The system lacks the time-reversal symmetry in contrast to the Cooper pair problem, thus the pairing between the inversion partners is more relevant than that of the time-reversal partner. Therefore we may focus on the $\Gamma(\vec{k}, \alpha, \beta) \propto \delta_{\alpha \beta}$ and $V_{\alpha \gamma \delta}(\vec{k}, \vec{k}') \propto \delta_{\alpha \beta} \delta_{\gamma \delta}$ case, which leads to

$$\langle (\vec{k}, -\vec{k}); \alpha, \alpha | \Psi^{(2)} \rangle = (E - 2\epsilon_k(\alpha)) \sum_{l, \text{odd}, m} a^l_{k, \alpha} Y_l^m(\hat{k}),$$

(S3)

$$\langle (\vec{k}, -\vec{k}); \alpha, \alpha | V | (\vec{k}', -\vec{k}'); \gamma, \gamma \rangle = - \sum_{l, \text{odd}, m} |\lambda^l_{\alpha \gamma}| w^l_{k, \alpha} w^l_{k', \gamma} Y^m(\hat{k}) Y^m(\hat{k}').$$

(S4)

We take an attractive factorizable potential with the interaction strength $|\lambda^l_{\alpha \gamma}|$ and assume that the intra-coupling constants are much larger than the inter-coupling constants, $|\lambda^l_{\alpha \gamma}| \gg |\lambda^l_{\alpha \neq \gamma}|$, for simplicity. The even $l$ channels are forbidden due to the antisymmetric nature of a two-fermion wave function,

$$\langle (\vec{k}, -\vec{k}); \alpha, \alpha | \Psi^{(2)} \rangle = - \langle (\vec{k}, -\vec{k}); \alpha, \alpha | \Psi^{(2)} \rangle,$$

(S5)

and the parity of spherical harmonics, $Y^m_l(\hat{k}) = (-1)^l Y^m_l(\hat{k})$.

The self-consistent equation with the quantum number $(l, \alpha)$ is

$$\frac{1}{|\lambda^l_{\alpha \alpha}|} = - \sum_k \frac{|w^l_{k, \alpha}|^2}{E_l^\alpha - 2\epsilon_k(\alpha)},$$

(S6)

$$= -N_{\alpha}(0) |w^l_{k, \alpha}|^2 \frac{d\epsilon}{E_l^\alpha - 2\epsilon}.$$
TABLE S1. A comparison of BG pair problem with original Cooper pair problem

|       | Cooper pair on FS | BG pair on BG-FS |
|-------|-------------------|------------------|
| Quasiparticle pairing |                   |                  |
| Time-reversal partner  |                   |                  |
| Inversion partner     |                   |                  |
| Instability           | U(1) instability   | Inversion instability |

We approximate the density of states and the averaged quantity at a BG-FS with a spin $\alpha$ by the constant $N_\alpha(0)$ and $W^\alpha_\alpha \equiv \langle |w^\alpha_{k,\alpha}|^2 \rangle_{FS}$. The momentum integration is replaced by an energy integration with a UV energy cut-off, $\Lambda$. We find that the eigenenergy with the quantum number $(l, \alpha)$ is

$$E^l_\alpha = -2\Lambda \exp \left( -\frac{2}{|\lambda^l_{\alpha\alpha}|N_\alpha(0)W^l_\alpha} \right), \quad \text{for } l: \text{odd},$$

for the weak attractive potential, $|\lambda^l_{\alpha\alpha}| \ll (N_\alpha(0)W^l_\alpha)^{-1}$. Hence, a bound state exists on a BG-FS for odd-parity channels.

One may generalize our results to a generic case with a discrete point group symmetry $G$. Then, the wave functions and interactions are decomposed into basis functions of an irreducible representation $R$ of group $G$ instead of spherical harmonics $Y^m_l (\hat{k})$.

FERMIONIC HAMILTONIAN OF NORMAL STATE

We consider a system with cubic and time-reversal symmetries which may realize a quadratic band touching energy spectrum in three spatial dimensions. The low energy Hamiltonian, so-called Luttinger Hamiltonian, is

$$H_0(\vec{k}) = (c_0 k^2 - \mu)\gamma^0 + \sum_a \hat{c}^+_a(\vec{k})\gamma^a.$$  

(S9)

We introduce the quadratic functions $d_a(\vec{k})$ and four dimensional Gamma matrices $(\gamma^a)$ with $a = 1, \cdots 5$ as,

$$d_1(\vec{k}) = \sqrt{3}k_x k_y, \quad d_2(\vec{k}) = \sqrt{3}k_y k_z, \quad d_3(\vec{k}) = \sqrt{3}k_z k_x,$$

$$d_4(\vec{k}) = \frac{\sqrt{3}}{2}(k_x^2 - k_y^2), \quad d_5(\vec{k}) = \frac{1}{2}(2k_z^2 - k_x^2 - k_y^2),$$

and

$$\gamma^1 = \sigma^y \otimes 1, \quad \gamma^2 = \sigma^z \otimes \sigma^y,$$

$$\gamma^3 = \sigma^z \otimes \sigma^x, \quad \gamma^4 = \sigma^x \otimes 1,$$

$$\gamma^5 = \sigma^z \otimes \sigma^z.$$  

(S10)

where the Clifford algebra $\{\gamma^a, \gamma^b\} = 2\delta_{ab}$ is satisfied as described in the previous literature [1]. The cubic symmetry allows the three independent parameters $c_0, c_1 = \hat{c}_1 = \hat{c}_2 = \hat{c}_3$ and $c_2 = \hat{c}_4 = \hat{c}_5$. The Hamiltonian may be expressed in terms of the $j = \frac{3}{2}$ angular momentum operators,

$$H_0(\vec{k}) = \alpha_1 k^2 + \alpha_2 (\vec{k} \cdot \vec{J})^2 + \alpha_3 (k_x^2 J_2^2 + k_y^2 J_3^2 + k_z^2 J_4^2),$$

(S11)

with

$$J_1 = \frac{\sqrt{3}}{2}\gamma^{25} + \frac{1}{2}(\gamma^{13} + \gamma^{24}),$$

$$J_2 = -\frac{\sqrt{3}}{2}\gamma^{35} - \frac{1}{2}(\gamma^{12} - \gamma^{35}),$$

$$J_3 = -\gamma^{14} - \frac{1}{2}\gamma^{23},$$

(S12)
where $\gamma^{ab} \equiv \frac{1}{2i}[\gamma^a, \gamma^b]$ is used. The doubly degenerate energy eigenvalues are $E_{0,\nu}(\vec{k}) = (c_0\vec{k}^2 - \mu) + \nu E_0(\vec{k})$ with $E_0(\vec{k}) = \sqrt{\sum_{a=1}^{5} c_a^2 d_a^2(\vec{k})}$ for $\nu = \pm 1$.

**BOGOLIUBOV FERMI-SURFACES IN SUPERCONDUCTORS WITH $j = \frac{3}{2}$ SYSTEMS**

We consider model Hamiltonians with different numbers of bands below. Namely, Hamiltonians with one, two, and four bands are considered, named one-band, two-band, and four-band models. Since we are interested in superconductivity, the sizes of the Bogoliubov-de Gennes (BdG) Hamiltonians are doubled. For example, one-band Hamiltonian is described by $2 \times 2$ matrices with a two component Nambu spinor.

**Four-band model**

Let us start with a $j = \frac{3}{2}$ superconductivity Hamiltonian. Its BdG Hamiltonian is generically written as,

$$H^0 = \sum_{\vec{k}} \chi^\dagger_{\vec{k}} \begin{pmatrix} H_0(\vec{k}) & \Delta(\vec{k}) \\ \Delta^\dagger(\vec{k}) & -H_0^T(-\vec{k}) \end{pmatrix} \chi_{\vec{k}},$$

with a Nambu spinor $\chi^T_{\vec{k}} = (\xi^T_{\vec{k}}, \xi^\dagger_{-\vec{k}})$ and a four-component transposed spinor $\xi^T_{\vec{k}} = (c_{\vec{k}, \frac{3}{2}}, c_{\vec{k}, \frac{1}{2}}, c_{\vec{k}, -\frac{1}{2}}, c_{\vec{k}, -\frac{3}{2}})$. The normal and pairing parts of BdG Hamiltonian $(H_0(\vec{k}), \Delta(\vec{k}))$ are described by $4 \times 4$ matrices.

To be specific, we consider a standard Hamiltonian in the literature [2], whose normal and pairing Hamiltonians are the Luttinger Hamiltonian with SO(3) symmetry ($c_1 = c_2$),

$$H_0(\vec{k}) = (c_0\vec{k}^2 - \mu)\gamma^0 + \sum_a c_a d_a(\vec{k})\gamma^a,$$  

and the time-reversal broken quintet pairing,

$$\Delta(\vec{k}) = \Delta_0(\gamma^3 + i\gamma^2)i\gamma^{12}. $$

We choose the pairing amplitude $\Delta_0$ as a real number. In the quintet pairing $(\gamma^3 + i\gamma^2)$, it is easy to see time-reversal symmetry breaking (TRSB), which is known to be a necessary condition for a BG-FS. Zero-energy surfaces in the Brilluion zone are illustrated in Fig. S1.

![Fig. S1. BG-FSs of a TRSB quintet state in momentum space. The spheroidal and toroidal Fermi surfaces are protected by a $Z_2$ topological invariant [2]. The dimensionless parameters $k_x,y,z/k_F$ are introduced, where $k_F$ is a momentum of the isotropic normal state Fermi surface.](image)

**Two-band model**

Construction of a two-band model is standard [2, 3]. One may construct a two-band model by projecting a four-band model onto either electron or hole bands of the normal state ($\nu = \pm 1$). In the model Hamiltonian (S14), the
condition $c_0 < c_1 = c_2$ gives well-defined electron and hole bands, so the sign of chemical potential determines a projected Hilbert space.

To be specific, let us consider positive chemical potential for electron bands ($\nu = +1$). Its BdG Hamiltonian is written as

$$H^{(2)}_+ = \sum_k \chi^\dagger_k \begin{pmatrix} H^+(\vec{k}) & \Delta^+_+(\vec{k}) \\ \Delta^+_+(\vec{k}) & -H^+_+(\vec{k}) \end{pmatrix} \chi_k,$$

with a two-band Nambu spinor $\chi^T_k = (\psi^T_{\vec{k},+}, \psi^\dagger_{\vec{k},+})$ and a two-component spinor $\psi_{\vec{k},+}$. We use the superscript $(2)$ to denote a two-band model.

Construction of $(H^+(\vec{k}), \Delta^+(\vec{k}))$ from $H^0$ is as follows. Consider an operator $J_k = \vec{k} \cdot \vec{J}$ to label two degenerate electron bands as $J_k = \pm 1/2$. By applying a local transformation, spinors with the $J_k$ basis may be transformed to spinors with a pseudo-spin basis labeled by $\sigma = \pm 1$.

$$\left( \begin{array}{c} c_{k,\nu=+} \sigma=+ \\ c_{k,\nu=+} \sigma=- \end{array} \right) \equiv \exp \left(-i \frac{\sigma_3}{2} \phi_k \right) \exp \left(-i \frac{\sigma_2}{2} \theta_k \right) \left( \begin{array}{c} c_{k,\nu=+} \sigma=+ \\ c_{k,\nu=+} \sigma=- \end{array} \right).$$

(S17)

Polar and azimuthal angles $(\theta_k, \phi_k)$ in momentum space are introduced. Note that a choice of the spinors is known to have an ambiguity, due to the degeneracy of a normal state energy [2].

The explicit forms of $(H^+(\vec{k}), \Delta^+(\vec{k}))$ with a spinor, $\psi^T_{\vec{k},+} = (c_{\vec{k},+}, c_{\vec{k},+})$, are

$$H^+(\vec{k}) = h^0_{+,+}(\vec{k}) I_{2 \times 2} + \tilde{h}_+(\vec{k}) \cdot \tilde{\sigma},$$

$$\Delta^+(\vec{k}) = \Delta_0(\hat{d}_3(\vec{k}) + i \hat{d}_2(\vec{k})) i \sigma_2,$$

(S18)

(S19)

with

$$h^0_{+,+}(\vec{k}) = E_{0,+}(\vec{k}) + \frac{\Delta_0^2}{2|d(\vec{k})|} (2 - \hat{d}_2(\vec{k})^2 - \hat{d}_3(\vec{k})^2),$$

$$\tilde{h}_+(\vec{k}) = \left| \frac{\Delta_0}{d(\vec{k})} \right| \left( \begin{array}{c} \hat{d}_3(\vec{k}) \hat{d}_2(\vec{k}) \\ \frac{1}{\sqrt{3}} \hat{d}_3(\vec{k}) \frac{1 - 4\hat{d}_5(\vec{k})}{3} \end{array} \right),$$

(S20)

(S21)

$$|\tilde{h}_+(\vec{k})| = \frac{\Delta_0^2}{|d(\vec{k})|} \sqrt{\hat{d}_1(\vec{k})^2 + \hat{d}_4(\vec{k})^2 + \hat{d}_5(\vec{k})^2}.$$  

(S22)

A normalized $d$-vector, $\hat{d}(\vec{k}) = \hat{d}(\vec{k})/|d(\vec{k})|$, is used. In $h^0_{+,+}(\vec{k})$ and $\tilde{h}_+(\vec{k})$, we only keep the corrections up to the second-order in terms of a pairing amplitude.

Note that the projection mixes the normal energy eigenvalue $(E_{0,+}(\vec{k}))$ of a normal state with the pairing term $(\Delta_0)$ of the four band model as manifested in Eq. (S20). The energy eigenvalues are given by,

$$E^{(2)}_{\alpha,\beta}(\vec{k}) = \alpha \sqrt{h^0_{+,+}(\vec{k})^2 + |\psi_{\alpha,+}(\vec{k})|^2} + \beta |\tilde{h}_+(\vec{k})|,$$

for $\alpha, \beta = \pm 1$,

(S23)

where $\psi_{\alpha,+}(\vec{k}) = \text{Tr} \left( \Delta^+(\vec{k})(i \sigma_2)^{\dagger} \right)/2 = \Delta_0(\hat{d}_3(\vec{k}) + i \hat{d}_2(\vec{k}))$. The zero-energy surface state may be generically possible for $(\alpha, \beta) = (\pm 1, \mp 1)$ with a non-zero pseudo-magnetic field which is a result of the TRSB quintet state.

The unitary transformation from a pseudo-spin basis into an energy eigenvector is well defined,

$$c_{\vec{k},\vec{\epsilon}^{(2)}_{\alpha,\beta}} = \left( \frac{\alpha \beta}{2} \right)^{1/2} \left( \begin{array}{c} \alpha \sqrt{1 + \alpha \frac{h_0}{h_0^{2} + |\psi_{\alpha,+}|^2}} \sqrt{\frac{1 + \beta h_0}{2}} \exp \left(i \frac{\phi_{\alpha,+} - \phi_{\alpha,-}}{2} \right) \\ \alpha \beta \sqrt{1 + \alpha \frac{h_0}{h_0^{2} + |\psi_{\alpha,+}|^2}} \sqrt{\frac{1 - \beta h_0}{2}} \exp \left(i \frac{\phi_{\alpha,+} + \phi_{\alpha,-}}{2} \right) \\ -\beta \sqrt{1 - \alpha \frac{h_0}{h_0^{2} + |\psi_{\alpha,+}|^2}} \sqrt{\frac{1 - \beta h_0}{2}} \exp \left(i \frac{\phi_{\alpha,+} + \phi_{\alpha,-}}{2} \right) \\ \beta \sqrt{1 - \alpha \frac{h_0}{h_0^{2} + |\psi_{\alpha,+}|^2}} \sqrt{\frac{1 + \beta h_0}{2}} \exp \left(i \frac{\phi_{\alpha,+} - \phi_{\alpha,-}}{2} \right) \end{array} \right)^T \left( \begin{array}{c} c_{\vec{k},\sigma=+} \\ c_{\vec{k},\sigma=-} \\ c_{\vec{k},\sigma=+}^{\dagger} \\ c_{\vec{k},\sigma=-}^{\dagger} \end{array} \right).$$

(S24)
We introduce a global U(1) phase \( \psi_s \) with \( \psi_s \equiv |\psi_s| e^{i\theta_s} \) and polar and azimuthal angles \( (\theta_s, \phi_s) \) defined in the pseudomagnetic field space \( \vec{h}_+ \). The normalized pseudo-spin vector \( \hat{h}_\mu(\vec{k}) = h_\mu^+ (\vec{k})/|h_\mu(\vec{k})| \) and the TRSB singlet channel \( \psi_s = \psi_{s,+}(\vec{k}) \) are used. One may easily check the relation \( c_{k,E_s}^{(2)} = c_{-k,E_s}^{(2 \ast)} \) from Eq. (S24).

**One-band model**

Similarly, a one-band model may be constructed by projecting a two-band Hamiltonian onto a Hilbert space associated with zero-energy surface states. In our SO(3) symmetric model, the surfaces may appear for \( (\alpha, \beta) = (\pm, \mp) \), manifested in \( E^{(2)}(\vec{k}) = \alpha \sqrt{|h_+^0(\vec{k})|^2 + |\psi_{s,+}(\vec{k})|^2 + \beta |h_+^0(\vec{k})|} \). We introduce a one-band Nambu basis \( \Psi_\vec{k}^\dagger = (c_{k,E_1}^{(2)}, c_{-k,E_2}^{(2)}) \), and the effective one-band Hamiltonian becomes

\[
H^{(1)}_\perp \equiv \sum_\vec{k} \Psi_\vec{k}^\dagger E_0(\vec{k}) \Psi_\vec{k},
\]

where \( E_0(\vec{k}) = E^{(2)}_{\mp \mp}(\vec{k}) \). The superscript (1) refers to the one-band model. We mainly use the one-band model in the following sections and use the notation \( H^{0}_{\text{TRSB}} \) instead of \( H^{(1)}_\perp \) for simplicity.

**INVERSION SYMMETRY BREAKING CHANNELS WITH \( j = 3/2 \) SYSTEM**

We introduce a generic term which couples to an inversion order parameter \( \phi \) in an effective Hamiltonian of a BG-FS. The Nambu spinors defined in section may determine the form of the matrices in the one, two, and four-band models.

**Four-band model**

Let us start with the four-band model, which allows the term with an inversion order parameter \( \phi \),

\[
\delta H^{0}_{\text{Inv}} = \phi \sum_{R,k} \chi^T_{k \bar{k}} \left( \begin{array}{cc} \eta_R(\vec{k}) & \delta_R(\vec{k}) \\ \delta_R^T(-\vec{k}) & -\eta_R^T(-\vec{k}) \end{array} \right) \chi_{\bar{k}},
\]

with a Nambu spinor \( \chi^T_{k \bar{k}} = (\xi^T_{k \bar{k}}, \xi_{-k \bar{k}}^\dagger) \) and a four-component spinor \( \xi^T_{k \bar{k}} = (c_{k,\frac{1}{2} + \frac{3}{2}}, c_{k,\frac{1}{2} - \frac{3}{2}}, c_{-k,\frac{1}{2} + \frac{3}{2}}, c_{-k,\frac{1}{2} - \frac{3}{2}}) \). The subscript \( R \) is for an irreducible representation. For a given \( R \), the 4x4 matrices \( (\eta_R, \delta_R) \) are decomposed as \( \eta_R(\vec{k}) = \sum_m a_m \eta_{R,m}(\vec{k}) \), \( \delta_R(\vec{k}) = \sum_m b_m \delta_{R,m}(\vec{k}) \) with \( m = 1, \cdots d_R \). The coefficients \( (a_m, b_m) \) are for different components of a \( d_R \)-dimensional irreducible representation.

In Table S2, pairing channels of \( O_h \) group with odd-parity, \( \delta_{R,m}(\vec{k}) \), are listed. \( O_h \) is a higher symmetry group than \( C_t \), which is a symmetry group of \( H^{0} \), hence all odd-parity representations of \( O_h \) may mix together and become \( A_{1u} \) representation of \( C_t \).

**Two-band model**

Similarly, the two-band model allows the term with \( \phi \),

\[
\delta H^{(2)}_{\text{Inv}} = \phi \sum_{R,k} \tilde{\chi}^T_{k \bar{k}} \left( \begin{array}{cc} \tilde{\eta}_R(\vec{k}) & \tilde{\delta}_R(\vec{k}) \\ \tilde{\delta}_R^T(-\vec{k}) & -\tilde{\eta}_R^T(-\vec{k}) \end{array} \right) \tilde{\chi}_{\bar{k}},
\]

with a Nambu spinor \( \tilde{\chi}^T_{k \bar{k}} = (\psi^T_{k,\bar{k} +}, \psi^\dagger_{-k,\bar{k} +}) \) and a two-component spinor \( \psi^T_{k,\bar{k} +} = (c_{k,+,\sigma=+}, c_{k,+,\sigma=-}) \). The 2x2 matrices \( (\tilde{\eta}_R, \tilde{\delta}_R) \) are introduced as \( \tilde{\eta}_R(\vec{k}) = \sum_m a_m \tilde{\eta}_{R,m}(\vec{k}) \), \( \tilde{\delta}_R(\vec{k}) = \sum_m b_m \tilde{\delta}_{R,m}(\vec{k}) \) with \( m = 1, \cdots d_R \). Each channel can be
ψ

TABLE S2. The odd-parity pairing matrices of $O_h$ symmetry. The channels of the two and four-band model ($\delta R_m(\tilde{k})$, $\tilde{\delta} R_m(\tilde{k})$) are listed. We consider a $L = 1$ pairing for the four-band model, for simplicity. We define $4 \times 4$ matrices $\tilde{J} = \begin{pmatrix} J_1 & J_2 & J_3 & J_4 \\ J_5 & J_6 & J_7 & J_8 \end{pmatrix}$ and bilinear operations of three-component vectors, $D_{\mu,\nu} = \begin{pmatrix} D_1 & D_2 \\ D_3 & D_4 \end{pmatrix}$ and $D_{\mu,\nu}^ \sigma = \begin{pmatrix} D_{1\sigma} & D_{2\sigma} \\ D_{3\sigma} & D_{4\sigma} \end{pmatrix}$, and the basis functions of $O_h$ group, $k_{A_{2u}} = k_x k_y k_z$, $k_{T_{1u}} = a(k_x, k_y, k_z) + b(k^3_x, k^3_y, k^3_z)$, $k_{T_{2u}} = (k_x(k_y - k^3_x), k_y(k_z - k^3_y), k_z(k_x - k^3_z))$ are used with constants $a, b$.

Explicitly expressed in terms of a four-band model ($\eta_R, \delta_R$),

$$\tilde{\eta}_R(\tilde{k}) = U^\dagger_{\tilde{k}} \eta_R(\tilde{k}) U_{\tilde{k}} = \sum_{\mu=0,1,2,3} \tilde{\eta}^\mu_R(\tilde{k}) \sigma_\mu, \quad \text{for } m = 1 \cdots d_R, \quad (S28)$$

$$\tilde{\delta}_R(\tilde{k}) = U^\dagger_{\tilde{k}} \delta_R(\tilde{k}) U_{\tilde{k}} = \sum_{\mu=1,2,3} \tilde{\psi}^\mu_R(\tilde{k}) \sigma_\mu(i \sigma_2), \quad \text{for } m = 1 \cdots d_R, \quad (S29)$$

with a $4 \times 2$ matrix $U_{\tilde{k}}$,

$$U_{\tilde{k}} = \begin{pmatrix} -\frac{\sqrt{2}}{2} e^{i\phi_\tilde{k}} \sin \theta_\tilde{k} & 0 \\ \frac{\cos \theta_\tilde{k}}{2} e^{-i\phi_\tilde{k}} \sin \theta_\tilde{k} & -\frac{\sqrt{2}}{2} e^{i\phi_\tilde{k}} \sin \theta_\tilde{k} \\ \frac{\cos \theta_\tilde{k}}{2} e^{-i\phi_\tilde{k}} \sin \theta_\tilde{k} & 0 \end{pmatrix}. \quad (S30)$$

The polar and azimuthal angles ($\theta_\tilde{k}, \phi_\tilde{k}$) in a momentum space are introduced. In Table S2, odd-parity pairing channels of the two-band model $\tilde{\delta}_R m$ and the four-band model $\delta_R m$ are compared.

**One-band model**

Similarly, the one-band model has the term with $\phi$,

$$\delta H^{(1)}_{\text{inv}} = \sum_{\mu=0,x,y} \phi \sum_{R,\tilde{k}} \Psi_{\tilde{k}}^\dagger \rho^R_{\mu}(\tilde{k}) \tau_\mu \Psi_{\tilde{k}}. \quad (S31)$$

with a two-component Nambu spinor $\Psi_{\tilde{k}}^T = (c_{\tilde{k},E_{+2}}, c_{\tilde{k},E_{-2}}^\dagger)$. We introduce a real-valued odd-parity function, $\rho^R_{\mu}(\tilde{k}) = \sum_{\mu=0,x,y} \phi \sum_{R,\tilde{k}} \Psi_{\tilde{k}}^\dagger \rho^R_{\mu}(\tilde{k}) \tau_\mu \Psi_{\tilde{k}}$, which is a function of ($\tilde{\eta}_R$, $\tilde{\delta}_R$) of the two-band model. Note that one channel, $\rho^R_{\mu}(\tilde{k})$, is forbidden by particle-hole symmetry.

One can express $\rho^R_{\mu}$ in terms of a normalized pseudo-spin vector $\tilde{h} = \tilde{h}_+(\tilde{k})/|\tilde{h}_+(\tilde{k})|$, a TRSB singlet pairing $\psi_s = \psi_{s,+}(\tilde{k})$, and inversion symmetry breaking channels ($\tilde{\eta}_R$, $\tilde{\delta}_R$) in a two-band model, (See the previous section),

$$\rho^R_{0}(\tilde{k}) = \left( \tilde{\eta}_R \frac{h_0}{|\psi_s|^2 + h_0^2} \hat{\psi} \cdot \tilde{\eta}_R \right) - \text{Re} \left( \frac{\psi_s^*}{\sqrt{|\psi_s|^2 + h_0^2}} (\hat{h} \cdot \tilde{\psi}) \right). \quad (S32)$$
An inverse matrix \( g \) we focus on a separable potential \( \rho \).

Performing the Hubbard-Stratanovich transformation, the mean-field Hamiltonian becomes

\[
\rho^{R}(\vec{k}) = \frac{\psi_{s}}{\sqrt{\psi_{s}^{2} + h_{0}^{2}}} \hat{h}_{3}(\vec{h} \cdot \vec{R}) - \vec{h}_{R}^{2} - \text{Re} \left( \frac{h_{0}}{\sqrt{\psi_{s}^{2} + h_{0}^{2}}} \psi_{s}^{*} \hat{h}_{3}(\vec{h} \cdot \vec{R}) - \vec{h}_{R}^{2} \right) + \text{Im} \left( \frac{\psi_{s}}{\sqrt{\psi_{s}^{2} + h_{0}^{2}}} \right),
\]

\[
\rho^{R}(\vec{k}) = \frac{\psi_{s}}{\sqrt{\psi_{s}^{2} + h_{0}^{2}}} \hat{h}_{1}(\vec{h} \cdot \vec{R}) - \vec{h}_{R}^{2} - \text{Re} \left( \frac{h_{0}}{\sqrt{\psi_{s}^{2} + h_{0}^{2}}} \psi_{s}^{*} \hat{h}_{1}(\vec{h} \cdot \vec{R}) - \vec{h}_{R}^{2} \right) - \text{Im} \left( \frac{\psi_{s}}{\sqrt{\psi_{s}^{2} + h_{0}^{2}}} \right)
\]

where the three-component vector notations, \( \vec{h}^{R} = (\vec{h}, \vec{h}, \vec{h}) \) and \( \vec{h} = (\vec{h}, \vec{h}, \vec{h}) \) are used.

### Mean-Field Analysis

Let us consider a BdG Hamiltonian of a one-band model (See section ),

\[
H_{0}^{\text{eff}} = \sum_{\vec{k}} \Psi_{k}^{\dagger} E_{0}(\vec{k}) T^{\mu} \Psi_{k}.
\]

\[
H_{\text{int}}^{\text{eff}} = -\frac{1}{2} \sum_{\mu,\nu=0,\pi} g_{\mu\nu} \sum_{\vec{k},\vec{k}'} V_{\mu\nu}(\vec{k},\vec{k}')(\Psi_{k}^{\dagger} T_{\mu} \Psi_{k})(\Psi_{k}^{\dagger} T_{\nu} \Psi_{k}).
\]

We focus on a separable potential \( V_{\mu\nu}(\vec{k},\vec{k}') = \rho_{\mu}(\vec{k}) \rho_{\nu}(\vec{k}') \) with \( \rho_{\mu}(\vec{k}) = -\rho_{\mu}(\vec{k}) \) at a BG-FS. For simplicity, we consider only two channels \( (\tau_{0}, \tau_{z}) \) with three coupling constants \( (g_{00}, g_{0x}, g_{xx}) \), and its generalization including other channels \( (\tau_{y}, \tau_{z}) \) is straightforward. The superscript \( \text{eff} \) is dropped hereafter.

Performing the Hubbard-Stratanovich transformation, the mean-field Hamiltonian becomes

\[
H_{\text{MF}}(\vec{\phi}) = H_{0} - \sum_{\mu,\vec{k}} \phi^{\mu} \Psi_{k}^{\dagger} \rho_{\mu}(\vec{k}) T^{\mu} \Psi_{k} + \frac{1}{2} \sum_{\mu,\nu} \phi^{\mu} g_{\mu\nu}^{-1} \phi^{\nu},
\]

with an order parameter,

\[
\phi^{\mu} \equiv \left( \sum_{\nu,\vec{k}} g_{\mu\nu} \Psi_{k}^{\dagger} \rho_{\nu}(\vec{k}) T^{\nu} \Psi_{k} \right), \quad \text{for} \quad \mu = 0, x.
\]

An inverse matrix \( g_{\mu\nu}^{-1} \) is well-defined, unless the matrix \( g_{\mu\nu} \) is singular. The mean-field partition function and free energy are,

\[
Z_{\text{MF}}(\vec{\phi}) = \int D[\Psi] \exp \left[ -\frac{1}{T} \sum_{\vec{k}} \Psi_{k}(-i k_{n} + H_{\text{MF}}) \Psi_{k} \right] \exp \left[ -\frac{1}{2T} \sum_{\mu,\nu} \phi^{\mu} g_{\mu\nu}^{-1} \phi^{\nu} \right],
\]

\[
F_{\text{MF}}(\vec{\phi}) = -T \sum_{\vec{k}} \ln 2 \cosh \frac{E_{k}^{+}(\vec{\phi})}{T} + \ln 2 \cosh \frac{E_{k}^{-}(\vec{\phi})}{T} + \frac{1}{2} \sum_{\mu,\nu} \phi^{\mu} g_{\mu\nu}^{-1} \phi^{\nu},
\]

with \( H_{\text{MF}} = E_{0}(\vec{k}) - \sum_{\mu} \phi^{\mu} \rho_{\mu}(\vec{k}) T^{\mu} \) and its energy eigenvalues \( E_{k}^{\pm} \),

\[
E_{k}^{\pm}(\vec{\phi}) = \phi_{0} \rho_{0}(\vec{k}) \pm \sqrt{E_{0}(\vec{k})^{2} + \phi_{x}^{2} \rho_{x}(\vec{k})^{2}},
\]

showing particle-hole symmetry, \( E_{k}^{+}(\vec{\phi}) = -E_{-k}^{-}(\vec{\phi}) \).

A self-consistent equation,

\[
\begin{pmatrix}
\phi_{0} \\
\phi_{x}
\end{pmatrix} = \begin{pmatrix}
g_{00} & g_{0x} \\
g_{0x} & g_{xx}
\end{pmatrix} \begin{pmatrix}
A_{0}(\vec{\phi}) \\
A_{x}(\vec{\phi})
\end{pmatrix},
\]

(S41)
is obtained by minimizing the free energy with respect to $\vec{\phi}$. Explicit forms of $A_0(\vec{\phi})$ and $A_x(\vec{\phi})$ are

$$A_0(\vec{\phi}) = \frac{1}{2} \sum_k \rho_0(\vec{k}) \left( \frac{\tanh \frac{E^+_k(\vec{\phi})}{2T} + \tanh \frac{E^-_k(\vec{\phi})}{2T}}{\sqrt{E^+_0(\vec{k})^2 + \phi_x^2(\vec{k})^2}} \right), \quad A_x(\vec{\phi}) = \frac{1}{2} \sum_k \frac{\phi_x(\vec{k})^2}{\sqrt{E^+_0(\vec{k})^2 + \phi_x^2(\vec{k})^2}} \left( \frac{\tanh \frac{E^+_k(\vec{\phi})}{2T}}{\tanh \frac{E^-_k(\vec{\phi})}{2T}} - \tanh \frac{E^-_k(\vec{\phi})}{2T} \right).$$

The momentum summation can be replaced by an integration of energy ($\epsilon$) and angles ($\theta_{\vec{k}}, \phi_{\vec{k}}$),

$$\sum_k = \int d\epsilon \, d\Omega_{\vec{k}} \, D(\epsilon, \Omega_{\vec{k}}), \quad d\Omega_{\vec{k}} = d\theta_{\vec{k}} \, d\phi_{\vec{k}} \sin(\theta_{\vec{k}}). \quad (S42)$$

The density of states may be written as $D(\epsilon, \Omega_{\vec{k}}) = \sum_{\vec{k}} \delta(\epsilon - E_{\vec{k}}) \delta(\Omega_{\vec{k}} - \Omega_{\vec{E}})$. We focus on contributions near a Fermi surface of a BG-FS ($\epsilon = 0$), introducing a UV energy cutoff, $\Lambda$, as usual. Then, the summation may be approximated by

$$\sum_k O(\vec{k}) = \int d\epsilon \, d\Omega_{\vec{k}} \, D(\epsilon, \Omega_{\vec{k}}) \, O(\epsilon, \Omega_{\vec{k}}) \approx \int_{-\Lambda}^{\Lambda} d\epsilon \, (\delta(\epsilon - \epsilon_F) \delta(\Omega_{\vec{k}} - \Omega_{\vec{E}})) \Omega \quad (S43)$$

with an average over the angle variables at a fixed energy, $\langle \cdots \rangle_{\Omega}$. For example, a SO(3) symmetric energy spectrum, $E_0(\vec{k}) = k^2 - \epsilon_F$, simplifies the two functions. Introducing dimensionless variables ($A_0, \phi_0, \tilde{E}, \tilde{T}$, $\tilde{\rho}_0, \tilde{\phi}_x$),

$$\tilde{A}_0(\phi) = \int_{-1}^{1} d\tilde{E} \int d\Omega_{\vec{k}} \, \tilde{D}(\tilde{E}) \rho_0(\vec{k}) \left( \frac{\sinh \frac{\phi_0 \rho_0(\vec{k})}{T}}{\cosh \frac{\phi_0 \rho_0(\vec{k})}{T} + \cosh \sqrt{\tilde{E}^2 + \phi_x^2 \rho_x(\vec{k})^2}} \right), \quad (S44)$$

$$\tilde{A}_x(\phi) = \int_{-1}^{1} d\tilde{E} \int d\Omega_{\vec{k}} \, \tilde{D}(\tilde{E}) \frac{\phi_x \rho_x(\vec{k})}{\sqrt{\tilde{E}^2 + \phi_x^2 \rho_x(\vec{k})^2}} \left( \frac{\sinh \frac{\sqrt{\tilde{E}^2 + \phi_x^2 \rho_x(\vec{k})^2}}{T}}{\cosh \frac{\phi_0 \rho_0(\vec{k})}{T} + \cosh \sqrt{\tilde{E}^2 + \phi_x^2 \rho_x(\vec{k})^2}} \right). \quad (S45)$$

where the angle-independent density of states, $\tilde{D}(\tilde{E}) \equiv D(\tilde{E}, \Omega_{\vec{k}})$, is used. Hereafter, we remove the tildes, for convenience.

**Mean-field phase diagram**

In this section, mean-field phase diagrams are obtained by solving the self-consistent equations in Eq. (S41). Phase boundaries between inversion-symmetric and inversion-symmetry-broken phases are determined as a function of coupling constants ($g_{xx}, g_{zz}, g_{00}$) and temperature $T$. 

![FIG. S2. Temperature dependence of $C_{\mu}(T)/\langle \rho_{FS}^2 \rangle_{\mu}$. $\lim_{T\to0} C_{\mu}(T) = \infty$ indicates an inversion symmetry instability.](image)
At non-zero temperature, a phase boundary is determined by
\[(g_{00} - C_0(T)^{-1})(g_{xx} - C_x(T)^{-1}) = g_{0x}^2,\] (S46)
with
\[C_0(T) = \frac{\langle \rho_{0x}^2 \rangle_{\text{FS}}}{2T} \int_{-1}^{1} dE \sech^2 \frac{E}{2T}, \quad C_x(T) = \frac{\langle \rho_{x}^2 \rangle_{\text{FS}}}{2T} \int_{-1}^{1} dE \tanh \frac{E}{2T}.\] (S47)

A typical temperature dependence of \(C_\mu(T)\) is illustrated in Fig. S2. We focus on low temperatures \(T \ll \Lambda\) and the integration over the angle variables can be approximated as \(\langle D(E) \rho_{\mu}(\Omega_{k})^2 \rangle_{\Omega} \simeq \langle D(0) \rho_{\mu}(\Omega_{k})^2 \rangle_{\Omega} = \langle \rho_{\mu}^2 \rangle_{\text{FS}}\). The energy minimization condition enforces \(g_{00} < C_0(T)^{-1}, g_{xx} < C_x(T)^{-1}\).

In a symmetry-broken phase \((\phi_\mu \neq 0)\), a manifold of zero-energy excitations may be in two categories. One category is referred to as a gapped phase whose zero-energy manifold does not contain a surface. Namely, conventional nodeless, nodal point, and nodal line superconductors are in this category. The other one contains a surface, which happens with the condition \(|\phi_0\rho_0(\vec{k})| > |\phi_x\rho_x(\vec{k})|\) at all momentums where quasi-particle excitations are gapless in a centrosymmetric BG-FS.

In Fig. S3, we illustrate the phase diagram at three different temperatures, considering two cases, \((\rho_0 = \rho_x = \hat{k}_x)\) and \((\rho_0 = \hat{k}_y, \rho_x = \hat{k}_x)\). There is a finite phase space for a gapped phase for the former case \((|\phi_0| < |\phi_x|)\), while it is forbidden for the latter case. Note that there is no reason for \(\rho_0(\vec{k}) = \rho_x(\vec{k})\) in terms of symmetry unless fine-tuned.

At zero temperature, the ground state energy determines a phase diagram. The mean-field ground state energy \(E_{G}^{\text{MF}}\) is
\[E_{G}^{\text{MF}}[\phi] = -\sum_{\vec{k}} \sqrt{E_0(\vec{k})^2 + \phi_0^2 \rho_0(\vec{k})^2 + \phi_0 \rho_0(\vec{k})} + \frac{1}{2} \sum_{\mu,\nu} \phi_\mu g_{\mu,\nu}^{-1} \phi_\nu.\] (S48)
Note that the energy is independent of \(\phi_0\), due to an odd-parity property, which is an artifact of our choice of a separable potential (see the next subsection).

In Fig. S3, we illustrate phase diagrams at \(T = 0\), considering the two cases, \((\rho_0 = \rho_x = \hat{k}_x)\) and \((\rho_0 = \hat{k}_y, \rho_x = \hat{k}_x)\). Note that the phase boundary is \(g_{xx} = 0\), which demonstrates an inversion instability, and a non-centrosymmetric gapped phase is generically absent without a fine-tuning.

### High order fluctuations

Here, we consider higher order fluctuations at zero temperature. As mentioned in the main text, the absence of \(\rho_0(\vec{k})\) dependence in the ground state energy is an artifact of our mean-field analysis. To overcome the artifact, we introduce phenomenological terms to the mean-field energy. At the leading order, the ground state energy \(E_{G}^{\text{ph}}\) is
\[E_{G}^{\text{ph}}[\phi] = E_{G}^{\text{MF}}[\phi] - u_0 \rho_0(\vec{k}) \rho_x(\vec{k}) + \frac{u_2}{2} \rho_0(\vec{k})^2 + \frac{v_2}{2} \rho_x(\vec{k})^2 + \cdots,\] (S49)
with phenomenological constants \(u_0, u_2, v_2 > 0\). The variation of the energy is
\[\delta E_{G}^{\text{ph}} = \sum_{\vec{k}} \left( -u_0 \rho_x(\vec{k}) + u_2 \rho_0(\vec{k}) \right) \delta \rho(\vec{k}) + \frac{v_2}{2} \delta \rho(\vec{k})^2 + \cdots,\] (S50)
under the variation \(\rho_0 = \rho_0 + \delta \rho\).

The same channel condition \((\rho_0(\vec{k}) \propto \rho_x(\vec{k}))\) is obtained by ignoring the higher-order terms with \(" \cdots \"\), which realizes a gapped phase as discussed above. However, the inclusion of the higher order terms such as \(\rho_0^3\) prohibits the same channel condition, and it is generically impossible to realize a non-centrosymmetric gapped phase.
1. $\rho_0(\vec{k}) = \rho_x(\vec{k}) = \hat{k}_x$ case

2. $\rho_0(\vec{k}) = \hat{k}_y, \rho_x(\vec{k}) = \hat{k}_x$ case

FIG. S3. Mean-field phase diagrams at four different temperatures $T_1 > T_2 > T_3 > 0$ with two conditions, $(\rho_0 = \rho_x = \hat{k}_x), (\rho_0 = \hat{k}_y, \rho_x = \hat{k}_x)$. The ratio between coupling constants, $g_{xx}/g_{x0}$ and $g_{00}/g_{x0}$ are introduced for horizontal and vertical axes, respectively. The labels (a, b, c) refer a centrosymmetric BG-FS (a), a non-centrosymmetric BG-FS (b), a non-centrosymmetric line-nodal SC (c). At each temperature, a centrosymmetric BG-FS is stable for weak coupling regions (a) and becomes unstable for strong coupling regions, where an inversion symmetry is broken (b,c). The solid lines separate the two phases. At dark grey regions $g_{30} < g_{xx}g_{00}$, the mean-field free energy is not stable and needs higher order terms to cure it. For $\rho_0 = \rho_x = \hat{k}_x$ case, the dashed lines are obtained by the criteria ($\phi^0 = \phi^*$), which separates two different zero-energy states, a BG-FS (b) and a line-nodal state (c). It is clear that the phase space for a BG-FS shrinks at lower temperature and approaches to the vertical axis for $T \to 0$. On the other hand, the phase space for a gapped phase is forbidden for $\rho_0 = \hat{k}_y, \rho_x = \hat{k}_x$ case.

RENNORMALIZATION GROUP ANALYSIS

We perform the RG analysis on a one-band BdG Hamiltonian with interaction terms,

$$H = \sum_\vec{k} \Psi_\vec{k}^\dagger E_0(\vec{k}) \tau^z \Psi_\vec{k} - \frac{1}{2} \sum_{\mu, \nu = 0, x} g_{\mu \nu} \sum_{\vec{k}, \vec{k}'} (\Psi_{\vec{k}'}^\dagger \rho_\mu(\vec{k}) \tau_\mu \Psi_{\vec{k}})(\Psi_{\vec{k}'}^\dagger \rho_\nu(\vec{k}') \tau_\nu \Psi_{\vec{k}'})$$

with three coupling constants $(g_{xx}, g_{x0}, g_{00})$. One Feynman diagram as shown in Fig. S4 contributes to RG equations due to the momentum conservation.

The quantum correction to coupling constants are obtained by integrating out the fast modes, and the coupling
constants are modified as \( g_{\mu\nu} \rightarrow g_{\mu\nu} + \delta g_{\mu\nu} \) with

\[
\delta g_{xx} = -g_{xx}^2 \int_{\vec{k},\vec{\kappa}_n} \text{Tr} \left( G_f^{(1)}(k) \tau_x G_f^{(1)}(k) \tau_x \right) \rho_x(\vec{k})^2,
\]

\[
\delta g_{x0} = -g_{xx} g_{x0} \int_{\vec{k},\vec{\kappa}_n} \text{Tr} \left( G_f^{(1)}(k) \tau_x G_f^{(1)}(k) \tau_x \right) \rho_x(\vec{k})^2,
\]

\[
\delta g_{00} = -g_{x0}^2 \int_{\vec{k},\vec{\kappa}_n} \text{Tr} \left( G_f^{(1)}(k) \tau_x G_f^{(1)}(k) \tau_x \right) \rho_x(\vec{k})^2.
\]

(S52)

The energy shell integration, \( \int_{\vec{k},\vec{\kappa}_n} = \int \frac{d^4k}{(2\pi)^4} \int_{-\infty}^{\infty} \frac{dk_n}{2\pi} \), is used with an energy cut-off, \( \Lambda \), which may be an order of the Fermi energy. The bare fermion propagator \( G_f^{(1)}(k) \) is

\[
G_f^{(1)}(k) = \text{diag}(\frac{1}{-ik_n + E_0(\vec{k})}, \frac{1}{-ik_n - E_0(\vec{k})}).
\]

(S53)

For example, one of the integrations can be evaluated as

\[
\int_{\vec{k},\vec{\kappa}_n} \text{Tr} \left( G_f^{(1)}(k) \tau_x G_f^{(1)}(k) \tau_x \right) \rho_x(\vec{k})^2 = -\int_{\Lambda/b}^\Lambda d\epsilon d\Omega_k \frac{D(\epsilon, \Omega_k) \rho_x(\Omega_k)^2}{\epsilon},
\]

(S54)

with a angle-dependent density of states, \( D(\epsilon, \Omega_k) \) and approximated by using the average over an angle variable at a fixed energy, \( \langle D(\epsilon, \Omega_k) \rangle \approx \langle D(0, \Omega_k) \rangle \). The integration is simplified as,

\[
\int_{\Lambda/b}^\Lambda d\epsilon d\Omega_k \frac{D(\epsilon, \Omega_k) \rho_x(\Omega_k)^2}{\epsilon} \approx \int_{\Lambda/b}^\Lambda d\epsilon \langle D(0, \Omega_k) \rangle \rho_x(\Omega_k)^2 \Omega = \langle \rho_x^2 \rangle_{FS} \log b.
\]

(S55)

The flow equations of three coupling constants \( (b = e^l) \) are

\[
\frac{dg_{xx}}{dl} = g_{xx}^2, \quad \frac{dg_{x0}}{dl} = \hat{g}_{x0} g_{xx}, \quad \frac{dg_{00}}{dl} = g_{x0}^2,
\]

(S56)

with dimensionless coupling constants \( \hat{g}_{\mu\nu} \equiv \langle \rho_x^2 \rangle_{FS} g_{\mu\nu} \) up to one-loop calculations. Their analytic solutions are

\[
\hat{g}_{xx}(l) = \frac{\hat{g}_{xx}(0)}{1 - \hat{g}_{xx}(0) l}, \quad \hat{g}_{x0}(l) = \frac{\hat{g}_{x0}(0)}{1 - \hat{g}_{xx}(0) l}, \quad \hat{g}_{00}(l) = \hat{g}_{00}(0) + \left( \frac{\hat{g}_{x0}(0)^2 l}{1 - \hat{g}_{xx}(0) l} \right).
\]

(S57)

All three coupling constants diverge at the long wavelength limit \( l \rightarrow l_c \equiv \hat{g}_{xx}(0)^{-1} \), and thus a BG-FS becomes unstable.

Our results may be generalized by including additional coupling constants. We find the flow equations with six coupling constants,

\[
\frac{dg_{xx}}{dl} = g_{xx}^2 \langle \rho_x^2 \rangle_{FS} + g_{xy}^2 \langle \rho_y^2 \rangle_{FS}, \quad \frac{dg_{yy}}{dl} = g_{yy}^2 \langle \rho_y^2 \rangle_{FS} + g_{xy}^2 \langle \rho_y^2 \rangle_{FS},
\]

\[
\frac{dg_{xy}}{dl} = g_{xx} g_{xy} \langle \rho_x^2 \rangle_{FS} + g_{yy} g_{xy} \langle \rho_y^2 \rangle_{FS}, \quad \frac{dg_{x0}}{dl} = g_{x0} g_{xx} \langle \rho_x \rangle_{FS} + g_{y0} g_{xy} \langle \rho_y \rangle_{FS},
\]

\[
\frac{dg_{00}}{dl} = g_{x0} g_{xy} \langle \rho_y \rangle_{FS} + g_{y0} g_{yy} \langle \rho_y^2 \rangle_{FS}.
\]

(S58)

We check that the RG flows are away from the non-interacting fixed point in the long wavelength limit \( l \rightarrow \infty \), and hence an instability of inversion symmetry exists.

**BOSON SELF ENERGY CALCULATION FOR GINZBURG LANDAU THEORY**

A phenomenological Ginzburg-Landau(GL) theory of a BG-FS may be written as

\[
\mathcal{F}[\Delta, \phi] = r_\Delta \text{Tr} [\Delta^\dagger \Delta] + r_\phi \phi^2 + \cdots,
\]

(S59)
FIG. S4. A Feynman diagram contributing to the RG flow equations. Red line refers to Green’s function of a fermion with a fast momentum which is integrated out. We consider a separable four-fermion interaction here, hence there is only one Feynman diagram which contributes to RG equations at one-loop order.

with a superconducting order parameter of a BG-FS, $\Delta$, and an inversion order parameter, $\phi$.

We calculate a boson self-energy of $\phi$ from the interaction with gapless fermions at one loop order and determine dependence of the tuning parameter ($r_\phi$). With the effective fermion Hamiltonian,

$$H = \sum_{k} \Psi_k^\dagger E_0(k) \tau^z \Psi_k + \phi \sum_{\nu=0,x,y} \rho_\nu(k) \Psi_k^\dagger \tau_\nu \Psi_k,$$

the boson self-energy becomes

$$\Pi_{\phi}(0,0) = -\phi^2 \int_{E,N} \sum_{\nu,\sigma} \rho_\nu(k) \rho_\sigma(k) \text{Tr} \left[ G^{(1)}_\nu(k) \tau_\nu G^{(1)}_\sigma(k) \tau_\sigma \right] = \phi^2 \left( \sum_{\nu=x,y} \langle \rho^2_\nu \rangle_{FS} \right) \log \left( \frac{\Lambda}{\mu} \right).$$

Then, the correction term is

$$r_\phi = r_\phi^0 - \Pi_{\phi}(0,0).$$

The infrared divergence of self-energy ($\mu$) with a positive sign indicates the instability of an inversion order parameter.

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[1] S. Murakami, N. Nagosa, and S.-C. Zhang, Phys. Rev. B 69, 235206 (2004).
[2] D. F. Agterberg, P. M. R. Brydon, and C. Timm, Phys. Rev. Lett. 118, 127001 (2017).
[3] J. W. F. Venderbos, L. Savary, J. Ruhman, P. A. Lee, and L. Fu, Phys. Rev. X 8, 011029 (2018).