Monopole versus spherical harmonic superconductors: Topological repulsion and stability

Enrique Muñoz,1, 2 Rodrigo Soto-Garrido,1 and Vladimir Juričić3

1 Facultad de Física, Pontificia Universidad Católica de Chile, Víncula Mackenna 4860, Santiago, Chile
2 Research Center for Nanotechnology and Advanced Materials CIEN-UC, Pontificia Universidad Católica de Chile, Víncula Mackenna 4860, Santiago, Chile
3 Nordita, KTH Royal Institute of Technology and Stockholm University, Roslagstullsbacken 23, 10691 Stockholm, Sweden

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Monopole harmonic superconductor, proposed in doped Weyl semimetals as a pairing between the Fermi surfaces enclosing the Weyl points, is rather unusual, as it features the monopole charge inherited from the parent topological metal. However, this state can compete with more conventional spherical harmonic pairings, such as an s-wave. We here demonstrate that the monopole superconductor and a more conventional spherical harmonic pairing phase quite generically repel one another. As we explicitly show, this feature is a direct consequence of the topological nature of the monopole superconductor, and we dub it topological repulsion. Furthermore, the s-wave pairing is more stable both when the chemical potentials at the nodes are unequal, and in the presence of point-like charged impurities. Since the phase transition is discontinuous, close to the phase boundary, we predict the Majorana gapless modes at the interfaces between domains featuring the two phases as the experimental signature of the monopole superconductor.

Introduction. Topological semimetals feature the nodal points in the Brillouin zone where the conduction and the valence bands touch yielding a rather rich landscape of emergent low-energy quasiparticles [1, 6]. In particular, the exotic electronic properties in Weyl semimetals (WSMs), such as Fermi arc surface states and anomalous magnetotransport, arise from the two topological nodal points in the Brillouin zone giving rise to pseudorelativistic Weyl fermions [7–11], which were experimentally observed in mostly binary compounds, such as TaAs and NbP [12–15]. These Weyl points are the source and the sink of the abelian Berry curvature, yielding the monopole charge $C = \pm 1$, the topological invariant characterizing these semimetals. Weyl metals can also represent a platform for the realization of yet different states of matter. For instance, they can host interaction-driven fully gapped axionic insulator [16–19], which has been recently experimentally observed [20]. On the superconducting side, WSMs can accommodate a plethora of pairing states [21–27]. Monopole superconductor (SC), recently proposed as a pairing state between the two Fermi surfaces (FSs) enclosing the Weyl points in a doped WSM [28], is an exciting possibility because it features Berry flux inherited from the underlying WSM state, but its physical consequences have been so far only touched upon [29, 30].

An urgent issue in this respect is the competition of the monopole pairing, characterized by the monopole harmonic functions $Y_{q,j,m}(\theta, \phi)$ with more conventional spherical harmonic states $Y_{l,m}(\theta, \phi)$, as well as its stability in the presence of impurities. We here demonstrate that the monopole and the spherical harmonic SCs quite generically repel one another, as shown in Fig. 1(a). Most importantly, we explicitly show that this behavior originates from the topological nodal nature of the monopole SC manifested through a simple criterion for the repulsion of the phases: $q + m \neq m'$. To illustrate it, we show that when the monopole state is trivialized by removing the vortex around the node ($q + m$ set to zero), the coexistence with a finite-momentum $s$–wave can take place, as can be seen in Fig. 1(b). On the other hand, the offset between the chemical potentials at the Weyl points favors the s-wave pairing, as shown in Fig. 2. The same effect is at play in the presence of point-like non-magnetic impurities, see Fig. 3. Finally, since the transition between the two superconducting states is discontinuous, close to the phase boundary the interfaces between the two phases should host gapless Majorana modes which may be used as an experimental signature of the monopole SC.

Model. We start by considering the model describing the mean-field Cooper pairing between the Weyl quasiparticles living at the FSs enclosing the two nodal points with the opposite monopole charge $C = \pm 1$

$$\hat{H} = \hat{H}_{\text{WSM}} + \hat{H}_\Delta. \quad (1)$$

The continuum Hamiltonian corresponding to the time-reversal symmetry breaking WSM with the two nodal points is $\hat{H}_{\text{WSM}} = \sum_{\zeta = \pm, \mathbf{q}} \hat{c}_\zeta(\mathbf{k}_0 + \mathbf{q})^\dagger \hat{c}_\zeta(\mathbf{k}_0 + \mathbf{q})$, where

$$\hat{h}_\zeta(\mathbf{q}) = v_F(\sigma_x q_x + \sigma_y q_y + \zeta \sigma_z q_z) - \mu, \quad (2)$$

and the chemical potential $\mu > 0$. This Hamiltonian is obtained after expanding the corresponding lattice model about the two Weyl nodes along the $k_z$-direction located at $\zeta K_0 = (0, 0, \zeta K_0)$, see Supplemental Material (SM) for technical details [32]. We here consider only isotropic nodes with Fermi velocity $v_F$, fix the position of the nodes at $K_0 = \pi/2a$, with the lattice constant $a = 1$, and also set $\hbar = c = k_B = 1$ hereafter. The Hamiltonian for an
inter-FS s-wave pairing is

$$\hat{H}_\Delta = \sum_q \hat{c}^\dagger_{\mathbf{k}_0+q}[\Delta_0 i\hat{\sigma}_y]e^{-i\mathbf{k}_0\cdot \mathbf{q}} + H.c.,$$

with $\Delta_0$ as the order parameter. This is possibly the simplest pairing between the Fermi surfaces $FS_{\pm}$ enclosing the two nodal points at $q = \mathbf{K}_0$ and $-\mathbf{K}_0$, with the quasiparticles with momenta $\mathbf{k}_0 + \mathbf{q}$ and $-\mathbf{k}_0 - \mathbf{q}$, where $\pm \mathbf{q}$ lives on the sphere $S_\pm$ obtained after shifting $FS_\pm$ by $\mp \mathbf{K}_0$ toward the origin. Crucially, the Cooper pair wavefunction acquires the total Berry flux $4\pi$ inherited from the parent chiral Weyl fermions [22]. Consequently, its projection onto the sphere $S_+$ ($S_-$) features at least one vortex with the unit $(2\pi)$ vorticity, and the corresponding projected pairing is proportional to a monopole harmonic function $Y_{q,\pm,\alpha}(\theta, \phi)$, with $4\pi q$ counting the total Berry flux of the SC state [28]. The pairing is spin triplet because it originates from the quasiparticles at two different Weyl points.

More formally, the band basis on the Fermi surfaces $FS_{\pm}$ is $\hat{c}^\dagger_\pm (\pm \mathbf{q}) = \sum_{\sigma=\uparrow, \downarrow} \xi_{\pm,\sigma}(\pm \mathbf{q})e^{i\mathbf{k}_0\cdot \mathbf{q}}$, with the spinors $\xi_{\pm,\sigma}(\pm \mathbf{q}) = (u_{\sigma}, v_{\sigma})^T$, chosen so that the Dirac string pierces the sphere at the south pole (spherical polar angle $\theta_q = \pi$), since $u_{\sigma} = \cos(\theta_q/2)$ and $v_{\sigma} = \sin(\theta_q/2)e^{i\phi_{\sigma}}$, and $\phi_{\sigma}$ is the azimuthal angle. After projecting the pairing Hamiltonian in Eq. (3) onto the $FS_{\pm} [\pm \mathbf{q} \in FS_{\pm}]$ in the weak coupling (BCS) regime $|\Delta_0| \ll \mu$, we obtain

$$\hat{\Delta}_\Delta = \sum_q \hat{c}^\dagger_\pm (q)\hat{\Delta}(q)\hat{c}^\dagger_\pm (-q) + H.c.,$$

with the gap function $\hat{\Delta}(q) = -2\Delta_0 u_q v^*_q = -\Delta_0 \sin \theta_q e^{-i\phi_q} = -\Delta_0 \sqrt{\frac{4\pi}{3}} Y_{-1,1,0}(\theta_q, \phi_q)$, where $Y_{q,\pm,\alpha}(\theta, \phi)$ is the standard monopole harmonic function [31, 32]. Notice that for the monopole pairing in Eq. (3), $2q = 2C_- = -2$, since $C_\pm \to C_\mp$ under $q \to -q$.

In a WSM prone to a superconducting instability, a more conventional intra-FS spin-singlet pairing, which necessarily occurs at a finite momentum $2\mathbf{K}_0$, is also possible, and competes with the monopole SC. Furthermore, the inversion symmetry in Weyl materials may be broken, so to account for this effect, we consider slightly different chemical potentials at the two nodes, $\mu_-$ and $\mu_+$, with $|\delta \mu| = |\mu_+ - \mu_-| \ll \mu$, where $\mu = (\mu_+ + \mu_-)/2$ the average chemical potential. The mean-field Bogoliubov-de Gennes Hamiltonian that includes both pairing instabilities takes the form

$$\hat{H} = \sum_q \Psi_q^\dagger \hat{H}_{BCS}(q) \Psi_q,$$

with

$$\hat{H}_{BCS}(q) = \begin{bmatrix} \xi_q & \Delta_0 & 0 & \Delta_q \\ \Delta_0^* & -\xi_q & 0 & \Delta^*_q \\ 0 & 0 & \Delta_0 & \xi^*_q \\ \Delta^*_q & 0^* & -\xi^*_q & \Delta^* \end{bmatrix},$$

and the Nambu basis is $\Psi_q^\dagger = \begin{bmatrix} \alpha_- (q) & \alpha_+ (-q) & \alpha_- (q)^\dagger & \alpha_+ (-q)^\dagger \end{bmatrix}$, while $\xi^\pm_q = v_F|q| - \mu^\pm$.

**BCS mean-field gap equations: Clean limit.** The mean-field gap equations for the two competing superconducting orderings are obtained from the finite-temperature Green’s function for the effective Bogoliubov-de Gennes Hamiltonian in Eq. (3), which in terms of the valley sub-
blocks reads as
\[ \hat{G}_0(\omega_n, \mathbf{q}) = \left[ -i\omega_n + \hat{H}_{BCS}(\mathbf{q}) \right]^{-1} = \begin{bmatrix} \hat{G}_0^{-} & \hat{G}_0^{++} \\ \hat{G}_0^{+} & \hat{G}_0^{++} \end{bmatrix}, \] (7)

where \( \hat{G}_0^{\pm\pm} \), \( \rho, \zeta = \pm \), are the 2 \times 2 submatrices, and \( \omega_n = (2n+1)\pi T \) is the fermionic Matsubara frequency at temperature \( T \). The gap equations for the conventional intra-Fermi surface pairing and the monopole SC then can be compactly written as
\[ \Delta_y(\mathbf{q}) = -T \sum_{\mathbf{q}} V_y(\mathbf{q}, \mathbf{q}') \langle \hat{a}_{-\mathbf{q}}(\mathbf{q}') \hat{a}_{\mathbf{q}}(\mathbf{q}') \rangle, \] (8)

where \( \zeta = - (\zeta = +) \) for \( \eta = \text{intra} \) (\( \eta = \text{inter} \)) corresponding to the spherical harmonic (monopole) pairing, and \( V_y \) are the pairing potentials. In terms of the Green’s function in Eq. (7), \( \langle \hat{a}_{-\mathbf{q}}(\mathbf{q}') \hat{a}_{\mathbf{q}}(\mathbf{q}') \rangle = \left[ \hat{G}_0^{\zeta} \right]_{12} \). The explicit form of the gap equations is displayed in the SM [33], from which we can conclude that when these two superconducting orders compete new instabilities can be generated but in the insulating (particle-hole) channels. More specifically, when the intra-FS pairing is s-wave, the two \( p^- \)-wave charge-density wave orders in the \( x \)- and \( y \)-directions may get generated (see the SM). However, this is so only when the two orders coexist, a possibility which is excluded, except precisely at the phase boundary, as we show below.

The pairing potentials for the spherical harmonics and the monopole channels when \( \mu_+ = \mu_- = \mu \), dictated by the form of the corresponding pairing functions, are given by
\[ V_{\text{intra}}(\mathbf{q}, \mathbf{q}') = V_0 Y_{l,m}(\theta_\mathbf{q}, \phi_\mathbf{q}) Y^*_{l,m}(\theta_{\mathbf{q}'}, \phi_{\mathbf{q}'}) \]
\[ V_{\text{inter}}(\mathbf{q}, \mathbf{q}') = \tilde{V}_0 Y_{-1,1,0}(\theta_\mathbf{q}, \phi_\mathbf{q}) Y_{-1,1,0}(\theta_{\mathbf{q}'}, \phi_{\mathbf{q}'}) \] (9)

where \( Y_{l,m}(\theta, \phi) = f_l(\theta)e^{im\phi} \). The resulting BCS gap equations take the compact form
\[ \lambda_\eta^{-1} = \int \frac{d\Omega}{4\pi} \frac{2}\int d\phi \ln \left[ \frac{2\omega_D}{\sqrt{A_+ B \cos(m+1)\phi}} \right], \] (10)

with the same notation as in Eq. (8). \( \int d\Omega = \int_0^\pi \int_0^{2\pi} \sin \theta d\theta d\phi, \) \( d_{\text{inter}} = \sin \theta, \) \( d_{\text{intra}} = f_l(\theta) \), and \( \omega_D \) is the Debye frequency. Here, \( \lambda_{\eta} \) \( \text{intra} \) = \( \tilde{V}_0 \rho(\mu) \), and \( \lambda_{\eta} \) \( \text{inter} \) = \( \kappa \rho(\mu) \), with \( \rho(\mu) \) as the density of states at the FS, and
\[ A_\pm = 2\Delta_{\text{intra}} f_l^2(\theta) \pm 2\Delta_{\text{inter}} \sin^2 \theta, \] (11)
\[ B = 2\Delta_{\text{intra}} \Delta_{\text{inter}} \sin \theta f_l(\theta), \] (12)

while
\[ \kappa = \frac{\tilde{V}_0}{4\pi} \int d\Omega |Y_{-1,1,0}(\theta, \phi)|^2. \] (13)

For a function \( g[\cos m\phi] \), with \( m \neq 0 \), it holds that
\[ \int_0^{2\pi} d\phi g[\cos m\phi] = \int_0^{2\pi} d\phi g[\cos \phi], \] while
\[ \int_0^{2\pi} d\phi \ln(A_+ + B \cos \phi) = -4\pi \ln \left[ \frac{A_+}{A_+ + |A_-|} \right], \] (14)

implying that for a spherical harmonic pairing \( Y_{l,m}(\theta, \phi) \) and a monopole SC \( Y_{q,l,m}(\theta, \phi), \) since \( Y_{q,l,m}(\theta, \phi) \sim e^{i(q+m)\phi}, \) the dominant phase is one with the stronger coupling, as explicitly shown in the SM [33]. Furthermore, when \( q \neq m' - m \), the coexistence is excluded except at the phase boundary where \( \lambda_{\text{intra}} = \lambda_{\text{inter}} \). In particular, a conventional harmonic state with \( m' = 0 \) repels a monopole SC, unless \( q = -m \). Therefore, the repulsion between the phases is a direct consequence of the topological structure of the monopole pairing, and we thus dub it topological repulsion.

We plot the phase diagram for s-wave and above discussed monopole harmonic \( Y_{l,m}(\theta, \phi) \) in Fig. [1][a]. As it can be seen, the two phases repel one another: they are separated by a first-order phase transition and coexist only at the phase boundary. Consequently, the phase separation may take place in the vicinity of the phase boundary, yielding the Majorana modes at the interfaces between the domains hosting the two phases. To further corroborate the topological origin of this repulsion between the phases, we trivialize the monopole SC by dropping the vortex term and choose this order parameter to be purely imaginary, i.e. we write it as \( i\Delta \sin \theta \), with \( \Delta \) real. As it can be seen in Fig. [1][b], the s-wave and the trivialized monopole SC then coexist in a finite region of the phase diagram.

To include the effect of the inversion symmetry breaking, we take different chemical potentials at the two nodes. As a consequence, the value of the effective inter-
FS pairing potential at the phase boundary increases, implying that the intra-FS s-wave superconductor becomes more favorable, as shown in Fig. 2.

Impurity scattering. Let us now consider the effect of scattering by randomly distributed, non-magnetic impurities, with a concentration $n_{\text{imp}}$, on the superconducting instabilities. Within the first Born approximation, this can be captured through an averaged self-energy matrix [34]. We then use it to solve the Dyson equation by taking the ansatz for the fully dressed Green’s function [34]. We then use it to solve the Dyson equation by taking the ansatz for the fully dressed Green’s function [34].

The respective scattering times are $\tau_{\text{inter}}$ and $\tau_{\text{intra}}$ (in units of $1/\mu$). The change of the phase boundary shows that the s-wave pairing is more stable. Here, $\delta \lambda = \lambda_{\text{inter}}/\lambda_{\text{intra}} - 1$, and $\lambda_{\text{inter}} = 0.13$.

![Graph showing the ratio of inter- and intra-Fermi surface couplings at the phase boundary](image)

FIG. 3. The ratio of the inter- and intra-Fermi surface couplings at the phase boundary (two critical temperatures equal) between the s-wave and the monopole superconductor in the presence of inter- and intra-Fermi surface scattering by the point impurities. The respective scattering times are $\tau_{\text{inter}}$ and $\tau_{\text{intra}}$ (in units of $1/\mu$). The change of the phase boundary shows that the s-wave pairing is more stable. Here, $\delta \lambda = \lambda_{\text{inter}}/\lambda_{\text{intra}} - 1$, and $\lambda_{\text{inter}} = 0.13$.

where $\Gamma_c$ is an upper cutoff for the Matsubara frequency sum and $\psi(x)$ is the digamma function. When only the intra-FS scattering is present, the critical temperature remains unchanged, consistent with Anderson’s theorem [35], and its generalized version for unconventional pairing states in terms of the superconducting fitness [36, 37]. Notice that the density-wave nature of this superconducting order does not play a role, since the disorder preserves translational symmetry on average.

For the monopole superconductor, on the other hand, because of the form of its projection on the FS, the gap does not renormalize. Consequently, the effect of both intra- and inter-FS disorder is to lower its critical temperature

$$\frac{T_c}{\lambda_{\text{inter}}} = \ln \left( \frac{\Gamma_c}{2\pi T_c} \right) - \psi \left( \frac{1}{2} + \frac{\tau_{\text{intra}}^{-1} + \tau_{\text{inter}}^{-1}}{4\pi T_c} \right),$$

Notice that both types of disorder anticommute with the pairing matrix for the monopole SC, as can be directly checked from Eq. (16). Therefore, the superconducting fitness function is non-vanishing for either of them, consistent with the correction to $T_c$ given by Eq. (17).

To illustrate the competition of the two superconducting phases when the intra-FS scattering is turned on, we plot the ratio between the inter- and intra-FS pairing interactions, $\delta \lambda = \lambda_{\text{inter}}/\lambda_{\text{intra}} - 1$ at the phase boundary (the two critical temperatures equal) as a function of the intra-FS inverse scattering time, shown in Fig. 3. The intra-FS scattering suppresses the monopole SC, since as this scattering increases, the phase boundary moves toward larger values of the inter-FS pairing strength. A similar behavior is observed when the inter-FS scattering is turned for a fixed intra-FS disorder.

**Discussion & Outlook.** To summarize, our analysis implies that the monopole and conventional spherical harmonic superconducting phases quite generically repel one another which is a direct consequence of the topological nature of the monopole SC. We show that the finite-momentum s-wave pairing is more stable both for unequal chemical potentials at the nodes, and in the presence of point-like charged impurities. Close to the phase boundary, the system features gapless modes at the interface of the topologically nontrivial monopole harmonic and the trivial s-wave superconducting domains, providing an experimental signature of the monopole SC.

In spite of many realized Weyl metals, the signatures of the Weyl superconductivity have been only recently reported in UTe$_2$ [38]. Particularly relevant in this context is the observation that the superconducting state is a time-reversal symmetry breaking two-component spin-triplet order parameter, which as such may feature a monopole component, but the nature of the order parameter is still an open question.

Our work should motivate further studies of the monopole harmonic SCs, such as their competition with...
the insulating instabilities, particularly with those displaying the monopole structure [39]. Finally, observable consequences of these exotic states beyond the surface Majorana modes are yet to be explored, as, for instance, impurity resonances [40].

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