Topological Superconductivity in Dirac Semimetals

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Dirac semimetals host bulk band-touching Dirac points and a surface Fermi loop. We develop a theory of superconducting Dirac semimetals. Establishing a relation between the Dirac points and the surface Fermi loop, we clarify how the nontrivial topology of Dirac semimetals affects their superconducting state. We note that the unique orbital texture of Dirac points and a structural phase transition of the crystal favor symmetry-protected topological superconductivity with a quartet of surface Majorana fermions. We suggest the possible application of our theory to recently discovered superconducting states in Cd$_3$As$_2$.

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Dirac semimetals are three-dimensional (3D) materials that possess gapless (Dirac) points in the bulk Brillouin zone (BZ), whose low-energy excitations are effectively described as Dirac fermions. With time-reversal symmetry (TRS) and inversion symmetry (IS) preserved, a pair of Dirac points is formed at the crossing of two doubly degenerate bands on a high-symmetry axis. They are protected by discrete rotation ($C_n$) symmetry [1–4], which prohibits band mixing to open a gap. Furthermore, Dirac semimetals may host a surface Fermi loop (FL) [3–6]. This contrasts sharply with a surface Fermi arc in Weyl semimetals [7], because its topological origin is different. Several Dirac semimetals, including Na$_3$Bi [8–11] and Cd$_3$As$_2$ [5,6,12–17], have been demonstrated experimentally and predicted theoretically [18–22].

Superconducting phase transitions were reported recently in Cd$_3$As$_2$ [23–25] and Au$_2$Pb [26], both of which support Dirac points protected by $C_4$ symmetry. Bulk Cd$_3$As$_2$ exhibits superconductivity under high pressure (≈8.5 GPa) [25] accompanied by a structural phase transition of the crystal [27]. In addition, point contact measurements of Cd$_3$As$_2$ reportedly induce superconductivity around the point contact region, where the tunneling conductance shows a zero-bias conductance peak [23,24]. Au$_2$Pb also exhibits a superconducting phase transition after a structural phase transition [26].

In this Letter, we address the effect of the nontrivial topology, i.e., the Dirac points and FL, on the superconducting properties. Topological materials are a promising platform to realize topological superconductors (TSCs) owing to the nontrivial topology of the wave function in normal states [28–35]. For instance, surface Dirac fermions may realize a TSC even for an $s$-wave pairing state [28,29]. Also, the Fermi surface topology, which is the simplest topological structure in the normal state, directly affects the topological superconductivity of odd-parity superconductors [30,31,35]. For the carrier-doped topological insulator, topological superconductivity has been anticipated for the surface [29] or the bulk [31].

Here we present a general framework for studying superconductivity in Dirac semimetals. The key ingredients are symmetry-protected topological numbers in crystalline insulators and superconductors [36–47]. In particular, we examine the $C_4$ topological invariant and the mirror Chern number, which ensure the existence of Dirac points and FLs, respectively, in Dirac semimetals. First, we show that these two topological numbers are intrinsically related to each other, establishing a relation between Dirac points and surface FLs. Then, we elucidate how the nontrivial topology of Dirac semimetals affects their superconducting state. We find that, for a class of pairing symmetries, Dirac points and FLs in the normal state are inherited as bulk point nodes and surface Majorana fermions (MFs), respectively, in the superconducting state.

By carefully examining the low-energy effective Hamiltonian, we also reveal that doped Dirac semimetals favor an equal-spin odd-parity pairing rather than a conventional $s$-wave one. The former pairing exhibits a distinct quartet of surface MFs stemming from the FL, though point nodes exist when the system retains $C_4$ rotation symmetry. If the $C_4$ symmetry is reduced to $C_2$ by a structural phase transition, the nodes disappear, and a full-gapped symmetry-protected TSC is realized. The FL-induced MFs are clearly distinguished from those in other TSCs [48,49] including superfluid $^3$He-A [50,51] and Weyl superconductors [34,52–55]. We finally suggest the possible application of our theory to recently discovered superconducting states in Cd$_3$As$_2$ and Au$_2$Pb.

Stability of Dirac points and surface Fermi loop.—First, we provide a general argument on the topology of Dirac points. Our theory assumes TRS, IS, and uniaxial rotation symmetry, which are the most common symmetries for Dirac semimetals. In the presence of TRS and IS, Kramer's degeneracy exists at arbitrary $k$ in the BZ, ensuring fourfold degeneracy when the conduction and valence bands are in contact. Such an accidental band crossing is generally not stable owing to band repulsion. However, if the band-touching point is on the high-symmetry axis, a $C_n$ symmetry can retain the band crossing as a Dirac point [1–4]. Below, we clarify the relevant topological structures.
We focus on the $C_4$ symmetric Hamiltonian $C_4H(k)C_4^{-1} = H(R_4k)$, with $R_4k = (k_x, -k_y, k_z)$. Here, without losing generality, we have chosen the rotation axis as the $k_z$ axis. The commutation relations between the TRS operator $T$, IS operator $P$, and $C_4$ are summarized as $[T,P] = [T,C_4] = [P,C_4] = 0$. As illustrated in Fig. 1(a), for a $C_4$ symmetric tetragonal crystal, there are two $C_4$ symmetry lines: $TZ = (0, 0, k_z)$ and $MA = (\pi, \pi, k_z)$, with $k_z \in [0, \pi]$. On these $C_4$ symmetry lines, the Hamiltonian commutes with $C_4$; thus, any energy band along the high-symmetry lines has a definite eigenvalue of the $C_4$ operator, $\alpha_p = \exp\left[\left(i\pi/2\right)(p + \frac{1}{2})\right] (p = 0, 1, 2, 3)$.

The existence of Dirac points is ensured by the topological invariant defined below. The system is generally gapped at the $C_4$ symmetry points $k = \Gamma, Z, M, A$, so one can count the number of bands below the Fermi level at these points. Denoting the number of such bands with the $C_4$ eigenvalue $\alpha_p$ at $k$ as $N_p(k)$, we can introduce the topological number $Q_p = N_p(\Gamma) - N_p(Z)$ for Dirac points on the $TZ$ line, which we call the $C_4$ topological invariant.

$$Q_0 = -Q_1 = -Q_2 = Q_3 = Q.$$  

If $Q \neq 0$, any band with $\alpha_p$ has $Q$ gapless points on the $TZ$ lines, corresponding to the difference $N_p(\Gamma) - N_p(Z)$, which eventually form $Q$ Dirac points. In Fig. 1(b), we illustrate a Dirac point with $Q = -1$. Because band mixing between different $C_4$ eigensystems is prohibited, the resultant Dirac points are stable as long as $C_4$ symmetry is maintained.

Similarly, we can also introduce the $C_4$ invariant for Dirac points on the $MA$ line.

Because of IS and the $C_2$ subgroup for $C_4$ symmetry, the system also has mirror-reflection symmetry: $M_{x,y} H(k_x, k_y, k_z) M_{x,y}^{-1} = H(k_x, k_y, -k_z)$, with $M_{x,y} = C_2^p P$. In the mirror-invariant planes ($k_z = 0$ or $\pi$), the Hamiltonian is block diagonal in the basis of the eigenstates of $M_{x,y}$; thus, the mirror Chern number $\nu_M(k_z)$ with $k_z = 0, \pi$ is defined as $\nu_M(k_z) = \frac{1}{2\pi} \int_{BZ} dk_x dk_y F^z(k)$, with $\lambda_4 = 0$ if $\nu_M(k_z) = 1$ is an eigenstate of $H(k)$ in the mirror sector with the eigenvalue $\lambda = \pm i$ of $M_{x,y}$ and $F^z$ is the field strength of $\lambda_4$. Generalizing the relation between a band inversion and the Chern number in terms of eigenvalues of crystal symmetry [43,58–61], we obtain the following relation for the mirror Chern number:

$$e^{i\pi/2/\nu_M(0)} = \prod_p \left[ N_{\nu_M(0)}(\Gamma) - N_{\nu_M(0)}(Y) \right] \prod_q \xi_{\nu_M(0)}^{-N_{\nu_M(0)}(Y)},$$

where $\xi_q = \exp\left[i\pi(q + \frac{1}{2})\right]$ and $q = 0, 1$ is the eigenvalue of $C_2$, $N_{\nu_M(0)}(k)$ is the number of occupied bands at $k$ with a set of the $C_4$ and $M_{x,y}$ eigenvalues ($\alpha_p, \lambda$) and $N_{\nu_M(0)}(Y)$ are those at $\Gamma$ with a set of $C_2$ and $M_{x,y}$ eigenvalues ($\xi_q, \lambda$). $\nu_M$ is the $C_2$ symmetry point in Fig. 1(a). Note that occupied bands at the $C_4$ ($C_2$) symmetry points have a definite set of eigenvalues for $C_4$ ($C_2$) and $M_{x,y}$ because $[C_4, M_{x,y}] = [C_2, M_{x,y}] = 0$. We can also obtain a similar relation for $\nu_M(\pi)$ by replacing $\Gamma$, $M$, and $Y$ with $Z$, $A$, and $T$, respectively, in Fig. 1(b).

To see the close relationship between the $C_4$ invariant and the mirror Chern number, consider a process in which a pair of stable Dirac points is created at $\Gamma$ [4]. Band inversion at $\Gamma$ occurs in this process, so a Kramer’s pair of occupied bands, which have a set of eigenvalues $(\alpha_p, \lambda)$ and $(\alpha_{3p', \lambda})$, go above the Fermi level, and a Kramer’s pair of empty bands with the eigenvalues $(\alpha_p, \lambda)$ and $(\alpha_{3p', \lambda})$ go below it at $\Gamma$. As a result, $N_{\nu_M(0)}(\Gamma)$ changes by $\Delta N_{\nu_M(0)}(\Gamma) = \Delta N_{\nu_M(0)}(\Gamma) = -1$. To have a stable Dirac point, $Q_p$ should change at the same time, so $p' \neq p''$. Then, from Eq. (2), we find that this process induces a simultaneous change in the mirror Chern number $\Delta \nu_M(0)$:

$$\Delta \nu_M(0) = \sum_p \left( p + \frac{1}{2} \right) \Delta N_{\nu_M(0)}(\Gamma) \mod 4,$$

$$= (p'' - p') \neq 0 \mod 4.$$  

Therefore, the creation of stable Dirac points is always accompanied by a net change in the mirror Chern number. From the bulk-boundary correspondence, the resultant mirror Chern number ensures the existence of surface helical Dirac fermions, whose Fermi surfaces form FLs.

Although the surface FLs accompany bulk Dirac points, it can be stable even when $C_4$ symmetry is lost, so the Dirac points have gaps. Indeed, unless the $C_2$ subgroup is broken,
the system maintains mirror-reflection symmetry, which is sufficient to stabilize the surface FL. Therefore, the structural phase transition that breaks $C_4$ to $C_2$ retains the FL.

**Topology of superconducting Dirac semimetals.**—With a finite carrier density, Dirac semimetals have disconnected bulk Fermi surfaces, each of which surrounds one of the band-touching Dirac points. See Fig. 1(a). Now consider a superconducting state in Dirac semimetals. The system is described by the Bogoliubov–de Gennes (BdG) Hamiltonian

$$H_{\text{BdG}}(k) = \begin{pmatrix} H(k) - \mu & \Delta(k) \\ \Delta^\dagger(k) & -H^*(-k) + \mu \end{pmatrix},$$

where $H(k)$ is the Hamiltonian for Dirac semimetals discussed above, $\mu$ is the chemical potential corresponding to the finite carrier density, and $\Delta(k)$ is the gap function. The BdG Hamiltonian supports particle-hole symmetry, $CH_{\text{BdG}}(k)C^{-1} = -H_{\text{BdG}}(-k)$, $C = \tau_z K$, with the Pauli matrix $\tau_z$ in the Nambu space and the conjugation operator $K$. Moreover, it may retain the symmetries of Dirac semimetals, depending on the symmetry property of the gap function. In particular, for a gap function with $\Delta(k) C = \Delta^\dagger(k) C \tau_z$, $H_{\text{BdG}}(k)$ keeps $C_4$ symmetry, $\Delta(k) C \tau_z = \Delta^\dagger(-k) C \tau_z$, with $C_4 = \text{diag}[C_4, e^{2\pi i/2} C_4]$. For a mirror-even or mirror-odd gap function that satisfies $M_{xy} \Delta(k) M_{xy}^\dagger = \eta_M \Delta(k, x, y, -z_k)$ with $\eta_M = \pm 1$, the system retains mirror-reflection symmetry, $\tilde{M}_{xy} H_{\text{BdG}}(k) \tilde{M}_{xy}^\dagger = H_{\text{BdG}}(k, x, y, -z_k)$, with $\tilde{M}_{xy} = \text{diag}[M_{xy}, \eta_M M_{xy}^\dagger]$. Correspondingly, we can introduce the $C_4$-invariant $\tilde{Q}_p$ and the mirror Chern numbers $\tilde{\nu}_\lambda$ for $H_{\text{BdG}}(k)$ [41,42], in a manner similar to that used for those of $H(k)$.

The topological numbers $\tilde{Q}_p$ and $\tilde{\nu}_\lambda$ are responsible for the existence of bulk point nodes on the $I$Z line and surface MFs in the superconducting state, respectively.

To evaluate these topological numbers, we employ the weak pairing assumption [31,32,35], i.e., that the superconducting gap is much smaller than the Fermi energy. The gap function is reasonably negligible away from the Fermi surface, in which we can take $\Delta(k) \to 0$, leading to $H_{\text{BdG}}(k) \to \text{diag}[H(k) - \mu, -H^*(-k) + \mu]$. Therefore, at the symmetry points $k = \Gamma, Z, M, A$, we can relate the negative energy states of $H_{\text{BdG}}(k)$ to those of $H(k)$. By taking into account the contribution from holes as well as electrons, the number $\tilde{N}_p$ of negative energy states with the $\tilde{C}_4$ eigenvalue $\alpha_p$ is evaluated as $\tilde{N}_p(k) = N_p(k) + \lfloor N - N_p(k) \rfloor$, where $N$ is the total number of bands in $H(k)$, $p_h = 3 - p + r \text{ mod } 4$, and the (first) (second) term on the right-hand side comes from the electron (hole) contribution. From this equation, the $C_4$ invariant in the superconducting state is obtained as

$$\tilde{Q}_p = \begin{cases} 0 & r = 0 \text{ or } p = p_h, \\ 2Q_p & \text{otherwise}. \end{cases}$$

Similarly, the mirror Chern number in the superconducting state is calculated as the sum of the electron and hole mirror Chern numbers, $\tilde{\nu}_\lambda = \nu_+ + \nu_-$, with $\lambda_h = -\eta_M \lambda$. As TRS in Dirac semimetals implies $\nu_- = -\nu_+$, we have

$$\tilde{\nu}_\lambda = \begin{cases} 0 & \eta_M = 1, \\ 2\nu_\lambda & \eta_M = -1. \end{cases}$$

Relations (5) and (6) have important physical consequences. (i) In the presence of $C_4$ symmetry, any superconducting Dirac semimetal with a nontrivial $r$ ($r = 1, 2, 3$) hosts point nodes as a remnant of Dirac points. Indeed, Eqs. (1) and (5) imply that at least a couple of $\tilde{Q}_p$ are nonzero in this case. To open a point node gap, we need to break the $C_4$ rotation symmetry. (ii) If the gap function is mirror odd, the mirror Chern number of the superconducting Dirac semimetal is nonzero, resulting in double MFs. In Fig. 1(c), we illustrate how the double MFs are created. In general, the gap function mixes the surface FL of electrons with that of holes so as to open a gap for the FL. In the mirror-odd case, however, mixing is prohibited on the mirror-invariant line in the surface BZ, so a pair of gapless points remains for each FL, forming double MFs.

In addition to the double MFs on the mirror-invariant line, we also find that each FL in the mirror-odd superconductor creates another pair of MFS on the $k_z$ axis in the surface BZ. By combining with $C$ and $M_{xy}$, the BdG Hamiltonian for the surface FL on the $k_z$ axis, which we denote $H_{\text{BdG}}^\text{FL}(k_z)$, has an antiunitary antisymmetry, $C_M H_{\text{BdG}}^\text{FL}(k_z) C_M^{-1} = -H_{\text{BdG}}^\text{FL}(k_z)$, with $C_M = iM_{xy} C = iM_{xy} \tau_z K$. Because $C_M = 1$ in the mirror-odd superconductor, $H_{\text{BdG}}^\text{FL}(k_z) iM_{xy} \tau_z$ is found to be real antisymmetric; thus, by using the Pfaffian, we can introduce the zero-dimensional topological invariant $\chi(k_z) = \text{sgn} \{ \text{Pf} [H_{\text{BdG}}^\text{FL}(k_z) iM_{xy} \tau_z] \}$. In the weak pairing case, $\chi(k_z)$ is evaluated as $\chi(k_z) = \text{sgn} \{ \text{det} [H_{\text{BdG}}^\text{FL}(k_z) - \mu] \}$, where $H_{\text{BdG}}^\text{FL}(k_z) - \mu$ is the Hamiltonian of the surface FL on the $k_z$ axis [62]. Therefore, $\chi(k_z)$ has different signs inside and outside the FL, which implies that $H_{\text{BdG}}^\text{FL}(k_z)$ should have zero-energy states near the points of intersection between the FL and the $k_z$ axis. These zero-energy states form a pair of MFS on the $k_z$ axis. Consequently, we can conclude that each FL has a quartet of MFS, as shown in Fig. 1(c). The quartet of MFS can stay gapless even when $C_4$ symmetry is broken, as long as mirror symmetry is preserved.

**Low-energy analysis and application to Cd$_4$As$_2$.**—For definiteness, we study the low-energy effective Hamiltonian, which describes a class of Dirac semimetals including Cd$_4$As$_2$ and Au$_3$Pb. Because bands in Dirac semimetals are doubly degenerate owing to PT symmetry, band-touching Dirac points are minimally described by a $4 \times 4$ matrix Hamiltonian. Thus, in the minimal setup, we need orbital degrees of freedom in addition to spin degrees of freedom, which are given by the Pauli matrices $\tau_\mu$ and $s_\mu$ in the orbital (1,2) and spin (†,†) spaces, respectively. The form of the $4 \times 4$ Hamiltonian is uniquely determined by symmetry [3,4]. In particular, for $P = \pm \sigma_z$, the low-energy lattice Hamiltonian is given by [4]
\[ H(k) = \{ -M + t_z (\cos k_x + \cos k_y) - t_z \cos k_z \} \sigma_z s_0 
+ (\eta \sin k_x) \sigma_x s_z - (\eta \sin k_y) \sigma_y s_0 
+ (\beta + \gamma) \sin k_z (\cos k_y - \cos k_x) \sigma_x s_x 
- (\beta - \gamma) \sin k_z \cos k_z \sigma_y s_y, \] 
\]

with \( T = i\sigma_0 s_y K \) and \( C_4 = e^{i(\pi/4)(2 + \eta_1)} r_x \). Here \( M, t_{xy}, t_z, \eta, \beta, \) and \( \gamma \) are material-dependent real constants. If \( t_z > (M - 2t_{xy}) > 0 \), this model has a pair of Dirac points located at \( k = (0, 0, \pm k_0) \), with \( k_0 > 0 \) defined by \( M = t_z \cos k_0 + 2t_{xy} \). We find \( \zeta(0) = \pm 1 \) and \( |Q| = 1 \). Accordingly, the FL arises at the surface parallel to the \( k_z \) axis, and the Dirac points are protected by \( C_4 \).

Near the Dirac points at \( k = (0, 0, \pm k_0) \), the low-energy Hamiltonian takes the form of the Dirac Hamiltonian, \( H(k) = \pm t_z k_0 (k_z + k_0) \sigma_z s_0 + \eta (k_x \sigma_x s_z - k_y \sigma_y s_0) \), which exhibits nontrivial \( \text{orbit-momentum locking} \). In Fig. 2(a), we show orbital textures in the \( k_x k_y \) plane with \( k_z = \pm k_0 \) in each spin sector, where the orientation of the orbit is tightly locked to the direction of the momentum on the Fermi surface. Orbit-momentum locking critically affects the possible pairing symmetry in the superconducting state. Indeed, we can show that constant \( s \)-wave pairing is inconsistent with the orbital texture. First, in such a static pairing state, electrons forming the Cooper pair have opposite momentum to each other, so they must belong to different Dirac points. Furthermore, as an \( s \)-wave pairing is spin singlet, it must be formed between electrons in different spin sectors. However, for a Cooper pair between electrons in different Dirac points and different spin sectors, orbit-momentum locking requires a momentum-dependent orbital structure in the Cooper pair, as illustrated in Fig. 2(a). Therefore, even if the pairing interaction favors an \( s \)-wave superconducting state, the pairing function cannot be constant, suggesting a suppression of the critical temperature.

On the other hand, for a Cooper pair with parallel spins, orbit-momentum locking is consistent with a constant pairing function. Indeed, the orbital-singlet equal-spin pairing \( \Delta = \Delta_0 (c_{1,1} c_{1,2} - c_{1,2} c_{1,1}) + i\Delta_0 (c_{1,1} c_{1,2} + c_{1,2} c_{1,1}) (= \Delta_\parallel) \) is compatible with the orbital texture in Fig. 2(a). Such an orbital-singlet Cooper pair is realized when the effective pairing interaction is dominated by an attractive interorbital interaction \( \mathcal{H}_{\text{int}} = -2V n_{1\uparrow} n_{2\uparrow} \), with \( n_\sigma = \sum_{x=\pm} c_{x,\sigma}^\dagger c_{x,\sigma}(x) \) \((V > 0)\) [31,63–65]. Although the actual pairing interaction is material dependent, the above results imply that doped Dirac semimetals favor the latter gap function. Because \( \Delta_\parallel \) is \( C_4 \) symmetric with \( r = 2 \) and mirror odd, i.e., \( C_4 \Delta_\parallel C_4 = -\Delta_\parallel \), it realizes a symmetry-protected TSC with bulk point nodes and a surface MF quartet, as discussed previously. In Fig. 2(b), we illustrate the quartet of MFs in this phase by numerically calculating the surface energy spectrum of the BdG Hamiltonian with Eq. (7) and \( \Delta = \Delta_\parallel \). Here we have also taken into account a symmetry-breaking effect from \( C_4 \) to \( C_2 \) by phenomenologically adding \( (m_0 \sin k_x) \sigma_x s_x \) to Eq. (7). As expected, Fig. 2(b) proves the existence of MFs on the mirror-invariant line \((\bar{\Gamma} \bar{Y}), \bar{Y} \) and \( k_z \) axis \((\bar{\Gamma} \bar{Z}) \) and moreover shows a gap in the \( \bar{Z} \bar{\Gamma} \) direction due to the \( C_4 \)-breaking term [66]. The obtained MFs in the mirror-invariant plane stay gapless even if the interaction effects are taken into account [67,68].

Finally, we discuss the possible application of our theory to superconductivity in \( \text{Au}_3 \text{Pb} \) and \( \text{Cd}_3 \text{As}_2 \). For \( \text{Au}_3 \text{Pb} \), first-principles calculations show that the Fermi level of this material is inside the gap of the Dirac points [26]; thus, no electron near the Dirac points contributes to the Cooper pairs. Hence, no TSC as discussed above is expected in \( \text{Au}_3 \text{Pb} \). On the other hand, the analysis above is applicable to the recently discovered superconductor \( \text{Cd}_3 \text{As}_2 \). In \( \text{Cd}_3 \text{As}_2 \), under high pressure, the structural phase transition occurs before the superconducting transition. Together with the orbit-momentum locking discussed above, the symmetry-breaking effect may stabilize the TSC phase by increasing the condensation energy, as the point nodes in the TSC phase are gapped when \( C_4 \) is reduced to \( C_2 \). Therefore, it is likely that \( \text{Cd}_3 \text{As}_2 \) realizes the TSC phase. The mirror-odd gap function of the TSC is detectable via anomalous Josephson effects [31,69] with carefully fabricated junctions.

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