Higher-order topological superconductors in $P\tau$, $T$-odd quadrupolar Dirac materials

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(Dated: March 30, 2020)

Presence or absence of certain symmetries in the normal state (NS) also determines the symmetry of the Cooper pairs. Here we show that parity ($P$) and time-reversal ($T$) odd Dirac insulators (trivial or topological) or metals, sustain a local or intra-unit cell pairing that supports corner (in $d = 2$) or hinge (in $d = 3$) modes of Majorana fermions and stands as a higher-order topological superconductor (HOTSC), when the NS additionally breaks discrete four-fold ($C_4$) symmetry. Although these outcomes do not rely on the existence of a Fermi surface, around it (when the system is doped) the HOTSC takes the form of a mixed parity, $T$-odd (due to the lack of $P$ and $T$ in the NS, respectively) $p + id$ pairing, where the $p(d)$-wave component stems from the Dirac nature of quasiparticles (lack of $C_4$ symmetry) in the NS. Thus, when strained, magnetically ordered Dirac materials, such as doped magnetic topological insulators (MnBi₂Te₄), can harbor HOTSCs.

Introduction. Symmetry of the normal state (NS) plays an important role in understanding the nature of the Cooper wavefunctions inside the paired states at low temperatures [1]. For example, (1) lack of the inversion symmetry in the NS mixes the even- and odd-parity pairings [2], and (2) Dirac materials composed of linearly dispersing massive or massless quasiparticles in the NS, described by the angular momentum $\ell = 1$ harmonics, harbor a plethora of exotic $p$-wave pairings [3], analogous to the ones in the B- and polar phases of $^3$He [4]. Here we investigate the role of time-reversal ($T$), inversion ($P$), as well as discrete crystalline four-fold ($C_4$) symmetry breaking on the paired states in two- and three-dimensional Dirac materials (insulator or metal) and come to the following conclusions.

In Dirac materials $P$ and $T$ can be simultaneously broken by a Dirac mass [5, 6]. Here we show that both two- and three-dimensional Dirac systems allow one local or inter-unit cell or momentum independent pairing that anticommutes with such a Dirac mass [Tables 1 and II]. In addition, when it breaks the $C_4$ symmetry (thus named Wilson-Dirac (WD) mass), the boundary modes (with codimension $d_c = 1$) of such paired states suffer dimensional reduction, producing zero energy corner and hinge modes ($d_c = 2$) of neutral Majorana fermions, respectively in two and three dimensions [Figs. 1, 2 and 3]. The paired states then represent higher-order topological superconductor (HOTSC), a topic of immense current interest [7, 8, 9, 10]. By contrast, other topological $p$-wave pairings, which commute with the WD mass, continue to represent first-order TSCs.

We primarily support these outcomes by numerically diagonalizing the effective single-particle Hamiltonian for various local pairings in trivial Dirac insulators (devoid of any boundary modes) and in the absence of a Fermi surface (thus involving both intra- and inter-band couplings). Therefore, emergent topology can solely be attributed to the BdG quasiparticles [38]. In the presence of a Fermi surface (conforming to weak coupling pairing) the intraband component of a HOTSC mimics $p + id$ pairing. Respectively, the parity mixing and $T$-breaking arise from the lack of $P$ and $T$ symmetries, whereas the $d$-wave component roots into the $C_4$ symmetry breaking in the NS, as its restoration converts the paired state into a trivial $p + is$ pairing. Therefore, antiferromagnetic topological insulators [6, 39], such as MnBi₂Te₄ [10], can be the ideal platform to search for HOTSCs, when they are doped (yielding a pairing conducive Fermi surface) and strained (lifting the crystalline symmetry).

Two-dimensions. The Hamiltonian for 2D quadrupolar massive Dirac fermions is $H_{2D} = H_0 + H_1 + H_2(\theta)$, where

$$H_0 = t \left[ \gamma_{31,1} S_1 + \gamma_{302,2} S_2 \right],$$
$$H_1 = \gamma_{303} \sum_{j=1}^{2} C_j,$$
$$H_2(\theta) = \Delta g(k) \left[ \gamma_{011} \cos \theta + \gamma_{021} \sin \theta \right].$$

Here $S_j = \sin(k_j a)$, $C_j = \cos(k_j a)$ with $k_j$s as the components of spatial momenta, $a$ is the lattice spacing, and $\theta$ is an arbitrary parameter [41]. Eight-dimensional Hermitian matrices $\Gamma_{\lambda \nu \rho}$ = $\eta_{\lambda} \sigma_{\nu} \tau_{\rho}$, where $\lambda, \nu, \rho = 0, \cdots , 3$, and the Pauli matrices $\{ \tau_{\nu} \}$, $\{ \sigma_{\nu} \}$ and $\{ \eta_{\nu} \}$ operator on the parity, spin and particle-hole indices, respectively. The Nambu spinor basis is $\Psi_{\text{Nam}(k)} = \left[ \Psi_k^\dagger, \sigma_{20} (\Psi_k^\dagger)^T \right]$, where $\Psi_k^\dagger \equiv \left[ c_{k,\uparrow}, c_{k,\downarrow}^\dagger, c_{k,\uparrow}^\dagger, c_{k,\downarrow} \right]$, and $c_{k,\sigma}$ is fermion annihilation operator with parity $\tau = \pm$, spin projection $\sigma = \uparrow, \downarrow$ and momentum $k$. When $\Delta = 0$, $H_{2D}^\text{Dir}$ describes a quantum spin Hall insulator and a trivial or normal insulator (NI) for $|m/t_0| < 2$ and $|m/t_0| > 2$, respectively. Here we set $m/t_0 = 3$.

Notice that $H_2(\theta)$ is odd under $T: k \rightarrow -k$ and $T = \Gamma_{020} K$, where $K$ is the complex conjugation, and $P: r \rightarrow -r$ and $P \Psi_{\text{Nam}(k)}(r)^{-1} = \Gamma_{003} \Psi_{\text{Nam}(-k)}(r)$. In addition, $H_2(\theta)$ breaks $C_4$ symmetry, if $g(k) = C_1 - C_2$. Then it represents a WD mass, as $\{ H_2(\theta), H_1 + H_2 \} = 0$, and the excitations are massive quadrupolar Dirac fermions.

Now we address topology of the paired states in this system, described by the single-particle Hamiltonian

$$H_{\text{pair}}^{2D} = \Delta_1 \Gamma_{j22} + \Delta_2 \Gamma_{j32} + \Delta_3 \Gamma_{j12} + \Delta_4 \Gamma_{j00} + \Delta_5 \Gamma_{j01} + \Delta_6 \Gamma_{j03}.$$ (2)
where \( j = 1 \) or \( 2 \), reflecting the \( U(1) \) gauge freedom in the choice of superconducting phase, and \( \Delta_i's \) are the pairing amplitudes. We choose \( j = 1 \). Two s-wave pairings (\( \Delta_4, \Delta_6 \)) are topologically trivial. By contrast, \( \Delta_1 \) and \( \Delta_3 \) pairings fully anticommute with the Dirac kinetic energy \( H_0 \) and represent fully gapped topological superconductor when \( |\Delta_1| > |m - 2t_0| \) and \( \Delta = 0 \). They support one-dimensional edge modes \([\text{Figs. 1(a) and 1(c)}]\). Remaining two pairings (\( \Delta_2 \) and \( \Delta_5 \)) break rotational symmetry. Respectively, they produce two Dirac points along the \( k_x \) and \( k_y \) directions, and support Fermi arcs along the \( x \) \([\text{Fig. 1(b)}]\) and \( y \) \([\text{Fig. 1(d)}]\) directions.

The effect of the WD mass on the pairings and boundary modes can be anticipated from its (anti)commutation relations with the pairing matrices \([\text{Table I}]\). Here we consider \( \theta = 0 \) and \( \theta = \frac{\pi}{4} \) only. The \( \Delta_3(\Delta_1) \) pairing anticommutes with \( H_2(0)[H_2(\frac{\pi}{4})] \). As \( H_2(\theta) \) changes sign under four-fold rotation, it acts as a domain wall mass (see Ref. \([12]\)) for the one-dimensional counter propagating edge modes of \( \Delta_3(\Delta_1) \) pairing when \( \theta = 0(\frac{\pi}{4}) \). Consequently, the boundary modes of \( \Delta_3 \) pairing undergoes a dimensional reduction, yielding four corner localized Majorana zero modes with \( d_c = 2 \) when \( \theta = 0 \) \([\text{Fig. 1(g)}]\). And we realize a second-order TSC. By contrast, \( \Delta_1, \Delta_2 \) and \( \Delta_5 \) pairings anticommute with \( H_2(0) \). So, their boundary modes are mildly affected \([\text{Figs. 1(e), 1(f) and 1(h)}]\), and they continue to be first-order TSCs. Similarly, for \( \theta = \frac{\pi}{4} \), only the \( \Delta_1 \) pairing represents a HOTSC and supports four corner localized zero modes \([\text{Fig. 2}]\).

Based on this observation, we propose a general principle of realizing HOTSCs. If an effective single-particle

![Figure 1](image-url)

**FIG. 1:** Top (Bottom): Local density of states (LDOS) for near (due to finite system size) zero energy modes for various p-wave pairings, in the absence (presence) of \( C_4 \) symmetry breaking WD mass \( H_2(0) \). Here we set \( t_0 = 1, m = 3 \) (yielding a NI) and \( \mu = 0 \) (no Fermi surface). Only the \( \Delta_1 \) pairing anticommutes with \( H_2(0) \) and represents a HOTSC, supporting four Majorana corner modes. Remaining three pairings commute with \( H_2(0) \) and their boundary modes are mildly affected \([\text{Table I}]\).

| Pairing | Matrix | \( H_0 \) | \( H_1 \) | \( H_2(0) \) | \( H_2(\frac{\pi}{4}) \) | HOTSC |
|---------|--------|--------|--------|--------|----------------|--------|
| \( \Delta_1 \) | \( \Gamma_{131} \) | \( - \) | \( - \) | \( + \) | \( + \) | \( \times \) | \( \checkmark \) |
| \( \Delta_2 \) | \( \Gamma_{132} \) | \( + \) | \( - \) | \( + \) | \( + \) | \( \times \) | \( \times \) |
| \( \Delta_3 \) | \( \Gamma_{112} \) | \( - \) | \( - \) | \( + \) | \( - \) | \( \checkmark \) | \( \times \) |
| \( \Delta_4 \) | \( \Gamma_{100} \) | \( - \) | \( + \) | \( + \) | \( + \) | \( \checkmark \) |
| \( \Delta_5 \) | \( \Gamma_{101} \) | \( + \) | \( + \) | \( + \) | \( + \) | \( \checkmark \) |
| \( \Delta_6 \) | \( \Gamma_{103} \) | \( + \) | \( + \) | \( - \) | \( - \) | \( \times \) | \( \times \) |

**TABLE I:** Commutation (+)/anticommutation (−) relations of pairings \([\text{Eq. 2}]\) with various entries of \( H_2^{2D} \) \([\text{Eq. 1}]\). Two s-wave pairings \( \Delta_1, \Delta_3 \) are topologically trivial. Remaining ones correspond to p-wave pairings. The associated boundary modes are shown in \( \text{Fig. 1} \) (Top). When \( \theta = 0(\frac{\pi}{4}) \), only \( \Delta_1 \) pairing anticommutes with the WD mass \( H_2(\theta) \) and supports four corner modes \([\text{Figs. 1(Bottom) and 2}]\).
Hamiltonian \((H_{FO})\) describes a first-order TSC, supporting boundary modes of \(d_c = 1\), then addition of an appropriate discrete-symmetry breaking WD mass \((H_{WD})\) can covert the paired state into a HOTSC, when \(\{H_{FO}, H_{WD}\} = 0\). Next we show that this mechanism is operative in \(d = 3\), yielding 1D hinge modes of \(d_c = 2\).

The Hamiltonian for a collection of three-dimensional quadrupolar massive Dirac fermions is \(H^{3D}_{Dir} = H_0 + H_1 + H_2\), where \(H_2 = \Gamma_{02} \Delta g(k)\) is the WD mass,

\[
H_0 = \frac{\hbar^2}{2m} \sum_{j=1}^{3} \Gamma_{31j} S_j, \quad H_1 = \Gamma_{330} \left[ m - t_0 \sum_{j=1}^{3} C_j \right],
\]

and \(\Gamma_{\rho\lambda\nu} = \eta_{\rho} \tau_\lambda \sigma_\nu\). The spinor basis is \(\Psi_{\text{Nam}}(k) = [\Psi_k, \tau_0 \sigma_2 \Psi_{-k}^\dagger]^\dagger\), with \(\Psi_k^\dagger = [c_{k,\uparrow}, c_{-k,\downarrow}, c_{-k,\uparrow}, c_{k,\downarrow}]\). While \(H_0\) gives rise to massless Dirac fermions, \(H_1\) stands as the symmetry preserving Dirac mass. Under \(\mathcal{T} : k \rightarrow -k\) and \(\Psi_{\text{Nam}}(k) \rightarrow \Gamma_{002} \Psi_{\text{Nam}}(-k)\), and the corresponding antunitary operator is \(\mathcal{T} = \Gamma_{002} K\). Under \(\mathcal{P} : r \rightarrow -r\) and \(\mathcal{P} \Psi_{\text{Nam}}(k) \mathcal{P}^{-1} = \Gamma_{330} \Psi_{\text{Nam}}(-k)\). The WD mass \(H_2\) breaks both \(\mathcal{P}\) and \(\mathcal{T}\) symmetries, but preserves the conjugate \(\mathcal{PT}\) symmetry, and in addition also breaks the discrete \(C_4\) symmetry if \(g(k) = C_1 - C_2\).

For \(\Delta = 0\), the above model supports strong (weak) topological insulator for \(1 < m/t_0 < 3\) (\(-1 < m/t_0 < 1\)), and NIs for \(m/t_0 > 3\) and \(m/t_0 < -1\). Here we choose \(m/t_0 = 4\). So the Dirac insulator is always trivial, and we solely unveil the topology of the paired states.

The single-particle Hamiltonian for local pairings is

\[
H^{3D}_{\text{pair}} = \Delta_j \Gamma_{j00} + \Delta_{ps} \Gamma_{j10} + \Delta_0 \Gamma_{j30} + \sum_{i=1}^{3} \Delta_i \Gamma_{j2i},
\]

where \(j = 1\) or \(2\). In the Dirac language \(\Delta_j\) transforms as a scalar, while the odd-parity \(\Delta_{ps}\) transforms as a pseudoscalar (PS). On the other hand, \(\Delta_0\) and \(\Delta_i\) transform as the temporal and three spatial components \((i = 1, 2, 3)\) of vector pairing, respectively. The (anti)commutation relations of all pairings with various components of \(H_{3D}^{\text{Dir}}\) are shown in Table II, which determines their topology. First we set \(\Delta = 0\).

Two s-wave pairings \(\Delta_s\) and \(\Delta_0\) are topologically trivial. The PS pairing is a fully gapped class DIII TSC, supporting gapless Majorana modes on six surfaces of a cubic system [Fig. 3(a)], when \(\Delta_{ps} > |m - 3t_0|\). The spatial components of vector pairing break the rotational symmetry and represent nematic superconductors. The \(\Delta_i\) pairing supports two Dirac points along the \(k_i\) direction, and Fermi arc surface states (with \(d_c = 1\)) along the \(i\)th direction in the real space [Figs. 3(b)-3(d)].

Now we switch on the WD mass \(H_2\). It breaks the \(C_4\) symmetry and changes sign four times in the \(xy\) plane for any \(z\). The PS pairing anticommutes with \(H_2\) [Table II], which then acts as a domain wall mass for the surface Majorana fermions, yielding 1D hinge modes (with \(d_c = 2\)) along \(z\) direction [Fig. 3(e)]. The PS pairing then represents a second-order TSC. For \(g(k) = C_3 - C_1\) and \(C_2 - C_3\) the hinge modes are aligned along the \(y\) and \(x\) directions, respectively. By contrast, all vector pairings commute with \(H_2\), and thus the Fermi arcs are mildly affected [Figs. 3(f)-3(h)]. These outcomes are in agreement with the general principle of realizing HOTSC.

Finally, we anchor these findings by projecting the HOTSCs onto a Fermi surface when the chemical doping (here measured from the bottom of the conduction band) \(\mu > 0\). We return to two-dimensional Dirac system and consider its low-energy model for \(\theta = 0\)

\[
H^{2D}_{\text{Dir}} = v \left[ \Gamma_{331} k_1 + \Gamma_{302} k_2 \right] + \Gamma_{303} M + \Gamma_{011} \Delta (k_1^2 - k_2^2),
\]

obtained by expanding \(H^{2D}_{\text{Dir}}\) around the \(\Gamma = (0, 0, 0)\) point, where \(M = |m - 2t_0|\), \(v = ta\) bears the dimension of Fermi velocity, and \(\Delta = -\Delta a^2/2\). The corresponding band diagonalizing matrix is \(U = U(k, \Delta) \oplus U(k, -\Delta)\),

| Pairing | Matrix | \(H_0\) | \(H_1\) | \(H_2\) |
|---------|--------|--------|--------|--------|
| \(\Delta_s\) | \(\Gamma_{j00}\) | - | - | - | + | \(x\) |
| \(\Delta_{ps}\) | \(\Gamma_{j10}\) | - | - | - | + | \(\checkmark\) |
| \(\Delta_0\) | \(\Gamma_{j30}\) | + | + | + | - | \(x\) |
| \(\Delta_1\) | \(\Gamma_{j21}\) | + | - | + | + | \(x\) |
| \(\Delta_2\) | \(\Gamma_{j22}\) | + | - | + | + | \(x\) |
| \(\Delta_3\) | \(\Gamma_{j23}\) | + | - | + | + | \(x\) |

**TABLE II:** Commutation (+)/anticommutation (−) relations of local pairings [Eq. (4)] with various components of \(H^{2D}_{\text{Dir}}\) [Eq. (5)]. Two s-wave pairings \((\Delta_s, \Delta_0)\) are topologically trivial. Only the pseudoscalar (PS) pairing \((\Delta_{ps})\) anticommutates with the WD mass \((H_2)\), yielding a second-order TSC that supports one-dimensional hinge modes, see Fig. 3(e).
where

$$U(k, \Delta) = \begin{pmatrix}
\frac{-\lambda}{\sqrt{2k_x}} & 0 & \frac{\lambda}{\sqrt{2k_x}} & 0 \\
\frac{-\bar{\eta}(k)}{\sqrt{2\lambda_+}} & \frac{-\bar{\eta}(k)}{\sqrt{2\lambda_+}} & \frac{\bar{\eta}(k)}{\sqrt{2\lambda_+}} & \frac{-\bar{\eta}(k)}{\sqrt{2\lambda_+}} \\
0 & \frac{-\lambda}{\sqrt{2k_x}} & 0 & \frac{\lambda}{\sqrt{2k_x}} \\
\frac{\bar{g}(k)}{\sqrt{2\lambda_+}} & \frac{\bar{g}(k)}{\sqrt{2\lambda_+}} & \frac{-\bar{g}(k)}{\sqrt{2\lambda_+}} & \frac{-\bar{g}(k)}{\sqrt{2\lambda_+}}
\end{pmatrix}, \quad (6)$$

with $k_\pm = k_1 \pm ik_2$, $\lambda = \sqrt{\eta^2 k_+^2 + M^2}$, $\bar{\eta}(k) = \Delta(k_1^2 - k_2^2)$. In the presence of $\Delta_3$ pairing, the single-particle Hamiltonian in the vicinity of the Fermi surface for large mass ($M \gg \eta k, \Delta$) reads

$$H_{FS}^{3D} = \xi_k \Gamma_{30} + \Delta_1 M \left\{ v [k_x \Gamma_{11} - k_y \Gamma_{12}] + \bar{g}(k) \Gamma_{20} \right\}, \quad (7)$$

where $\xi_k = \sqrt{\eta^2 k_+^2 + M^2} - \mu$, and $\Gamma_{\mu\nu} = \eta_{\mu\nu}$. The Pauli matrices $\{\eta_{\mu}\}$ operate on the particle-hole (pseudospin) indices. For $\Delta = 0$, $H_{FS}^{3D}$ describes a $T$-symmetric fully gapped $p$-wave pairing. The $p$-wave BdG quasiparticles solely arises from the Dirac nature of NS fermions. If we set $\bar{g}(k) = g_0$ (constant), then $H_{FS}^{3D}$ describes a trivial $p + is$ pairing. The breaking of $T$ and mixing of parity inside the paired state stem from the lack of $T$ and $\mathcal{P}$ symmetries in the NS, respectively. By contrast, when $\bar{g}(k) = \Delta(k_1^2 - k_2^2)$, $H_{FS}^{3D}$ describes a HOT $p + id$ pairing, and the appearance of the $d$-wave component can now solely be attributed to the lack of $C_4$ symmetry in the NS. Therefore, absence of each symmetry in the NS plays crucial role in determining the symmetry and topology of the paired states \[18\]. Note that $H_{FS}^{3D}$ assumes the form of Dirac fermions ($p$-wave pairing), subject to inverted-band regular Dirac mass (yielding a Fermi surface when $\mu > 0$) and $\mathcal{P}$- and $T$-odd, $C_4$ symmetry breaking WD mass ($d$-wave pairing); together giving rise to a HOTSC and four corner localized Majorana zero modes \[Fig. 1(g)\]. The same argument is applicable for the $\Delta_1$ pairing when $\theta = \frac{\pi}{2}$.

Similarly, the single-particle Hamiltonian for the three-dimensional PS pairing around the Fermi surface takes the form $H_{FS}^{3D} = \xi_k \Gamma_{30} + H_{p+id}^{3D}$, with $M = |m - 3t_0|$ and

$$H_{p+id}^{3D} = \frac{\Delta_{ps}}{M} \left\{ v [k_x \Gamma_{11} - k_y \Gamma_{12} + k_z \Gamma_{13}] + \bar{g}(k) \Gamma_{20} \right\}. \quad (8)$$

It takes the form of the $\mathcal{P}$- and $T$-odd $p + id$ ($p + is$) pairing for $\bar{g}(k) = \Delta(k_1^2 - k_2^2)$ (constant), standing as HOT (axionic \[49\]) superconductor. Therefore, around the Fermi surface the PS pairing is described by Dirac fermions ($p$-wave pairing) in the presence of both regular ($\xi_k$) and $\mathcal{P}$- and $T$-odd, $C_4$ symmetry breaking ($d$-wave pairing) Dirac masses, which gives birth to 1D hinge modes \[Fig. 3 \[48\]. Imprint of each discrete symmetry in the paired state is identical to that for the 2D HOTSC.

**Discussion.** To summarize, here we demonstrate a general principle of realizing HOTSCs. In both $d = 2$ and 3, a first-order TSC can be converted into a HOTSC in the presence of a discrete symmetry breaking, $\mathcal{P}$- and
T-odd anticommuting WD mass [Tables III, I], respectively yielding corner and hinge modes of codimension $d_e = 2$ [Figs. 1, 2, 3]. Therefore, magnetically doped or ordered (due to strong electronic correlations) Dirac insulators (trivial or topological) can accommodate HOTSCs, when they supports a Fermi surface (conductive for weak coupling pairings) and are subject to external strain (breaking discrete rotational symmetry). Hopefully, the present discussion will stimulate a search for HOTSCs (both theoretically and experimentally) in strained but doped magnetic topological insulators [6, 39, 50], such as MnBi$_2$Te$_4$ [40]. In the future, it will also be worth investigating possible HOTSCs in candidate HOT insulators, such as Bi [11] and strained Luttinger materials [51].

Acknowledgments. B.R. was supported by the startup grant from Lehigh University.

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