

Supplementary Notes for “Topological triplet-superconductivity in spin-1 semimetal”

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SUPPLEMENTARY NOTE 1 : TRIPLE POINT SEMIMETAL TIGHT-BINDING EXAMPLE

Here, we follow Ref.[1] and provide a band structure in space group 199 which realize triple point fermions at two inequivalent high symmetry points, $\pm P$. We consider a tight-binding model with four sites in each unit cell where the coordinates are given by $r_1 = (0, 0, 0)$, $r_2 = (1/2, 1/2, 0)$, $r_3 = (1/2, 0, 1/2)$, and $r_4 = (0, 1/2, 1/2)$. [2] Here, we take the primitive lattice vectors as $a_1 = (1/2, 1/2, 1/2)$, $a_2 = (0, 1, 0)$, and $a_3 = (0, 0, 1)$. We consider s-orbital on each site and define an electron annihilation operator $c_s^{A,R}$, where s corresponds to up and down spin, which are quantized along a crystalline z -axis. A and R indices represent the position of unit cell and the site within the unit cell respectively. The tight-binding Hamiltonian is given by

$$H^{\delta A, R, R', t, \lambda}(\mathbf{q}) = e^{-i\mathbf{k} \cdot \delta A} c_q^{R, s \dagger} (t \delta_{ss'} + i(\boldsymbol{\lambda} \cdot \boldsymbol{\sigma})_{ss'}) c_q^{R', s'} + \text{h.c.} \quad (1)$$

where δA is a lattice vector. In Supplementary Table I, we give the complete Hamiltonian by listing all terms in above notation.

Supplementary Table I: A complete list of terms in the tight-binding example.

$\mathbf{q} \cdot \delta A$	R	t	$\boldsymbol{\lambda}$	R'
0	4	$\sqrt{2}t_1$	$(\sqrt{3}t_1, -t_1, 0)$	1
0	3	$-\sqrt{2}t_1$	$(-\sqrt{3}t_1, t_1, 0)$	2
0	2	0	$(t_1, \sqrt{3}t_1, -\sqrt{2}t_1)$	1
q_y	4	0	$(t_1, \sqrt{3}t_1, \sqrt{2}t_1)$	3
$\frac{1}{2}(q_x - q_y - q_z)$	3	$-\sqrt{2}t_1$	$(-\sqrt{3}t_1, t_1, 0)$	1
$\frac{1}{2}(-q_x + q_y - q_z)$	4	$-\sqrt{2}t_1$	$(-\sqrt{3}t_1, t_1, 0)$	2
$-q_z$	4	$-\sqrt{2}t_2$	$(\sqrt{3}t_2, t_2, 0)$	1
$-q_z$	3	$\sqrt{2}t_2$	$(-\sqrt{3}t_2, -t_2, 0)$	2
$-q_y$	2	0	$(-t_2, \sqrt{3}t_2, \sqrt{2}t_2)$	1
0	4	0	$(-t_2, \sqrt{3}t_2, -\sqrt{2}t_2)$	3
$\frac{1}{2}(-q_x - q_y - q_z)$	3	$\sqrt{2}t_2$	$(-\sqrt{3}t_2, -t_2, 0)$	1
$\frac{1}{2}(q_x + q_y - q_z)$	4	$\sqrt{2}t_2$	$(-\sqrt{3}t_2, -t_2, 0)$	2

The corresponding eight electronic bands are plotted in Supplementary Figure 1 when $t_2/t_1 = 2$. This model realizes two distinct pairs of triple point fermions at momenta $\pm P$. Close to the band crossing points, $\mathbf{q} = \pm \mathbf{K} + \mathbf{k}$, the Hamiltonian can be expanded up to the linear order as,

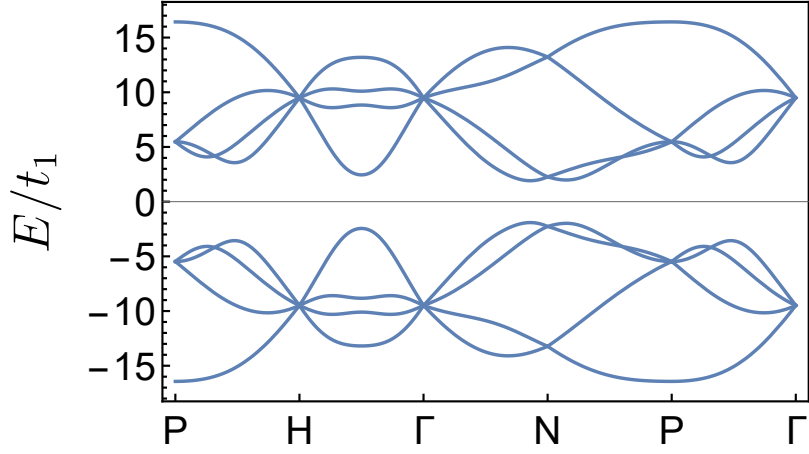
$$h_{\pm}(\mathbf{k}) = \psi_{\pm, \mathbf{k}}^{\dagger} \left[\left(\frac{\sqrt{6} - \sqrt{6}t_2^2}{2\sqrt{t_2^2 + 1}} \right) \mathbf{k} \cdot \mathbf{J} \right] \psi_{\pm, \mathbf{k}} \quad (2)$$

with $t_1 = 1$ which displays $SO(3)$ symmetry.

SUPPLEMENTARY NOTE 2 : SPIN PAIRING MATRICES M_S OF $j = 1$ ELECTRONS

In this section, we give the explicit form of the spin pairing matrices M_S which are used in the main text. First, $M_{S=0}$ is equal to 3×3 identity matrix $\mathbb{I}_3$ and remains invariant under spin rotation transformation. Each $M_{S=1}$ is proportional to J_a and behaves as one of three magnetic dipole matrices under the rotation transformation. J_a are explicitly written as,

$$J_x = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, J_y = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}, J_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad (3)$$



Supplementary Figure 1: (color online) An example of band structure in space group 199 which realize triple point fermions at two inequivalent high symmetry points, $\pm P$. [1]

and one can write down three $M_{S=1}$ as $\sqrt{\frac{3}{2}}J_x$, $\sqrt{\frac{3}{2}}J_y$ and $\sqrt{\frac{3}{2}}J_z$ which satisfy the normalization condition, $\text{tr}[M_S(M_S)^\dagger] = 3$. Five $M_{S=2}$ transform as five quadrupole matrices and are given by

$$\begin{aligned} \Gamma_{x^2-y^2} &= \sqrt{\frac{3}{2}}(J_x^2 - J_y^2), \Gamma_{3z^2-r^2} = \sqrt{\frac{1}{2}}(2J_z^2 - J_x^2 - J_y^2), \\ \Gamma_{yz} &= \sqrt{\frac{3}{2}}(J_y J_z + J_z J_y), \Gamma_{zx} = \sqrt{\frac{3}{2}}(J_z J_x + J_x J_z), \Gamma_{xy} = \sqrt{\frac{3}{2}}(J_x J_y + J_y J_x). \end{aligned} \quad (4)$$

SUPPLEMENTARY NOTE 3 : FIERZ IDENTITY WITH $j=1$ FERMIONS

In this section, we give Fierz identities for the spherically symmetric and the anisotropic cases. Any 3×3 Hermitian matrix can be represented using a basis set $\{\Sigma^A\}_{A=1,\dots,9}$ which contains 9 elements. Assume the basis to be orthogonal : $\text{tr}[\Sigma^A \Sigma^B] = 3\delta^{AB}$. A choice of basis consists in $\Sigma_A \rightarrow \Gamma_A$ with

$$\{\Gamma^A\} = \{M_0, M_1, M_2\}, \quad (5)$$

where M_S are the multipole matrices of $j = 1$ electrons. Let $\psi = (\psi_1, \psi_2, \psi_3)$ be a three component vector with Grassmann variables ψ_a . Then, any interaction term can be decomposed as

$$(\psi^\dagger P \psi)(\psi^\dagger Q \psi) = -\frac{1}{9} \text{tr}(P \Sigma^A Q \Sigma^B) (\psi^\dagger \Sigma^A \psi) (\psi^\dagger \Sigma^B \psi), \quad (6)$$

$$(\psi^\dagger P \psi^*)(\psi^T Q \psi) = \frac{1}{9} \text{tr}(P \Sigma^A Q \Sigma^B) (\psi^\dagger (\Sigma^A)^T \psi) (\psi^\dagger \Sigma^B \psi), \quad (7)$$

respectively. See Ref.[3] for the discussion of Fierz identities in generic situation.

We first consider the spherically symmetric case. Let

$$X_1 = (\psi^\dagger \psi)^2, \quad (8)$$

$$X_2 = \sum_{a=1,2,3} (\psi^\dagger M_1^a \psi)^2, \quad (9)$$

$$X_3 = \sum_{a=1\dots 5} (\psi^\dagger M_2^a \psi)^2 \quad (10)$$

be the interactions terms which are allowed by $SO(3)$ symmetry. With Supplementary Equation (6), we get

$$\mathbf{X} = F\mathbf{X} \quad (11)$$

with $\mathbf{X} = (X_1, X_2, X_3)$ and

$$F = \begin{pmatrix} -1/3 & -1/3 & -1/3 \\ -1 & -1/2 & 1/2 \\ -3/5 & 5/6 & -1/6 \end{pmatrix}. \quad (12)$$

Then, we can define $F' = F - \mathbb{I}_3$, which has matrix rank 1. After doing the row reduction, F' is given as

$$F' \sim \begin{pmatrix} 1 & 0 & 2/5 \\ 0 & 1 & -3/5 \\ 0 & 0 & 0 \end{pmatrix}, \quad (13)$$

from which we get the Fierz identities which are given as below.

$$\begin{aligned} 0 &= (\psi^\dagger \psi)^2 + \frac{2}{5} \sum_{a=1\dots 5} (\psi^\dagger M_2^a \psi)^2, \\ 0 &= \sum_{a=1,2,3} (\psi^\dagger M_1^a \psi)^2 - \frac{3}{5} \sum_{a=1\dots 5} (\psi^\dagger M_2^a \psi)^2 \end{aligned} \quad (14)$$

These relations allow to eliminate two kinds of interactions terms, X_1 and X_3 , from the analysis of the spherically symmetric case.

Next consider the cubic symmetric case with $\mathbf{L} = (L_1, L_2, L_3, L_4)$ and the L_i are defined as

$$L_1 = (\psi^\dagger \psi)^2, \quad (15)$$

$$L_2 = \sum_{a=1,2,3} (\psi^\dagger M_1^a \psi)^2, \quad (16)$$

$$L_3 = \sum_{a=1,2} (\psi^\dagger M_2^a \psi)^2 \quad (17)$$

$$L_4 = \sum_{a=3,4,5} (\psi^\dagger M_2^a \psi)^2 \quad (18)$$

After doing the same procedure as in the spherically symmetric case, we obtain

$$\mathbf{L} = F\mathbf{L} \quad (19)$$

with

$$F = \begin{pmatrix} -1/3 & -1/3 & -1/3 & -1/3 \\ -1 & -1/2 & 1/2 & 1/2 \\ -2/3 & 1/3 & -2/3 & 1/3 \\ -1 & 1/2 & 1/2 & -1/2 \end{pmatrix}. \quad (20)$$

For $F' = F - \mathbb{I}_4$, the row reduction gives

$$F' \sim \begin{pmatrix} 1 & 0 & 0 & 2/3 \\ 0 & 1 & 0 & -1 \\ 0 & 0 & 1 & -2/3 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad (21)$$

from which we get the Fierz identities which are given as below.

$$\begin{aligned} 0 &= (\psi^\dagger \psi)^2 + \frac{2}{3} \sum_{a=3,4,5} (\psi^\dagger M_2^a \psi)^2, \\ 0 &= \sum_{a=1,2,3} (\psi^\dagger M_1^a \psi)^2 - \sum_{a=3,4,5} (\psi^\dagger M_2^a \psi)^2, \\ 0 &= \sum_{a=1,2} (\psi^\dagger M_2^a \psi)^2 - \frac{2}{3} \sum_{a=3,4,5} (\psi^\dagger M_2^a \psi)^2 \end{aligned} \quad (22)$$

Finally, we consider the tetragonal symmetric case with $\mathbf{T} = (T_1, \dots, T_7)$ and the T_i are defined as

$$T_1 = (\psi^\dagger \psi)^2, \quad (23)$$

$$T_2 = \sum_{a=1,2} (\psi^\dagger M_1^a \psi)^2, \quad (24)$$

$$T_3 = (\psi^\dagger M_1^3 \psi)^2 \quad (25)$$

$$T_4 = (\psi^\dagger M_2^1 \psi)^2 \quad (26)$$

$$T_5 = (\psi^\dagger M_2^2 \psi)^2 \quad (27)$$

$$T_6 = \sum_{a=3,4} (\psi^\dagger M_2^a \psi)^2 \quad (28)$$

$$T_7 = (\psi^\dagger M_2^5 \psi)^2 \quad (29)$$

Using Supplementary Equation (6), we get seven identities that are given below.

$$T_1 = -\frac{1}{3}(T_1 + T_2 + T_3 + T_4 + T_5 + T_6 + T_7) \quad (30)$$

$$T_2 = -\frac{2}{3}T_1 - \frac{1}{2}T_2 + \frac{2}{3}T_5 + \frac{1}{2}T_6 + \frac{1}{3\sqrt{2}}((\psi^\dagger \psi)(\psi^\dagger M_2^2 \psi) + (\psi^\dagger M_2^2 \psi)(\psi^\dagger \psi)) \quad (31)$$

$$T_3 = -\frac{1}{3}T_1 - \frac{1}{2}T_3 + \frac{1}{2}T_4 - \frac{1}{6}T_5 + \frac{1}{2}T_7 - \frac{1}{3\sqrt{2}}((\psi^\dagger \psi)(\psi^\dagger M_2^2 \psi) + (\psi^\dagger M_2^2 \psi)(\psi^\dagger \psi)) \quad (32)$$

$$T_4 = -\frac{1}{3}T_1 + \frac{1}{2}T_3 - \frac{1}{2}T_4 - \frac{1}{6}T_5 + \frac{1}{2}T_7 - \frac{1}{3\sqrt{2}}((\psi^\dagger \psi)(\psi^\dagger M_2^2 \psi) + (\psi^\dagger M_2^2 \psi)(\psi^\dagger \psi)) \quad (33)$$

$$T_5 = -\frac{1}{3}T_1 + \frac{1}{3}T_2 - \frac{1}{6}T_3 - \frac{1}{6}T_4 - \frac{1}{2}T_5 + \frac{1}{3}T_6 - \frac{1}{6}T_7 + \frac{1}{9}\left(2\sqrt{2} - \frac{1}{\sqrt{2}}\right)((\psi^\dagger \psi)(\psi^\dagger M_2^2 \psi) + (\psi^\dagger M_2^2 \psi)(\psi^\dagger \psi)) \quad (34)$$

$$T_6 = -\frac{2}{3}T_1 + \frac{1}{2}T_2 + \frac{2}{3}T_5 - \frac{1}{2}T_6 + \frac{1}{3\sqrt{2}}((\psi^\dagger \psi)(\psi^\dagger M_2^2 \psi) + (\psi^\dagger M_2^2 \psi)(\psi^\dagger \psi)) \quad (35)$$

$$T_7 = -\frac{1}{3}T_1 + \frac{1}{2}T_3 + \frac{1}{2}T_4 - \frac{1}{6}T_5 - \frac{1}{2}T_7 - \frac{1}{3\sqrt{2}}((\psi^\dagger \psi)(\psi^\dagger M_2^2 \psi) + (\psi^\dagger M_2^2 \psi)(\psi^\dagger \psi)) \quad (36)$$

SUPPLEMENTARY NOTE 4 : IDENTIFICATION OF MICROSCOPIC SYMMETRY ALLOWED INTERACTIONS

In this section, we identify a way to realize a special form of interactions between triple point fermions, which are given in the main text, starting from microscopic symmetry allowed interactions in the lattice model. We start from the tight-binding model, which is given in Supplementary Equation (1), with $t_2/t_1 = 2$.

We first consider the usual on site Hubbard interactions,

$$H_{int} = U \sum_i (n_{i,\uparrow} n_{i,\downarrow} + n_{i,\downarrow} n_{i,\uparrow}) \quad (37)$$

where i labels lattice site and $\uparrow$ and $\downarrow$ represent up and down spin respectively. After performing the Fourier transformation and projecting into the triple-band crossing point, we get the following form of interactions between triple point fermions.

$$h_{int} = \frac{U}{5} [(\psi_{+,0}^\dagger \psi_{+,0})(\psi_{-,0}^\dagger \psi_{-,0}) + \frac{2}{3} \sum_{a=3,4,5} (\psi_{+,0}^\dagger M_2^a \psi_{+,0})(\psi_{-,0}^\dagger M_2^a \psi_{-,0})] \quad (38)$$

Here, $\psi_{\pm,0} = (\psi_{\pm,\mathbf{k}=0,1}, \psi_{\pm,\mathbf{k}=0,0}, \psi_{\pm,\mathbf{k}=0,-1})$. Remarkably, one can easily show that Supplementary Equation (38) vanishes using Supplementary Equation (22).

Next we consider the nearest neighbor Hubbard interactions which has the following form.

$$H_{int} = V \sum_{a,b} \sum_{i,j} n_{i,a} n_{j,b} \quad (39)$$

Here, i and j label nearest neighbour sites. After doing similar procedure, which is stated above, we get the following form of interactions between triple point fermions.

$$h_{int} = V [3(\psi_{+,0}^\dagger \psi_{+,0})(\psi_{-,0}^\dagger \psi_{-,0}) - \frac{2}{3} \sum_{a=3,4,5} (\psi_{+,0}^\dagger M_2^a \psi_{+,0})(\psi_{-,0}^\dagger M_2^a \psi_{-,0})] \quad (40)$$

One can easily show that Supplementary Equation (40) can be rewritten as the following using Supplementary Equation (22).

$$\begin{aligned} h_{int} &= \frac{-8V}{3} \sum_{a=1,2,3} (\psi_{+,0}^\dagger M_1^a \psi_{+,0}) (\psi_{-,0}^\dagger M_1^a \psi_{-,0}) \\ &= -4V \sum_{a=x,y,z} (\psi_{+,0}^\dagger J_a \psi_{+,0}) (\psi_{-,0}^\dagger J_a \psi_{-,0}) \end{aligned} \quad (41)$$

Then, Supplementary Equation (41) can be rewritten as the following by employing Supplementary Equation (7).

$$h_{int} = 2V \sum_{a=x,y,z} (\psi_{+,0}^\dagger J_a \gamma \psi_{-,0}^*) (\psi_{-,0}^T (J_a \gamma)^\dagger \psi_{+,0}) \quad (42)$$

Supplementary Equation (42) clearly shows that attractive nearest neighbor Hubbard interactions ($V < 0$) can induce pairing instability towards spin-triplet superconducting states.

Lastly, we consider the spin-dependent interactions which has the following form.

$$H_{int} = J \sum_{a,b} \sum_{i,j} (c_{i,a}^\dagger \sigma_{ab} c_{i,b}^\dagger) (c_{j,a}^\dagger \sigma_{ab} c_{j,b}^\dagger) \quad (43)$$

Here, i and j label nearest neighbour sites. We get the following form of interactions between triple point fermions.

$$h_{int} = \frac{J}{20} \left[-7(\psi_{+,0}^\dagger \psi_{+,0}) (\psi_{-,0}^\dagger \psi_{-,0}) + \frac{10}{3} \sum_{a=3,4,5} (\psi_{+,0}^\dagger M_2^a \psi_{+,0}) (\psi_{-,0}^\dagger M_2^a \psi_{-,0}) - \frac{16}{3} (\psi_{+,0}^\dagger M_2^5 \psi_{+,0}) (\psi_{-,0}^\dagger M_2^5 \psi_{-,0}) \right] \quad (44)$$

One can easily show that Supplementary Equation (44) can be rewritten as the following using Supplementary Equation (22).

$$\begin{aligned} h_{int} &= \frac{J}{20} \left[8 \sum_{a=1,2,3} (\psi_{+,0}^\dagger M_1^a \psi_{+,0}) (\psi_{-,0}^\dagger M_1^a \psi_{-,0}) - \frac{16}{3} (\psi_{+,0}^\dagger M_2^5 \psi_{+,0}) (\psi_{-,0}^\dagger M_2^5 \psi_{-,0}) \right] \\ &= \frac{J}{20} \left[12 \sum_{a=x,y,z} (\psi_{+,0}^\dagger J_a \psi_{+,0}) (\psi_{-,0}^\dagger J_a \psi_{-,0}) - 8(\psi_{+,0}^\dagger (J_x J_y + J_y J_x) \psi_{+,0}) (\psi_{-,0}^\dagger (J_x J_y + J_y J_x) \psi_{-,0}) \right] \end{aligned} \quad (45)$$

Then, Supplementary Equation (45) can be rewritten as the following by employing Supplementary Equation (7).

$$h_{int} = -\frac{3J}{10} \sum_{a=x,y,z} (\psi_{+,0}^\dagger J_a \gamma \psi_{-,0}^*) (\psi_{-,0}^T (J_a \gamma)^\dagger \psi_{+,0}) + \frac{J}{5} (\psi_{+,0}^\dagger J_z \gamma \psi_{-,0}^*) (\psi_{-,0}^T (J_z \gamma)^\dagger \psi_{+,0}) \quad (46)$$

Supplementary Equation (46) shows that antiferromagnetic interactions, $J > 0$, can induce pairing instability towards spin-triplet superconducting states.

SUPPLEMENTARY REFERENCES

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