Eightfold Degenerate Fermions in Two Dimensions

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Multifold degenerate fermions have attracted a lot of research interest in condensed matter physics and materials science, but always lack in two dimensions. In this Letter, from symmetry analysis and lattice model construction, we demonstrate that eightfold degenerate fermions can be realized in two-dimensional systems. In nonmagnetic materials with negligible spin-orbit coupling, the gray magnetic space groups together with SU(2) spin rotation symmetry can protect the two-dimensional eightfold degenerate fermions on a certain high-symmetry axis in the Brillouin zone, no matter whether the system is centrosymmetric or noncentrosymmetric. In antiferromagnetic materials, the eightfold degenerate fermions can also be protected by certain “spin space groups.” Furthermore, by first-principles electronic structure calculations, we predict that the paramagnetic phase of the monolayer LaB6 on a suitable substrate is a two-dimensional eightfold degenerate as well as Dirac node-line semimetal. Especially, the eightfold degenerate points are close to the Fermi level, which makes monolayer LaB6 a good platform to study the exotic physical properties of two-dimensional eightfold degenerate fermions.

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Introduction.—In high-energy physics, relativistic massless Dirac fermions and Weyl fermions are the representations of the Poincaré group. At zero momentum, the massless Dirac fermions and Weyl fermions are four- and twofold degenerate, respectively. In condensed matter physics, the massless Dirac and Weyl fermions have been realized as the low-energy quasiparticle excitations [1–7]. The physical properties of massless Dirac and Weyl particles known in high-energy physics, such as the chiral anomaly, have also been observed in condensed matter physics [8,9].

On the other hand, 230 space groups are subgroups of the Poincaré symmetry; thus condensed matter systems have less constraints and new fermionic quasiparticles beyond high-energy physics can emerge [10–16]. For instance, three-, six-, and eightfold degenerate fermionic quasiparticles were proposed theoretically [10–16] and later realized in experiments [17,18]. So far, the new types of quasiparticles beyond the Dirac and Weyl fermions have been only studied in three-dimensional semimetals.

Two-dimensional (2D) systems contain rich physics in condensed matter. For instance, the first example of Dirac semimetal was realized in a 2D material—the graphene [19]. Furthermore, some special phenomena only exist in two dimensions (or at the surface of three-dimensional lattice systems), such as the integer and fractional quantum Hall effect and the quantum spin Hall effect [20–22]. In 2D systems, the point groups are uniaxial and the highest point group symmetry is $D_{oh}$. The relatively lowered symmetries thus strongly restrict the types of quasiparticles. For instance, the threefold degeneracy can never be protected in 2D materials since the uniaxial point groups do not have three-dimensional irreducible (projective) representations. The previously mentioned new types of nontrivial quasiparticles, if they exist in 2D, must be protected by nonsymmorphic space groups supporting layered structures.

In this Letter, based on group theory analysis and lattice model calculations, we demonstrate that the highest degeneracy of quasiparticles is eight, which is located on a high-symmetry line (HSL) in the Brillouin zone (BZ). Among the space groups supporting layered structures, four can protect eightfold degeneracy, including three centrosymmetric space groups (i.e., 51, 55, 127, with little cogroup $E \times \{L, T\}$), where $I$ and $T$, respectively, stand for space-inversion and time-reversal operation) and one noncentrosymmetric space group (i.e., 26 with little cogroup $2km^*m = \{E, C_{2v}, T, M, \bar{T}, \bar{M}\}$). More importantly, as long as the intrinsic spin-orbit coupling is negligible, the eightfold degenerate fermions can also stably exist in magnetic semimetals with collinear antiferromagnetic order, even if the Zeeman coupling between the spins of itinerary electrons and the local magnetic momentum essentially gives rise to spin-orbit coupling. These magnetic semimetals belong to two type-III magnetic space groups (51.293, 55.355) and six type-IV magnetic space groups (51.299, 51.300, 51.302, 55.360, 55.361, 127.396). Strictly speaking, in these systems, the magnetic space groups are
enhanced to spin space groups in which the spin rotations are (partially) unlocked with the lattice rotations; accordingly the little corgroups of the HSLs are enhanced to a “spin point group” containing $\mathcal{C}'_{2y}$ as a subgroup (for details, see the Supplemental Material [23]). Finally, by first-principles electronic structure calculations, we predict that the monolayer LaB$_6$ on a suitable substrate is a 2D eightfold degenerate as well as Dirac node-line semimetal in paramagnetic phase.

**Symmetry analysis.**—Because of fractional translations associated with point-group operations, the little corgroup of some $k$ points at the boundary of the BZ may have high-dimensional projective representations. These high-dimensional projective representations lead to extra degeneracies in the electronic energy band structure. There are a portion of the Dirac semimetals and Dirac node-line semimetals protected by nonsymmorphic space groups [39–43].

To understand the emergence of the eightfold degeneracy, we check the $P4/mibm$ (127) space group symmetry as an example. The elementary symmetry operations of the $P4/mibm$ space group include $C_{4z}$, $C_{2z}(1/2, 1/2, 0)$, and $T$, which yield the point group $D_{4h}$. Since there is no fractional translation along the $z$ direction, the space group $P4/mibm$ can support quasi-2D lattice structure. In the following, our discussion is restricted to the $xy$ plane with the BZ shown in Fig. 1(a). Obviously, any $k$ point on the $X_{s}$-M line is invariant under the following symmetry operations: the screw rotation $C_{2y}(1/2, 1/2): (x, y) \rightarrow (-x + 1/2, y + 1/2)$, the glide mirror $M_{y}(1/2, 1/2): (x, y) \rightarrow (-x + 1/2, y + 1/2)$, and the mirror $M_{z}: (x, y) \rightarrow (x, y)$. Furthermore, since $T$ is always a symmetry element of nonmagnetic materials, the $X_{s}$-M line is also invariant under the combined symmetry operations $\mathcal{I}T$. Noticing that the square of the symmetry operation $C_{2y}(1/2, 1/2)\mathcal{I}T = M_{y}(1/2, 1/2)T$ is $[M_{y}(1/2, 1/2)T]^{2} = (1, 0)$, the square of the representation of $M_{y}(1/2, 1/2)T$ is equal to $-1$, resulting in a Kramers degeneracy in the energy spectrum. In other words, the fractional translations of the nonsymmorphic group give rise to two-dimensional irreducible projective representations of the little corgroup of the $X_{s}$-M line, i.e., $\mathcal{C}'_{2y} \times Z^{\mathcal{I}T}_{2}$ with $\mathcal{C}'_{2y} = \{E, C_{2y}, M_{z}, M_{z}\}$ and $Z^{\mathcal{I}T}_{2} = \{E, IT\}$. This projective representation makes $X_{s}$-M a nodal line [see Fig. 1(b)].

On the other hand, since $M_{y}(1/2, 1/2)T$ commutes with $M_{z}$, the $X_{s}$-M axis has two inequivalent Kramers pairs distinguished by the quantum number $\pm 1$, the eigenvalues of $M_{z}$. This can be seen more clearly from the character table (Table I) of the unitary part of the little corgroup $\mathcal{C}'_{2y}$ and the action of the antunitary operation $\mathcal{I}T$. Obviously, the two one-dimensional irreducible representations $D^{(1)}$ and $D^{(2)}$ form a Kramers pair, while $D^{(3)}$ and $D^{(4)}$ form another Kramers pair. Because of different quantum numbers of $M_{z}$, the two Kramers pairs are not equivalent; also see the group theory analysis in the Supplemental Material [23].

If a band with the first Kramers pair crosses another band with the second Kramers pair, a pair of crossing points are formed on the $X_{s}$-M axis, as shown in Fig. 1(c). On the other hand, since spin-orbital coupling is not taken into account, the spin space has SU(2) symmetry, which protects the spin degeneracy. Therefore, the pair of crossing points are eightfold degenerate. Because of the $C_{4z}$ symmetry, another pair of eightfold degenerate points can be found on the $X_{s}$-M axis.

**Effective lattice model.**—Here we provide a lattice model to illustrate the eightfold degeneracy protected by the $P4/mibm$ space group symmetry. The minimal model is on a square lattice including four sublattices, as shown in Fig. 2(a). We begin with a Hamiltonian composed of $s$ orbitals, including the hopping between the nearest and next-nearest neighbors as follows:

$$
h_{k} = t(1 + \cos k_{x})\Sigma_{01} + t \sin k_{x}\Sigma_{12} + t(1 + \cos k_{y})\Sigma_{11}$$
$$- t \sin k_{y}\Sigma_{21} + t'2[1 + \cos(k_{x} + k_{y})]\Sigma_{10}$$
$$+ t'2[1 - \cos(k_{x} + k_{y})]\Sigma_{13}$$
$$- t'2\sin(k_{x} + k_{y})(\Sigma_{20} - \Sigma_{21}).$$

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**TABLE I.** Character table of $\mathcal{C}'_{2y}$ group at the $X_{s}$-M axis.

<table>
<thead>
<tr>
<th>$\mathcal{C}'_{2y}$</th>
<th>$E$</th>
<th>$C_{2y}(1/2, 1/2)$</th>
<th>$M_{z}$</th>
<th>$M_{y}(1/2, 1/2)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$D^{(1)}$</td>
<td>1</td>
<td>$-i$</td>
<td>1</td>
<td>$-i$</td>
</tr>
<tr>
<td>$D^{(2)}$</td>
<td>1</td>
<td>$i$</td>
<td>1</td>
<td>$i$</td>
</tr>
<tr>
<td>$D^{(3)}$</td>
<td>1</td>
<td>$-i$</td>
<td>$-1$</td>
<td>$-i$</td>
</tr>
<tr>
<td>$D^{(4)}$</td>
<td>1</td>
<td>$i$</td>
<td>$-1$</td>
<td>$i$</td>
</tr>
</tbody>
</table>
where \( \Sigma_{ij} = s_i \otimes s_j \) describes the sublattice degrees of freedom, \( s_0 \) is the \( 2 \times 2 \) identity matrix, \( s_1, s_2, \) and \( s_3 \) are the Pauli matrices, and \( t \) and \( t' \) are the nearest neighbor and next-nearest neighbor hopping integrals, respectively. It is obvious that the system preserves both \( T \) and \( \mathcal{T} \) symmetries. The spin index is omitted since spin-orbital coupling is open boundaries in the \( x \) direction. As shown in Fig. 2(d), there are no edge states connecting the two eightfold degenerate points, which is different from the Dirac semimetals caused by band inversion [2,3].

Furthermore, we break \( \mathcal{T} \) symmetry by distinguishing the red and black sites in Fig. 3(a) by adding an on-site different potential energy on the red and black sites in Fig. 3(a) by adding an on-site potential energy. The new Hamiltonian \( H_k' = H_k + t_0 \Sigma_{30} \) preserves \( C_{2v}(1/2, 1/2) \mathcal{T}, \) \( M_z(1/2, 1/2) \mathcal{T} \), and \( M_z \) symmetries. As expected, the eightfold degenerate point on the \( X_y-M \) axis is lifted, but the one on the \( X_y-M \) axis remains, as shown in Fig. 3(b) plotted with \( t_0 = 0.5t \). Thus the 2D eightfold degenerate semimetals can stably exist in noncentrosymmetric systems.

Now we provide all the space groups that can protect the eightfold degeneracy in 2D semimetals. First, there are only 17 nonsymmetric space groups supporting 2D layered structures as listed in Table II, which may protect 2D eightfold degenerate fermions. Second, we have just shown that with extra \( SU(2) \) spin rotation symmetry there are two kinds of little cospins that can protect the eightfold degeneracy, namely, \( C_{2v} \times Z_2^{\mathcal{T}} \) and \( 2' m'm \). Since time reversal \( \mathcal{T} \) is always a symmetry of the system, the unitary point group of the required space group

**TABLE II.** The relationship of two-dimensional nonsymmetric space group and eightfold degenerate semimetals.

<table>
<thead>
<tr>
<th>Point group</th>
<th>Space groups</th>
<th>Eightfold degeneracy</th>
</tr>
</thead>
<tbody>
<tr>
<td>( C_{2v} )</td>
<td>26</td>
<td>Yes</td>
</tr>
<tr>
<td>( D_{2h} )</td>
<td>27, 28, 29, 30, 31</td>
<td>No</td>
</tr>
<tr>
<td>( D_{2d} )</td>
<td>49, 50, 53, 54, 57, 59</td>
<td>No</td>
</tr>
<tr>
<td>( D_{2h} )</td>
<td>51, 55</td>
<td>Yes</td>
</tr>
<tr>
<td>( D_{4h} )</td>
<td>125, 129</td>
<td>No</td>
</tr>
<tr>
<td>( D_{4h} )</td>
<td>127</td>
<td>Yes</td>
</tr>
</tbody>
</table>
should contain \( \mathcal{E}_{2v} \times \{ E, \mathcal{I} \} = D_{2h} \) if \( \mathcal{I} \) is present or \( \mathcal{E}_{2v} = \{ E, M_x, M_z, C_{2v} \} \) if \( \mathcal{I} \) is absent as its subgroup. It turns out that all of the 17 space groups satisfy the second requirement.

Third, the fractional translation associated with the little cogroup elements (on a HSL) should support two inequivalent Kramers degeneracies. The Kramers degeneracy can be protected by one of the following symmetry elements: \( M_x(1/2, 1/2) \mathcal{T} \), \( M_z(0, 1/2) \mathcal{T} \), \( C_{2v}(1/2, 1/2) \mathcal{T} \), \( C_{2v}(1/2, 0) \mathcal{T} \), \( M_x(1/2, 1/2) \mathcal{T} \), \( M_z(1/2, 0) \mathcal{T} \), \( C_{2z}(1/2, 1/2) \mathcal{T} \), or \( C_{2z}(0, 1/2) \mathcal{T} \). We further need the operation \( M_z \) to provide the quantum numbers \( \pm 1 \) to distinguish two inequivalent Kramers pairs. It turns out that only four space groups (51, 55, 127, and 26) satisfy the above requirements, as shown in Table II. Different from the 127 \((P4/mbm)\) space group, the eightfold degenerate points protected by the 26\((P-nc21)\) or the 51\((P-nm2)\) space group can only locate at one boundary axis of the 2D BZ. The 55\((P-cbm)\) space group is special, the eightfold degenerate points can locate at either one or two boundary axes in the 2D BZ.

Finally, we consider an out-of-plane collinear antiferromagnetic order that breaks the \( \mathcal{I} \) and \( \mathcal{T} \) symmetry but preserves the combined \( \mathcal{I} \mathcal{T} \) symmetry, as shown in Fig. 3(c). Then the new Hamiltonian becomes \( H'_k = H_k + 2t_\sigma \Sigma_x \sigma_z / 2 \) \((\sigma_z \text{ the z component spin operator})\). While the Zeeman term introduces spin-orbit coupling to the Hamiltonian, the operations \( C_{2v}(1/2, 1/2) \mathcal{T} \), \( M_z(1/2, 1/2) \mathcal{T} \), \( M_z(1/2, 0) \mathcal{T} \), and \( \mathcal{I} \mathcal{T} \) remain to be symmetries of the Hamiltonian \( H'_k \) if each operation is interpreted as a combination of lattice operation and the corresponding spin rotation. If the intrinsic kinetic term \( H_k \) has negligible spin-orbit coupling, then the total Hamiltonian \( H'_k \) has extra symmetries since the system is invariant under spin rotation \( (C_{2v}\{E\}) \) and lattice mirror reflection \( (E\{M_z\}) \) \((\text{here } C_{2v} \text{ acts on spin only, while } M_z \text{ acts on lattice only})\). In other words, the little cogroup on the \( X-M \) line is enlarged into a spin point group containing the Shubnikov magnetic point group \( \mathcal{C}_{2v} \times Z_2^{(i)} \) as a subgroup. This spin point group can protect the eightfold degenerate points on the \( X-M \) axis (see the Supplemental Material [23] for details). The dispersion of a lattice model with \( t_m = 0.2t \) is shown in Fig. 3(d). Notice that the eightfold degenerate point on the \( X-M \) axis is lifted due to the absence of \( C_{2v}(1/2, 1/2) \) and \( M_x(1/2, 1/2) \) symmetry as shown in Fig. 3(d).

Therefore, the sufficient conditions of the eightfold degeneracy include the following: (1) the system contains out-of-plane collinear antiferromagnetic order, (2) the intrinsic spin-orbit coupling for the electrons is negligible, and (3) the Shubnikov little cogroup on a high-symmetry line is \( \mathcal{C}_{2v} \times Z_2^{(i)} \). It turns out that only eight magnetic space groups satisfy the above condition, including two type-III magnetic space groups (51.293, 55.355) and six type-IV magnetic space groups (51.299, 51.300, 51.302, 55.360, 55.361, 127.369).

**Material calculations.**—In terms of realistic materials, since 2D eightfold degenerate semimetals are fragile when considering spin-orbit coupling (SOC), we can find 2D eightfold degenerate semimetals in layered light element compounds. Here, we propose a new 2D structure \( \text{LaB}_8 \) which is constructed from the bulk \( \text{LaB}_6 \) [44] under space group \( P4/mbm \). The monolayer \( \text{LaB}_8 \) is made up of two layers of B atoms and one layer of La atoms as shown in Figs. 4(a)–4(c). The B atomic layer is made up of B atomic octahedron and B atoms [Fig. 4(a)].

In order to confirm the structural stability, we calculated the phonon spectrum of monolayer \( \text{LaB}_8 \) as shown in Fig. 4(d). Clearly, the phonon spectrum of monolayer \( \text{LaB}_8 \) has no imaginary frequency, thus the crystal structure is dynamically stable. As shown in Fig. 4(e), the electronic band structure of monolayer \( \text{LaB}_8 \) has six Dirac nodal lines around the Fermi level, which can be divided into two kinds. One kind derives from the band inversion around the time-reversal invariant \( \Gamma \) point and is protected by nonsymmorphic symmetry as the above symmetry analysis. Without strain, the monolayer \( \text{LaB}_8 \) unfortunately does not support the eightfold degenerate fermions. But the two Dirac nodal lines along the \( X-M \) direction have different quantum numbers of \( M_z \) and are very close around the high-symmetry point \( X \) [Fig. 4(e)]. By applying lattice strain, the nodal lines could
probably touch each other and produce the eightfold degenerate points. When compressing the lattice constant by 3%, the nonmagnetic state of a monolayer LaB$_8$ indeed contains eightfold degenerate fermions as shown in Fig. 4(f). Although the stressed LaB$_8$ actually exhibits ferromagnetic order at zero temperature, it is argued in the Supplemental Material [23] that the eightfold degenerate fermions still exist at finite temperatures. Because of the SOC has very weak influence on the bands around the Fermi level [23], the degenerate points. Moreover, since the SOC has very weak influence on the bands around the Fermi level [23], the monolayer LaB$_8$ has eight eightfold degenerate fermions at finite temperatures. Because of the SOC has very weak influence on the bands around the Fermi level [23], the monolayer LaB$_8$ may indeed exhibit ferromagnetic order belonging to two type-III magnetic space groups (51, 55, 127) and one noncentrosymmetric space group (26). (iv) As long as the intrinsic spin-orbit coupling is negligible, the eightfold degenerate fermions can also stably exist in magnetic semimetals with collinear antiferromagnetic order belonging to two type-III magnetic space groups (51, 55, 127) and one noncentrosymmetric space group (26). (v) The monolayer LaB$_8$ on a suitable substrate may be an ideal platform for studying the exotic properties of 2D eightfold degenerate fermions in the paramagnetic phase.

In summary, based on symmetry analysis, lattice model, and the first-principles electronic calculations, we obtain five main results: (i) The eightfold degenerate fermions can stably exist in 2D systems. (ii) The little cogroups $C_2 \times \{E, \bar{I}T\}$ and $2m\bar{m}\bar{m} = \{E, C_2, T, M, \bar{T}, M, \bar{T}\}$ on a certain HSL in the Brillouin zone can protect the 2D eightfold degenerate fermions in centrosymmetric or noncentrosymmetric nonmagnetic systems, respectively. (iii) There are four space groups that can protect eightfold degenerate fermions, including three centrosymmetric space groups (51, 55, 127) and one noncentrosymmetric space group (26). (iv) As long as the intrinsic spin-orbit coupling is negligible, the eightfold degenerate fermions can also stably exist in magnetic semimetals with collinear antiferromagnetic order belonging to two type-III magnetic space groups (51, 55, 127) and one noncentrosymmetric space group (26). (v) The monolayer LaB$_8$ on a suitable substrate may be an ideal platform for studying the exotic properties of 2D eightfold degenerate fermions.

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