New Journal of Physics
The open access journal at the forefront of physics
Deutsche Physikalische Gesellschaft DPG
IOP Institute of Physics

PAPER • OPEN ACCESS

Systematic analysis for triple points in all magnetic symmorphic systems and symmetry-allowed coexistence of Dirac points and triple points

To cite this article: Chi-Ho Cheung *et al* 2018 *New J. Phys.* **20** 123002

New Journal of Physics
The open access journal at the forefront of physics

Deutsche Physikalische Gesellschaft DPG
IOP Institute of Physics

Published in partnership with: Deutsche Physikalische Gesellschaft and the Institute of Physics

CrossMark

OPEN ACCESS

RECEIVED
28 April 2018

REVISED
12 November 2018

ACCEPTED FOR PUBLICATION
15 November 2018

PUBLISHED
5 December 2018

PAPER

Systematic analysis for triple points in all magnetic symmorphic systems and symmetry-allowed coexistence of Dirac points and triple points

Chi-Ho Cheung[1,2], R C Xiao[3,4], Ming-Chien Hsu[5], Huei-Ru Fuh[6], Yeu-Chung Lin[7] and Ching-Ray Chang[7]

1 Graduate Institute of Applied Physics, National Taiwan University, Taipei 10617, Taiwan
2 Wuhan National High Magnetic Field Center and School of Physics, Huazhong University of Science and Technology, Wuhan 430074, People's Republic of China
3 Key Laboratory of Materials Physics, Institute of Solid State Physics, Chinese Academy of Sciences, Hefei 230031, People's Republic of People's Republic of China
4 School of Physical Science and Technology and Institute for Advanced Study, Soochow University, Suzhou 215006, People's Republic of China
5 National Sun Yat-sen University, Department of Physics Kaohsiung, Taiwan
6 Yuan Ze University, Department of Chemical Engineering and Materials Science Chung-Li, Taoyuan, Taiwan
7 Department of Physics, National Taiwan University, Taipei 10617, Taiwan

E-mail: f98245017@ntu.edu.tw

Keywords: topological materials, Dirac fermions, electronic structure, Weyl fermions, topological phase transition, triple points

Abstract

Similar to Weyl fermions, a recently discovered topological fermion 'triple point' can be generated from the splitting of Dirac fermion in the systems with inversion symmetry (IS) breaking or time-reversal symmetry (TRS) breaking. Inducing triple points in IS breaking symmorphic systems have been well studied, but the same cannot be said for the TRS breaking symmorphic systems. In this work, we extend the theory of searching for triple points to all symmorphic magnetic systems. We list among all symmorphic systems all the *k* paths which allow the existence of triple points. With this systematic study, we also found that the coexistence of Dirac points and triple points is allowed in some particular symmetric systems. Besides theoretical analysis, we carried out numerical analysis as well. According to our first-principles calculations, B_3Re_7 and As_2Ni_5 are the candidates for realizing the coexistence of Dirac and triple points. We have not only provided an exhaustive triple point search mechanism for the symmorphic systems, but also identified material systems that host the Dirac and the triple points.

1. Introduction

Over the past few decades, topology has been emerging in condensed matter physics. The development started from the quantum Hall effect [1, 2] which is the quantum-mechanical version of the Hall effect. The second stage of development is the quantum anomalous Hall effect [3–6] which is a quantum Hall effect without external magnetic field. The third stage of development is the quantum spin Hall effect [7–12] which is a quantum Hall effect without the breaking of time-reversal symmetry (TRS). Analogous to quantum spin Hall effect which pumps spin, there are topological crystalline insulators [13–16] which can pump the eigenvalues of mirror symmetry. All these four topological phenomena are insulating in bulk band, but have topologically protected surface states which are conducting.

Besides looking for topological phenomena in bulk insulating materials, scientists also look for topological phenomenon in bulk metallic materials. Recently, topological metals such as Dirac semimetal [17–21], Weyl semimetal [22–29] and triple point semimetal [29–42] have been discovered. These topological metals have topologically protected surface states just like those quantum Hall effects. No matter metallic in bulk or insulating in bulk, as long as their surface state are topologically protected, they can be promising candidates for electronic devices or even spintronic devices. Thus they can be valuable for industrial applications. On the other hand, topological metal provides a different playground and relatively lower price to search for those elementary particles described by relativistic quantum field theory. Since topological metal is valuable for both academic research and industrial applications, it has drawn a lot of attention in recent years.

One of the topological metals hosting a quasiparticle analogue of an elementary particle is the Dirac semimetal. The earliest found Dirac semimetal is Na_3Bi [19]. Na_3Bi has both inversion symmetry (IS) and TRS, thus all bands at every k points in the Brillouin zone are at least doubly degenerate. When a doubly degenerate band linearly crosses over another doubly degenerate band at a k point, a four-fold degenerate Dirac point is formed. Such a Dirac point can be an analogue of the Dirac fermion described by relativistic quantum field theory in high energy physics.

In high energy physics, breaking TRS or IS causes Dirac fermion to split into Weyl fermions. In condensed matter physics, bands can be non-degenerate when system does not have TRS or IS. When a non-degenerate band linearly crosses over another non-degenerate band at a k point, a two-fold degenerate Weyl point is formed. Such a Weyl point can be an analogue of Weyl fermion in high energy physics too.

However, in condensed matter physics, fermions in crystal are constrained by magnetic space group (MSG) symmetries rather than by Lorentz invariance. This gives rise to the uncertainty that doubly degenerate bands may or may not split when TRS or IS is broken. In this paper, we will discuss a new fermion-triple point which has no counterparts in high energy physics and can be formed by a non-degenerate band linearly crossing over a doubly degenerate band at a k point. In general, the formations of triple points can be caused by the nonsymmorphic or the symmorphic MSG symmetries, but as we emphasize in the title, we only discuss those triple points which are caused by the symmorphic MSG symmetries.

If Dirac fermions in condensed matter must has TRS and IS just like the Dirac fermions in high energy physics, then it cannot coexist with triple points which need to break either TRS or IS. However, recent research shows that Dirac fermions in condensed matter can exist in a system without TRS $\cdot$ IS [43, 44]. This gives rise to the possibility of finding several systems which have two k paths with two different symmetry groups: one allows the existence of Dirac points while another one allows the existence of triple points.

We organize this paper as follows. In section 2, we review the condition of forming triple points by discussing a special case [19, 33, 43]. In section 3, we generalize this condition to all magnetic point groups (MPGs) and list all possible k paths of all possible symmorphic systems which allow the existence of triple points. In section 4, we point out that the coexistence of Dirac points and triple points is symmetrically allowed in some particular symmetric systems. In section 5, we provide examples, B_3Re_7 and As_2Ni_5, to realize the coexistence of Dirac points and triple points. In section 6, we summarize the contributions of this paper.

2. The condition of forming triple points

Similar to Weyl fermions in high energy physics, triple points in condensed matter physics can be split from Dirac fermions when TRS or IS of the system is broken. It is well known that Dirac fermions can exist in a system which has both TRS and D_{6h} point group symmetry (D_{6h} is a Schoenflies notation for origin point group, please refer to [45] for all origin point groups in Schoenflies notation). In this section, we are going to use this system as an example to show how triple points split from Dirac fermions and point out the necessary condition of forming triple points.

D_{6h} point group includes C_{3z}, C_{2z}, M_x and IS (please refer to [46, 47] for symbols' meaning and orientation of the symmetry operators of any origin point groups). Since the system has TRS and IS, all bands have spin degeneracy at any k point. As Dirac fermions are a crossing point of two 2-fold degenerate bands, Dirac fermion is a point of 4-fold degeneracy.

If all bands have spin degeneracy at any k point, triple point cannot be formed (triple point is a point of 3-fold degeneracy). Thus TRS or IS must be broken to induce triple points. However, at a high symmetry k point/path/plane, TRS and IS are not the only symmetries which protect the degeneracy of bands. Therefore, other crystal symmetries need to be considered.

To be more specific, we assume that the irreducible representations of the bands which form the Dirac points are $\overline{E}_{1g/u}$ and $\overline{E}_{3g/u}$ (the symbols of irreducible representations are written in extended Mulliken notation). With the irreducible representations, the matrix forms of the symmetry operators are as follows:

$$
\begin{aligned}
&\textit{for basis}: \bar{E}_{1g/u}\\
&\quad\ \text{TRO} \qquad\qquad \text{IS} \qquad\qquad\quad M_x \quad C_{2z} \quad C_{3z}\\
&\pm\begin{bmatrix}0 & -1\\ 1 & 0\end{bmatrix}K \pm \begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix} \ \pm\ \begin{bmatrix}0 & i\\ i & 0\end{bmatrix}\begin{bmatrix}i & 0\\ 0 & -i\end{bmatrix}\begin{bmatrix}e^{\frac{i\pi}{3}} & 0\\ 0 & e^{\frac{-i\pi}{3}}\end{bmatrix},\\
&\textit{for basis}: \bar{E}_{3g/u}\\
&\quad\ \text{TRO} \qquad\qquad \text{IS} \qquad\qquad\quad M_x \quad C_{2z} \quad C_{3z}\\
&\pm\begin{bmatrix}0 & 1\\ -1 & 0\end{bmatrix}K \mp \begin{bmatrix}-1 & 0\\ 0 & -1\end{bmatrix} \ \mp\ \begin{bmatrix}0 & i\\ i & 0\end{bmatrix}\begin{bmatrix}-i & 0\\ 0 & i\end{bmatrix}\begin{bmatrix}e^{i\pi} & 0\\ 0 & e^{-i\pi}\end{bmatrix},
\end{aligned}
\tag{1}
$$

where TRO is the operator of TRS and K is complex conjugate operator.

If a symmetry operator S (S can be a unitary or an anti-unitary operator) acts on a k_h vector, such that $Sk_h = k_h + nG$, where G is any reciprocal lattice vector and n is any integer number, then all such symmetry operators form the little group of k_h.

Firstly, we only consider the unitary subgroup of the little group of k_h. Hamiltonian $H(k_h)$ has to commute with all the symmetry operators of the unitary subgroup of the little group of k_h. If any symmetry operators of this unitary subgroup does not commute with each other in a subspace of the Hilbert space, then $H(k_h)$ has to be degenerate in this subspace, otherwise $H(k_h)$ cannot commute with all the symmetry operators of the unitary subgroup simultaneously.

Furthermore, those anti-unitary symmetry operators of the little group of k_h could cause extra degeneracy. In symmorphic system, in order to consider all the symmetry operators of the little group of k_h, we have to treat the little group as an MPG rather than the original point group, regardless if the system does or does not have any magnetic moment. If the system does not have any magnetic moment, then it has TRS. Thus the symmetry group of the system is one of the grey groups of the 122 MPGs. The little group of k_h of this system is a subgroup of the grey group. Therefore, the little group of k_h of a paramagnetic system could be any MPG. All 122 MPGs can be classified into three types: 32 ordinary point groups, 32 'grey' point groups and 58 'black and white' MPGs (grey point groups are the groups contain TRS symmetry and their point group symbols always have '$1'$' at the end. For example '$6/mmm1'$' is a grey point group. Similar denotations are for MSG. MSG symbol always has $1'$ at the end if the space group has TRS. Please refer to [45] for further details of MPG and MSG symbols). The degeneracies of the ordinary point groups have been discussed hereinabove. The extra degeneracies caused by the TRS of any grey point groups are known as the Kramers degeneracy which have well discussed too [47]. The extra degeneracies caused by the anti-unitary symmetry operators of any black and white MPGs are discussed in the appendix of this paper.

In the system with D_{6h} and TRS, any k point on $\Gamma-Z$ axis-k_z is invariant under C_{3z}, C_{2z} rotation or M_x reflection or (TRO·IS) operation, thus the symmetry group of $\Gamma-Z$ axis is $6/m'mm$ which is a black and white MPG. According to equation (1), C_{2z} does not commute with M_x in both $\bar{E}_{1g/u}$ and $\bar{E}_{3g/u}$. Furthermore, according to table A1, the anti-unitary operators in $6/m'mm$ do not cause any extra degeneracy. Thus, $\bar{E}_{1g/u}$ and $\bar{E}_{3g/u}$ are both 2-fold degenerate along the k_z path. Besides, $\bar{E}_{1g/u}$ and $\bar{E}_{3g/u}$ are two different irreducible representations in k_z path, so any coupling between these two representations (bands) are forbidden. Hence, there will be no gap opening when these two bands come across each other at k_z path. Therefore, under such symmetry condition, a linear crossing between two 2-fold degenerate bands is allowed and so is the 4-fold degenerate Dirac point.

The symmetry condition that allows the existence of Dirac points can be streamlined and generalized as follows: Dirac points can exist at a k path whose symmetry group has two or more than two 2-dimensional double group irreducible representations. We will simply call this symmetry condition Condition A.

If the TRS of the system is broken, the symmetry group of k_z path is reduced from $6/m'mm$ to C_{6v}. Since the 2-fold degeneracy of $\bar{E}_{1g/u}$ and of $\bar{E}_{3g/u}$ remain protected by C_{2z} and M_x, the Dirac points on k_z path do not split just because of TRS breaking. If M_x symmetry is chosen for further symmetry breaking, all symmetry operators of the little group of k_z path commute with each other. Both $\bar{E}_{1g/u}$ and $\bar{E}_{3g/u}$ will split. If we want to induce triple points, breaking M_x symmetry is not an option. If C_{2z} is chosen for the further symmetry breaking, the symmetry group of the little group of k_z path becomes C_{3v}. All symmetry operators in $\bar{E}_{3g/u}$ commute with each other, the symmetry operators in $\bar{E}_{1g/u}$ do not commute with each other. Thus $\bar{E}_{1g/u}$ remains a 2-fold degeneracy whereas $\bar{E}_{3g/u}$ splits into two non-degenerate bands. On k_z path, since C_{3z} symmetry can prevent any coupling between $\bar{E}_{1g/u}$ and $\bar{E}_{3g/u}$, these representations still belong to different irreducible representations. Therefore, the crossing point will not be gapped. Thus each Dirac point will split into two triple points when the C_{2z} and TRS are broken. The variations of band structures and of system symmetry are shown in figure 1.

This physical phenomenon will be further clarified if we use the $k \cdot P$ expansion and method of invariants to calculate the Hamiltonian around Γ point for k_z path:

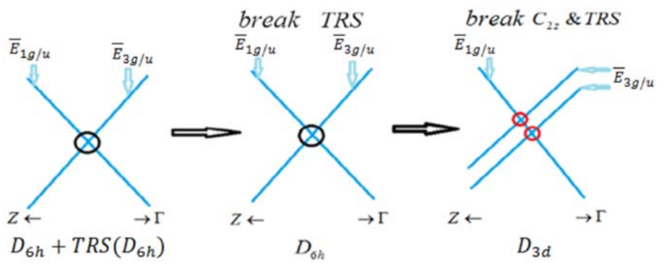

Figure 1. The schematic figure of the symmetry reduction processes of the system. After the system symmetry has been reduced from D_{6h} + TRS(D_{6h}) to D_{6h}, both $\bar{E}_{1g/u}$ and $\bar{E}_{3g/u}$ do not split. When the symmetry of the system becomes D_{3d}, $\bar{E}_{1g/u}$ remains 2-fold degenerate whereas $\bar{E}_{3g/u}$ splits into two non-degenerate bands. The Dirac points are marked in black circles and the triple points are marked in red circles.

$$H_{D_{3d}}(k_z) = \varepsilon_0(k_z) + \begin{pmatrix} C_0 - C_1k_z^2 & 0 & 0 & 0 \\ 0 & C_0 - C_1k_z^2 & 0 & 0 \\ 0 & 0 & -C_0 + C_1k_z^2 & D \\ 0 & 0 & D & -C_0 + C_1k_z^2 \end{pmatrix}, \quad (2)$$

this is the Hamiltonian for the system with D_{3d} symmetry and without TRS; the expansion is only up to the first order of k for off-diagonal matrix elements and up to the second order of k for diagonal matrix elements; $\varepsilon_0(k_z) = A_0 + A_1k_z^2$. C_0 and C_1 are real positive k independent coefficients. A_0, A_1 and D are real k independent coefficients.

When the C_{3z} operator acts on the effective Hamiltonian $C_{3z}H_{D_{3d}}(k)C_{3z}^{-1}$, according to the C_{3z} symmetry operator of equation (1), a phase factor $e^{\frac{2i\pi}{3}}$ or $-e^{\frac{i\pi}{3}}$ will be generated on the matrix elements H_{12}, H_{21} and the matrix elements of off-diagonal block. Therefore these matrix elements must have k_+ or k_- ($k_\pm = k_x \pm ik_y$) factor to match the C_{3z} symmetry condition $C_{3z}H_{D_{3d}}(k)C_{3z}^{-1} = H_{D_{3d}}(C_{3z}^{-1}k)$. If only considering the Hamiltonian of $\Gamma-Z$ axis, all these matrix elements become zero. This explains: 'on k_z path, C_{3z} symmetry can prevent any coupling between $\bar{E}_{1g/u}$ and $\bar{E}_{3g/u}$, such that these representations belong to different irreducible representations.' Furthermore breaking C_{2z} symmetry and TRS induces $D(\tau_0\sigma_x - \tau_z\sigma_x)/2$ (τ is the Hilbert space of the combined $\bar{E}_{1g/u}$ and $\bar{E}_{3g/u}$; σ is the Hilbert space within $\bar{E}_{1g/u}$ or within $\bar{E}_{3g/u}$). This term splits $\bar{E}_{3g/u}$ into two 1-dimensional irreducible representations. Thus the 4-fold degenerate Dirac point splits into two 3-fold degenerate triple points.

Base on the above analysis, the symmetry condition that allows the existence of triple points can be streamlined as follows: triple points can only exist at a k path whose symmetry group contains both 1-dimensional and 2-dimensional double group irreducible representations [33]. We will simply call this symmetry condition Condition B.

3. Triple points in all symmorphic systems

In this section, we are going to find among all possible symmorphic systems all possible k paths that allow the existence of triple points.

In a symmorphic system, symmetry group of any k points is one of the MPGs. So the first step is to check among the 122 types of MPGs and list all the MPGs which can match the symmetry condition that allows the existence of triple points.

Among the 32 types of ordinary point groups, there are 3 types, namely C_{3v}, D_3 and D_{3d}, of point groups that satisfy Condition B. In all the Brillouin zone of the 14 types of Bravais lattice, only 6 types of k path contain C_3 symmetry (there is no k plane contains C_3 symmetry). These 6 types of k path are Λ and P of the trigonal; $\Gamma-Z$ and $K-H$ of the hexagonal; 1 1 1 direction of cubic P (simple cubic), cubic F (face-centered cubic) and cubic I (body-centered cubic); F of cubic I (since there is no unified k path symbol, the Brillouin zones are demonstrated in figure 2 to define the 6 symbols which are used for marking the 6 types of k path). These 6 types of k path can only contain C_{3v}, none of them can contain D_3 or D_{3d}. Therefore, among the ordinary point groups only C_{3v} can match the symmetry condition that allows the existence of triple points.

Since operating TRO on k is to change the sign of k, only k points, not k paths, allow grey point group to be their symmetry group. Thus, if the symmetry group of k is a grey point group, triple point cannot exist on this k.

All black and white MPGs contain a set of unitary operators which form a unitary subgroup (one of the ordinary point group), and this unitary subgroup has a set of double group irreducible representations. The rest of the operators of the black and white MPG are anti-unitary operators. These anti-unitary operators cannot

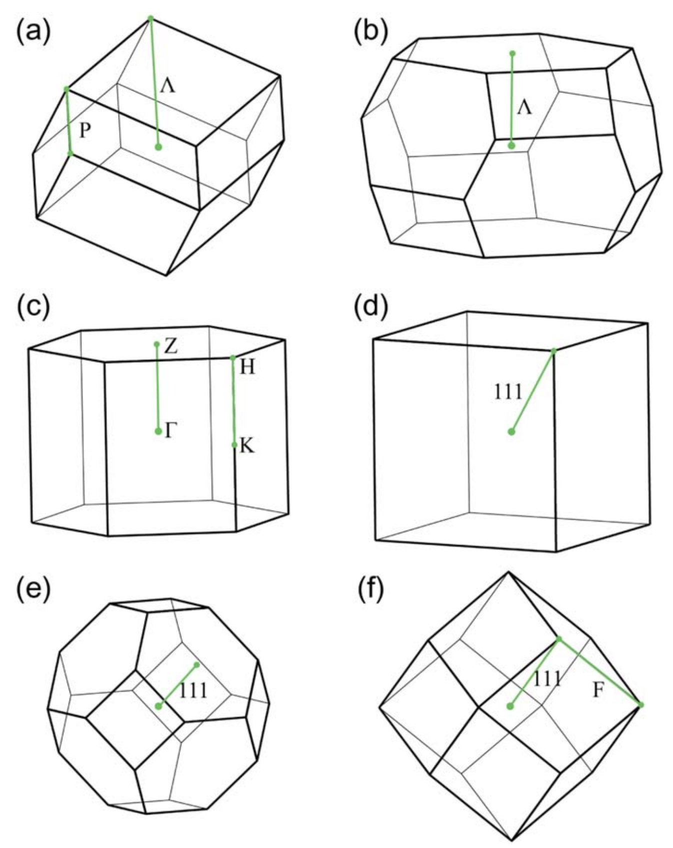

Figure 2. The Brillouin zone for (a) trigonal with $a > \sqrt{2}\,c$, (b) trigonal with $a < \sqrt{2}\,c$, (c) hexagonal, (d) cubic *P*, (e) cubic *F* and (f) cubic *I*. All the *k* paths, which contain C_3 symmetry, are marked in green. Other Brillouin zones, which cannot contain C_3 symmetry, are omitted.

generate any double group irreducible representation, but they can further 'degenerate' the ordinary double group irreducible representations (as shown in appendix). The further degeneracies could allow the existence of triple points, whereas the ordinary double group irreducible representations forbid that. Or contrarily, the further degeneracies forbid the existence of triple points, whereas the ordinary double group irreducible representations allow that.

Among all the 58 types of black and white MPGs, 17 types have further degeneracies (as shown in table A1). Among the 17 types, only $-6'$ allows the existence of triple points, whereas the double group irreducible representations of its unitary subgroup forbid that. All the other 16 types forbid the existence of triple points due to one or more of the following reasons: (1) the presence of element-TRS · IS, (2) the absence of 1-dimensional double group irreducible representation, (3) the absence of *k* path belonging to the black and white MPG. Among the 16 types, $-3'm$ is the one that forbids the existence of triple points, whereas the double group irreducible representations of its unitary subgroup (its unitary subgroup is C_{3v}) allow that. For later discussion, it would be important to notice that $-3'm$ has the element of $-1'$ ($-1'$ is IS · TRS).

Next step is to look for *k* paths, in all symmorphic systems, which allow the existence of triple points. We can directly look for these *k* paths in all the symmorphic MSGs. However, there are too many symmorphic MSGs. Thus we choose to analyze MPG of the symmorphic MSG first. In this way a large number of unqualified MSGs can be excluded. Then we contrast those qualified MPG systems with their MSG symbols.

As mentioned above, there are two kinds of *k* paths allowing the existence of triple points: the first kind is the *k* paths which belong to $-6'$ black and white MPG; the second kind is the *k* paths whose unitary subgroup belongs to C_{3v} while the *k* paths do not have $-1'$ symmetry. We will search for these two kinds of *k* paths separately.

Firstly, we search for the *k* paths which belong to $-6'$. If the Brillouin zone of a system contains the $-6'$ *k* path, the crystal symmetry (directions of magnetic moments are not counted for crystal symmetry) of the system must contains C_{3h} symmetry. According to the subgroup decomposition of the 32 point groups in [47], the crystal symmetry of the system contains C_{3h} symmetry only if the crystal symmetry of the system is D_{6h} or D_{3h} or C_{6h} or C_{3h}. The Bravais lattice of these four kinds of crystal symmetry is Hexagonal. In the Brillouin zone of Hexagonal Bravais lattice, only $\Gamma - Z$ can contain all the symmetry elements of $-6'$. Thus we only need to

Table 1. The list of MPG system that might contain k path of the first kind. The first column is the label of MPG systems. Answer of 'Does Γ–Z of the system belong to $-6'$?' is given in the second column.

Label of MPG systems	Does $\Gamma-Z$ belong to $-6'$?
(C_{6h}) 6/m	no
6/m1′	no
6′/m′	yes
6′/m	no
6/m′	no
(D_{3h}) −6m2	no
−6m21′	no
−6m′2′	no
−6′m2′	no
−6′m′2	yes
(D_{6h}) 6/mmm	no
6/mmm1′	no
6/m′mm	no
6/mm′m′	no
6/m′m′m′	no
6′/mmm′	no
6′/m′mm′	no
(C_{3h}) −6	no
−61′	yes
−6′	yes

determine whether the $\Gamma-Z$ of all MPG systems of D_{6h}, D_{3h}, C_{6h} and C_{3h} belong to $-6'$. The results are shown at table 1.

Secondly, we search for the k paths whose unitary subgroup belongs to C_{3v} while the k paths do not have $-1'$ symmetry. If the Brillouin zone of a system contains such k path, the symmetry group of the system must contain C_{3v} symmetry. According to the subgroup decomposition of the 32 point groups in [47], the symmetry group of the system contains C_{3v} symmetry only if the crystal symmetry of the system is one of the seven symmetries, namely C_{3v}, T_d, O_h, C_{6v}, D_{3d}, D_{3h} and D_{6h}. Furthermore, as (TRO · IS) acting on any k is equal to k, any k point in the Brillouin zone contains (TRO · IS) symmetry if and only if the system contains (TRO · IS) symmetry. Thus we can use two symmetry conditions to filter most of the MPGs which belong to the seven crystal symmetry: 1. the system must contain C_{3v} symmetry; 2. the system must not contain (TRO · IS) symmetry. Besides, the k paths which contain C_{3v} symmetry must contain C_3 symmetry. Hence, as mentioned above, the k path whose unitary subgroup is C_{3v} symmetry must be one of the following: Λ and P of trigonal; $\Gamma-Z$ and $K-H$ of hexagonal; 111 direction of cubic P, cubic F and cubic I; F of cubic I. All we need to do is to determine whether the unitary subgroup, of these 6 types of k paths in the Brillouin zone of the filtered MPG systems, is C_{3v} symmetry. The determining processes and results are given in table 2. Notice that for the Brillouin zone of trigonal Bravais lattice, the k path-P appears only if lattice constants fulfill the condition of $a > \sqrt{2}\,c$ (please refer to table 3.1 of [45] for the definitions of lattice constant a and lattice constant c). Sometimes, the k path-$K-H$ of the Hexagonal Bravais lattice is not contained in the mirror plane of C_{3v} symmetry, such that $K-H$ does not contain C_{3v} symmetry. Hence, we need the MSG to determine whether the existence of triple points is allowed on this k path. Thus, some answers in the fifth column of table 2 are 'MSG is needed'. Combining table 1 and table 2, then contrasting with MSG, we can get among all symmorphic systems all the k paths which allow the existence of triple points (as shown in table 3).

4. Symmetry-allowed coexistence of Dirac point and triple point

The degeneracy of a Dirac fermion in high energy physics is protected by TRS and IS. However, the degeneracy of a Dirac fermion in condensed matter can be preserved in a k path whose symmetry group satisfy Condition A (as mentioned in section 2). That means Dirac fermion can exist in a system which does not contain (TRO · IS) symmetry. This gives rise to the possibility of the coexistence of Dirac fermion and odd-fold degenerate fermion. We know that triple points can exist in a k path whose symmetry group satisfy Condition B (as mentioned in section 2 too). Combining the condition of existence for the Dirac fermion with the condition of existence for the triple point, we find that there are several systems which allow the coexistence of Dirac points and triple

Table 2. The list of system symmetry that might contain k paths of the second kind. The first column is the label of MPG systems. The second column shows whether the system is filtered out by the symmetry condition of 'containing C_{3v} but not $-1'$'. The third column is the class of the Brillouin zone. The fourth column is the label of the k path. The fifth column shows answers for whether the k path allows the existence of the triple points. Sometimes, the k path-K–H of the Hexagonal Bravais lattice is not contained in the mirror plane of C_{3v} symmetry and consequently K–H does not contain C_{3v} symmetry. Hence, we need the MSG to determine whether the existence of the triple points is allowed on this k path. Thus, some answers in the fifth column are 'MSG is needed'. For the Brillouin zone of the trigonal Bravais lattice, the k path-P appears only if lattice constants fulfill the condition of $a > \sqrt{2}c$.

Symmetry of the system	Contains C_{3v} or not? contains $-1'$ or not?	Brillouin zone	k path	The existence of triple points
(C_{3v}) 3 m	contains C_{3v}, but no $-1'$	trigonal	Λ	yes
			P	yes
		Hexagonal	$\Gamma-Z$	yes
			$K-H$	MSG is needed
3m1′	contains C_{3v}, but no $-1'$	trigonal	Λ	yes
			P	yes
		Hexagonal	$\Gamma-Z$	yes
			$K-H$	MSG is needed
3m′	no C_{3v}			
(T_d) −43 m	contains C_{3v}, but no $-1'$	cubic P	1 1 1	yes
		cubic F	1 1 1	yes
		cubic I	1 1 1	yes
			F	yes
−43m1′	contains C_{3v}, but no $-1'$	cubic P	1 1 1	yes
		cubic F	1 1 1	yes
		cubic I	1 1 1	yes
			F	yes
−4′3m′	no C_{3v}			
(O_h) m-3 m	contains C_{3v}, but no $-1'$	cubic P	1 1 1	yes
		cubic F	1 1 1	yes
		cubic I	1 1 1	yes
			F	yes
m-3m1′	contains $-1'$			
m′-3′m	contains $-1'$			
m-3m′	no C_{3v}			
m′-3′m′	contains $-1'$			
(C_{6v}) 6 mm	contains C_{3v}, but no $-1'$	Hexagonal	$\Gamma-Z$	no
			$K-H$	yes
6mm1′	contains C_{3v}, but no $-1'$	Hexagonal	$\Gamma-Z$	no
			$K-H$	yes
6′mm′	contains C_{3v}, but no $-1'$	Hexagonal	$\Gamma-Z$	yes
			$K-H$	MSG is needed
6m′m′	no C_{3v}			
(D_{3d}) -3 m	contains C_{3v}, but no $-1'$	trigonal	Λ	yes
			P	yes
		Hexagonal	$\Gamma-Z$	yes
			$K-H$	MSG is needed
−3m1′	contains $-1'$			
−3′m	contains $-1'$			
−3′m′	no C_{3v}			
−3m′	no C_{3v}			
(D_{3h}) −6m2	contains C_{3v}, but no $-1'$	Hexagonal	$\Gamma-Z$	yes
			$K-H$	MSG is needed
-6m21′	contains C_{3v}, but no $-1'$	Hexagonal	$\Gamma-Z$	yes
			$K-H$	MSG is needed
−6m′2′	no C_{3v}			
−6′m2′	contains C_{3v}, but no $-1'$	Hexagonal	$\Gamma-Z$	yes
			$K-H$	MSG is needed
−6′m′2	no C_{3v}			
(D_{6h}) 6/mmm	contains C_{3v}, but no $-1'$	Hexagonal	$\Gamma-Z$	no
			$K-H$	yes
6/mmm1′	contains $-1'$			
6/m′mm	contains $-1'$			
6/mm′m′	no C_{3v}			
6/m′m′m′	contains $-1'$			
6′/mmm′	contains $-1'$			
6′/m′mm′	contains C_{3v}, but no $-1'$	Hexagonal	$\Gamma-Z$	yes
			$K-H$	MSG is needed

Table 3. The list of all k paths which allow the existence of triple points. The first column is the label of MSG systems which allow the existence of triple points. The second column are the k paths of the system which allow the existence of triple points. The third column is the kind of the k path. The first kind of k paths is from table 1 and the second kind is from table 2.

Label of MSG systems	k path	the kind of k path
P3m1	$\Gamma-Z$	first kind
P3m11′	$\Gamma-Z$	first kind
P31m	$\Gamma-Z$	first kind
	$K-H$	first kind
P31m1′	$\Gamma-Z$	first kind
	$K-H$	first kind
R3m	Λ	first kind
	P	first kind
R3m1′	Λ	first kind
	P	first kind
P-31 m	$\Gamma-Z$	first kind
	$K-H$	first kind
P-3m1	$\Gamma-Z$	first kind
R-3 m	Λ	first kind
	P	first kind
P-61′	$\Gamma-Z$	second kind
P-6′	$\Gamma-Z$	second kind
P6′/m′	$\Gamma-Z$	second kind
P6mm	$K-H$	first kind
P6mm1′	$K-H$	first kind
P6′m′m	$\Gamma-Z$	first kind
P6′mm′	$\Gamma-Z$	first kind
	$K-H$	first kind
P-6m2	$\Gamma-Z$	first kind
P-6m21′	$\Gamma-Z$	first kind
P-6′m′2	$\Gamma-Z$	second kind
P-6′m2′	$\Gamma-Z$	first kind
P-62 m	$\Gamma-Z$	first kind
	$K-H$	first kind
P-62m1′	$\Gamma-Z$	first kind
	$K-H$	first kind
P-6′2′m	$\Gamma-Z$	first kind
	$K-H$	first kind
P-6′2m′	$\Gamma-Z$	second kind
P6/mmm	$K-H$	first kind
P6′/m′m′m	$\Gamma-Z$	first kind
P6′/m′mm′	$\Gamma-Z$	first kind
	$K-H$	first kind
P-43 m	1 1 1	first kind
P-43m1′	1 1 1	first kind
F-43 m	1 1 1	first kind
F-43m1′	1 1 1	first kind
I-43 m	1 1 1	first kind
	F	first kind
I-43m1′	1 1 1	first kind
	F	first kind
Pm3m	1 1 1	first kind
Fm3m	1 1 1	first kind
Im3m	1 1 1	first kind
	F	first kind

points. T and Δ of $Pm3m$, Δ of $Fm3m$, Δ of $Im3m$, $\Gamma-Z$ of $P6/mmm$, $\Gamma-Z$ of $P6mm$ and $\Gamma-Z$ of $P6mm1'$ allow the existence of Dirac points while the k paths of these several systems, which allow the existence of triple points, are given in table 3. The Brillouin zone of these several systems and definitions of T and Δ are shown in figure 3.

Then two questions surfaced:

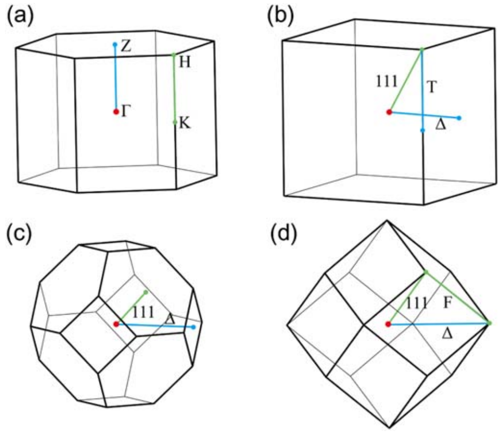

Figure 3. The Brillouin zone of the systems which allow the coexistence of Dirac points and triple points. The Brillouin zone of (a) P6/mmm, P6mm and P6mm1'. The Brillouin zone of (b) Pm3m, (c) Fm3m and (d) Im3m. The k paths, which allow the existence of triple points, are marked in green. The k paths, which allow the existence of Dirac points, are marked in blue.

(1) Is the condition of existence for the Weyl points similar to the condition of existence for the triple points? More specifically, can Weyl points exist in a k path whose symmetry group contains two 1-dimensional double group irreducible representations?

(2) Can the coexistence of Dirac points, triple points and Weyl points be allowed in some symmetric systems?

To answer question (1), we analyze two systems: the first system has D_{3d} point group symmetry with hexagonal Bravais lattice. The symmetry group of $\Gamma - Z$ in its Brillouin zone is C_{3v}. C_{3v} contains two 1-dimensional double group irreducible representations. These two representations have different mirror symmetry eigenvalues (i and $-i$) which means they are two different representations in the mirror plane of C_{3v} symmetry. Thus the crossing point in $\Gamma - Z$ must extend onto the mirror planes of C_{3v} symmetry to form a Weyl nodal line other than discrete points. This means, in this case, Weyl points are not able to exist in a k path whose symmetry group contains two 1-dimensional double group irreducible representations.

The second system has C_{3i} point group symmetry with hexagonal Bravais lattice. The symmetry group of $\Gamma - Z$ is C_3. C_3 contains two 1-dimensional double group irreducible representations. This system can be viewed as the first system to which a uniform magnetic field-B_z, in parallel with principle axis, is applied. The B_z breaks the mirror symmetry of C_{3v} and the Weyl nodal line break up into nodal points. Furthermore, the band structure along k_z path can be described by equation (2) plus several B_z induced terms:

$$H_{C_{3i}}(k_z) = \varepsilon_0(k_z) + \begin{pmatrix} M(k_z) + \beta_1 & 0 & 0 & 0 \\ 0 & M(k_z) + \beta_2 & 0 & 0 \\ 0 & 0 & -M(k_z) + \beta_3 & D + \beta_5 \\ 0 & 0 & D + \beta_5^* & -M(k_z) + \beta_4 \end{pmatrix}, \quad (3)$$

where β_1, β_2, β_3 and β_4 are real while β_5 is complex; $M(k_z)$ is $C_0 - C_1 k_z^2$. Solving the eigenvalues of equation (3), we find that the 2-dimensional double group irreducible representation-$\overline{E}_{1g/u}$ in equation (2) splits into two 1-dimensional double group irreducible representations. That means each triple point in equation (2) splits into two crossing points. Using $k \cdot P$ expansion and method of invariants to calculate the Hamiltonian around these crossing points can prove that these crossing points are Weyl points [48]. Therefore, the two 1-dimensional double group irreducible representations of $\Gamma - Z$ in this system allow the existence of Weyl points.

According to the above analysis for the two systems, the Weyl points can exist or not exist in a k path whose symmetry group contains two 1-dimensional double group irreducible representations. Thus, the answer to question (1) is negative.

For answering question (2):

The $\Gamma - Z$ of two of the above mentioned systems does not allow the coexistence of Dirac points, triple points and Weyl points, but recent research shows that triple point and Weyl point are able to coexist with each other [30, 35].

The symmetry requirement of Weyl points is much lower than that of the triple points. Weyl points are robust against the perturbations of most of the symmetry breaking. Weyl points can even exist at the k points whose symmetry group belongs to C_1 [49]. Such Weyl points in the bulk of 3-dimensional systems only need periodic symmetry in the absence of (TRO · IS).

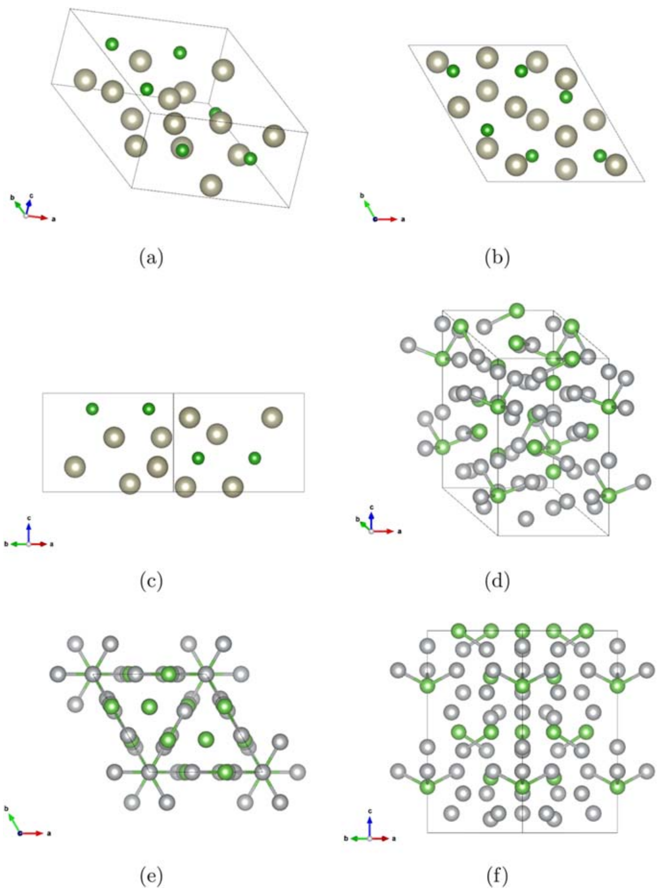

Figure 4. (a), (b) and (c) are the crystal structure of B_3Re_7. (b) is the top view of B_3Re_7 while (c) is the profile view. Green atoms in (a), (b) and (c) are B while grey atoms are Re. (d), (e) and (f) are the crystal structure of As_2Ni_5. (e) is the top view of As_2Ni_5 while (f) is the profile view. Green atoms in (d), (e) and (f) are As while grey atoms are Ni. The Bravais lattice of B_3Re_7 and As_2Ni_5 is hexagonal. The directions are marked at the corner of each subfigure, *c* axis is the *Z* axis of hexagonal.

Therefore, in view of the symmetry analysis hereinabove, the coexistence of Dirac points, triple points and Weyl points is allowed in some systems. If that happens, it will be chaotic whether the systems are to be defined as Dirac semimetal, triple point topological metal or Weyl semimetal. There is a viewpoint that triple point topological metal is an intermediate phase between Dirac and Weyl semimetal [33]. It can be true, but there are overlaps among these three phases and the boundary of the phases is still obscure so far. Such a state of chaos raises due to the use of symmetry to classify these three phases. In condensed matter systems, the symmetry group of a system is unique, but, in the Brillouin zone of a system, there are many different *k* paths/planes belonging to different symmetry groups. Usually, the existence of Dirac points or triple points in a *k* path depends on the symmetry group of the *k* path, other than depending only on the symmetry group of the system. As a result, the coexistence of Dirac points, triple points and Weyl points is symmetry-allowed.

5. Coexistence of Dirac points and triple points in B_3Re_7 and As_2Ni_5

In this section, we show that there are two materials- B_3Re_7 and As_2Ni_5 which allow the coexistence of Dirac points with triple points. More interestingly, those Dirac points and triple points can exist near the Fermi level with or without electron–hole doping.

The crystal structures of B_3Re_7 and As_2Ni_5 are plotted in figure 4. and the Brillouin zone of these two systems is shown in figure 3(a). According to [50, 51], both B_3Re_7 and As_2Ni_5 belong to $P6_3mc1'$. Their MPG symmetry is the same as $P6mm1'$ which has been mentioned in section 4. Even though the C_{2z} symmetry of $P6_3mc1'$ is accompanied by a fractional translation, the translation is to shift $1/2$ lattice constant along the *Z* axis. Thus the translation does not change the irreducible representations of $\Gamma - Z$ and of $K - H$ (except *Z* point and *H* point). Therefore, it is possible to identify the coexistence of the Dirac points with triple points in the $P6_3mc1'$ system.

The following first-principles calculations are performed by the Vienna *Ab initio* Simulation Package [52, 53]. For self-consistent total energy calculations, we use the generalized gradient approximation plus *U* (*GGA*+ *U*) and the Perdew–Burke–Ernzerhof exchange-correlation functional with projector-augmented wave

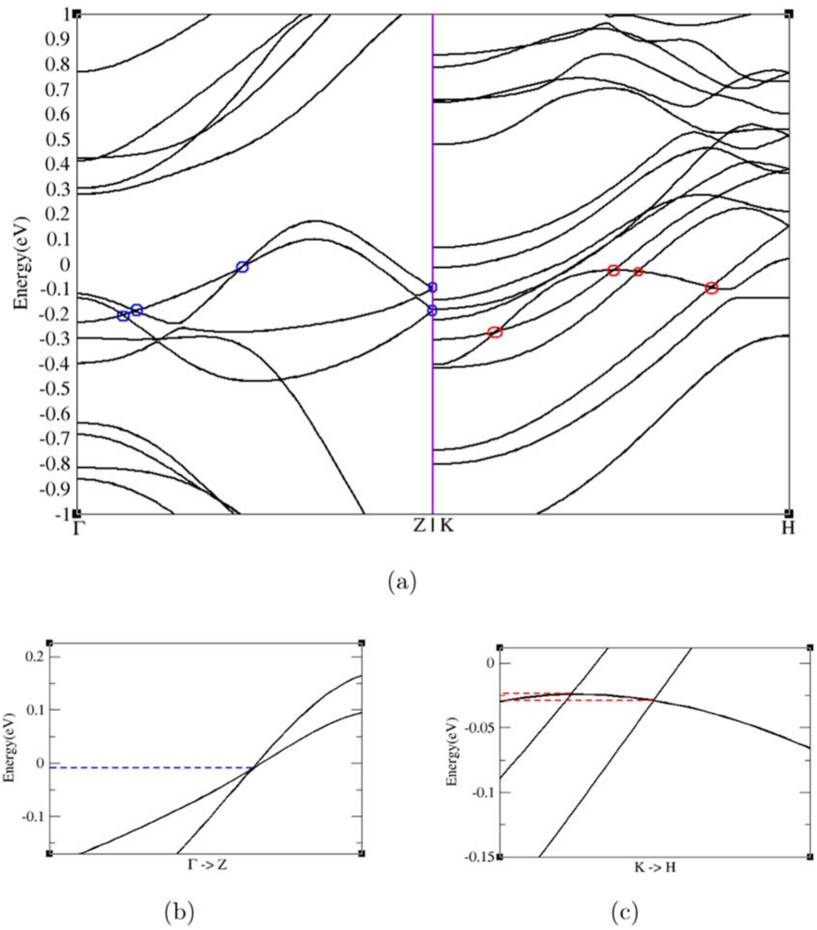

Figure 5. The band structures of B_3Re_7. The Fermi energy is set to be zero. (a) The band structure along $\Gamma-Z$ and K–H. The Dirac points, which are close to Fermi level and coexist with triple points, are marked in blue while triple points are marked in red. (b) is the zoom picture of Dirac point which is closest to Fermi level. (c) is the zoom picture of triple points which are closest to Fermi level. The dashed lines in (b) and (c) are merely a guide for viewing the energy level of Dirac point and triple points.

potentials. The parameters U are given by [50], we do not tune U in our calculation. Using Gamma-centered grid method, the reciprocal space is meshed at $4 \times 4 \times 6$ and $4 \times 4 \times 2$ for B_3Re_7 and As_2Ni_5, respectively. The energy convergence criteria for electronic iterations are set to be smaller than 10^{-4} eV. The cutoff energies for the plane wave basis are 980 eV and 515.123 eV for B_3Re_7 and As_2Ni_5, respectively.

According to the first-principles calculations for B_3Re_7 (as shown in figure 5), B_3Re_7 has one Dirac point and two triple points, and these three points are very close to Fermi level (within 30 meV). Besides, B_3Re_7 has other Dirac-triple pairs in the range of 0–0.3 eV, which means B_3Re_7 can host the coexistence of Dirac points and triple points with or without electron–hole doping [48, 54]. According to the first-principles calculations of As_2Ni_5 (as shown in figure 6), As_2Ni_5 does not have Dirac-triple pair around the Fermi level. However, As_2Ni_5 has 4 Dirac points and 7 triple points in a short energy range (0.25–0.37 eV), which means As_2Ni_5 can host the coexistence of Dirac points and triple points with electron–hole doping [48, 54].

Generally, any magnetic moment in a system will break TRS for sure. However, in similar crystal structure (C_{6v}), since the Dirac points on $\Gamma-Z$ (Z point is not included) and the triple points on $K-H$ are not protected by TRS, they may present while magnetic moments exist. If all magnetic moments point to same direction and along Z axis, all mirror symmetries of C_{6v} will be broken while C_6 maintained. Consequently, each Dirac point on $\Gamma-Z$ (Z point is not included) splits into 4 Weyl points while each triple point on $K-H$ splits into 2 Weyl points. If the mirror symmetries-M_x (the subscript-x means the mirror plane contains the a and c axis of figure 4) is broken by the magnetic moment while mirror symmetry-M_y (the subscript-y means the normal vector of M_y is perpendicular to the normal vector of M_x and c axis in figure 4) is preserved, then C_{6v} will be down to C_{3v}. Consequently, each Dirac point on $\Gamma-Z$ (Z point is not included) splits into 2 triple points while triple points on $K-H$ remain intact.

Since the primitive unit cells of B_3Re_7 and of As_2Ni_5 are too large (B_3Re_7 has 20 atoms and As_2Ni_5 has 42), it is quite difficult to include the Heyd–Scuseria–Ernzerhof (HSE) hybrid functional in the first-principles calculations. However, HSE hybrid functional is a small perturbation and there are a lot of Dirac-triple pairs in B_3Re_7 and As_2Ni_5. It is quite impossible to eliminate all the Dirac-triple pairs with such a small perturbation.

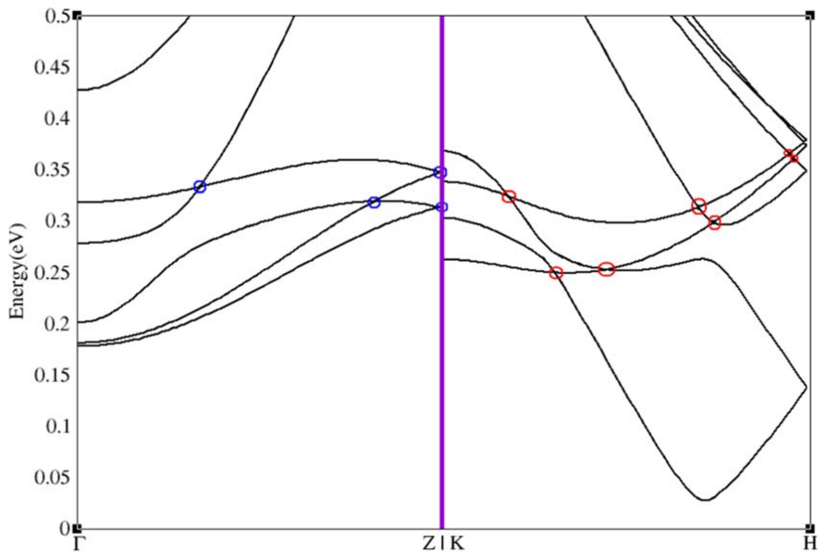

Figure 6. The band structure along $\Gamma - Z$ and $K - H$ for As_2Ni_5. The Fermi energy is set to be zero. Those Dirac points and triple points, which are in the energy range of 0.25 eV–0.37 eV, are marked in blue and red, respectively.

6. Conclusion

In high energy physics, breaking TRS or IS and keeping Lorentz invariance, one Dirac fermion will split into two Weyl fermions. In condensed matter systems, breaking TRS or IS, Dirac point may remain intact, split into triple points or split into Weyl points. One Dirac point can split into two triple points, two triple points can split into four Weyl points. The existence of triple point between the Dirac phase and the Weyl phase was well hidden in the past. The recent discovery of the triple point motivates researchers further to study many of its unknown characteristics. Therefore, we extend the theory of searching for triple points to all symmorphic magnetic systems, and list among all symmorphic systems all the k paths which allow the existence of triple points. Our study is helpful for a systematic search of the triple points in various systems. Besides, we also found that the coexistence of the Dirac points with the triple points is symmetrically allowed in some particular symmetric systems. According to our first-principles calculations, B_3Re_7 and As_2Ni_5 can be the candidates for realizing the coexistence of Dirac points with the triple points. We have not only provided an exhaustive triple point search mechanism for the symmorphic systems, but also identified material systems that host the Dirac and the triple points.

Acknowledgments

This work is supported by the Ministry of Science and Technology of Taiwan under Grant No. MOST 107-2112-M-002-013-MY3.

Appendix: Corepresentations of black and white MPG

All black and white point groups can be expressed as follows [45]:

$$M = H + \mathrm{TRO}(G - H), \tag{4}$$

where M is black and white point group, H is the unitary subgroup of M and G is one of the ordinary point groups.

Here, we denote element of H by U, and element of $\mathrm{TRO}(G - H)$ by V. We suppose that Δ is a unitary irreducible representation of H (the dimension of Δ can be greater than 1) and $|\varphi\rangle$ is the basis of Δ (the dimension of Δ is same as the dimension of $|\varphi\rangle$), therefore:

$$U\langle\varphi| = \langle\varphi|\ \Delta(U). \tag{5}$$

Now we introduce a basis $|\phi\rangle$ which is produced by operating V on $|\varphi\rangle$:

$$V\langle\varphi| = \langle\phi|. \tag{6}$$

Table A1. The list of all the black and white MPGs which have representations belonging to case (2) or case (3). The first column is the label for M. The second column is the label for H. The third column is the label for the irreducible representation of H (the symbols of irreducible representations are written in extended Mulliken notation). The fourth column is the classification of the irreducible representation of H.

M	H	Irreducible representation of H	Case
$-1'$	$1\,(C_1)$	$\overline{A}$	2
$2'/\mathrm{m}$	$\mathrm{m}\,(C_{1h})$	${}^1\overline{E}$, ${}^2\overline{E}$	3
$2/\mathrm{m}'$	$2\,(C_2)$	${}^1\overline{E}$, ${}^2\overline{E}$	3
$4'$	$2\,(C_2)$	${}^1\overline{E}$, ${}^2\overline{E}$	3
$-4'$	$2\,(C_2)$	${}^1\overline{E}$, ${}^2\overline{E}$	3
$4'/\mathrm{m}$	$2/\mathrm{m}\,(C_{2h})$	${}^1\overline{E}_g$, ${}^2\overline{E}_g$, ${}^1\overline{E}_u$, ${}^2\overline{E}_u$	3
$4/\mathrm{m}'$	$4\,(C_4)$	${}^1\overline{E}_2$, ${}^2\overline{E}_1$, ${}^1\overline{E}_1$, ${}^2\overline{E}_2$	3
$4'/\mathrm{m}'$	$\text{-}4\,(S_4)$	${}^1\overline{E}_2$, ${}^2\overline{E}_1$, ${}^1\overline{E}_1$, ${}^2\overline{E}_2$	3
$-3'$	$3\,(C_3)$	$\overline{A}$	2
		${}^1\overline{E}$, ${}^2\overline{E}$	3
$-3'\mathrm{m}$	$3\,\mathrm{m}\,(C_{3v})$	${}^1\overline{E}$, ${}^2\overline{E}$	3
		$\overline{E}_1$	1
$-3'\mathrm{m}'$	$32\,(D_3)$	${}^1\overline{E}$, ${}^2\overline{E}$	3
		$\overline{E}_1$	1
$6'$	$3\,(C_3)$	${}^1\overline{E}$, ${}^2\overline{E}$	3
		$\overline{A}$	1
$-6'$	$3\,(C_3)$	${}^1\overline{E}$, ${}^2\overline{E}$	3
		$\overline{A}$	1
$6'/\mathrm{m}$	$\text{-}6\,(C_{3h})$	${}^1\overline{E}_1$, ${}^2\overline{E}_3$, ${}^1\overline{E}_2$, ${}^2\overline{E}_2$, ${}^2\overline{E}_1$, ${}^1\overline{E}_3$	3
$6/\mathrm{m}'$	$6\,(C_6)$	${}^1\overline{E}_1$, ${}^2\overline{E}_3$, ${}^1\overline{E}_2$, ${}^2\overline{E}_2$, ${}^2\overline{E}_1$, ${}^1\overline{E}_3$	3
$6'/\mathrm{m}'$	$-3\,(C_{3i})$	${}^1\overline{E}_g$, ${}^2\overline{E}_g$, ${}^1\overline{E}_u$, ${}^2\overline{E}_u$	3
		$\overline{A}_g$, $\overline{A}_u$	1
$\mathrm{m}'3$	$23\,(T)$	${}^1\overline{F}$, ${}^2\overline{F}$	3
		$\overline{E}$	1

From equations (5), (6) and $V^{-1}\,UV$ belongs to H, we can obtain:

$$U\langle\phi| = UV\langle\varphi| \;=\; V(V^{-1}UV)\langle\varphi| = V\langle\varphi|\;\Delta(V^{-1}UV) \;=\; \langle\phi|\;\Delta^{*}(V^{-1}UV), \tag{7}$$

complex conjugate is denoted by asterisk. Let

$$\langle\zeta| \;=\; \langle\varphi,\,\phi|. \tag{8}$$

From equations (5), (7) and (8), we have:

$$U\langle\zeta| \;=\; \langle\zeta|\;D(U), \tag{9}$$

where

$$D(U) = \begin{pmatrix}\Delta(U) & 0\\ 0 & \Delta^{*}(V^{-1}UV)\end{pmatrix}, \tag{10}$$

for all U that belong to H. Since $\Delta^{*}(V^{-1}UV)$ is also a representation of H [55], the anti-unitary operators of M do not create any extra irreducible representation. Anti-unitary operators only cause the irreducible representations of H to become degenerate with each other or with itself, but usually anti-unitary operators do not cause any extra degeneracy.

If $\Delta(U)$ and $\Delta^{*}(V^{-1}UV)$ are equivalent, then there exists an unitary operator P such that:

$$\Delta(U) = P\Delta^{*}(V^{-1}UV)P^{-1}, \tag{11}$$

for all U belonging to H.

If

$$PP^{*} = \Delta(V^{2}), \tag{12}$$

then anti-unitary operators do not cause any extra degeneracy, and we call it case(1).

If

$$PP^{*} = -\Delta(V^{2}), \tag{13}$$

then anti-unitary operators cause the irreducible representation Δ to become degenerate with itself, and we call it case(2).

If $\Delta(U)$ and $\Delta^{*}(V^{-1}UV)$ are not equivalent, then they are degenerate with each other, and we call it case(3).

Now we can classify all the representations of all the black and white point groups. All those black and white point groups contain representations belonging to case(2) or case(3) are listed in table A1.

ORCID iDs

Chi-Ho Cheung https://orcid.org/0000-0002-3927-2914
R C Xiao https://orcid.org/0000-0001-8085-2251

References

[1] Ando T, Matsumoto Y and Uemura Y 1975 *J. Phys. Soc. Jpn.* **39** 279–88
[2] Laughlin R B 1981 *Phys. Rev.* B **23** 5632(R)
[3] Chang C Z *et al* 2013 *Science* **340** 6129
[4] Liu C X, Zhang S C and Qi X L 2016 *Annu. Rev. Condens. Matter Phys.* **7** 301–21
[5] Haldane F D M 1988 *Phys. Rev. Lett.* **61** 2015
[6] Xu G, Weng H, Wang Z, Dai X and Fang Z 2011 *Phys. Rev. Lett.* **107** 186806
[7] Weng H *et al* 2015 *Phys. Rev.* B **92** 075436
[8] Kane C L and Mele E J 2005 *Phys. Rev. Lett.* **95** 226801
[9] Kane C L and Mele E J 2005 *Phys. Rev. Lett.* **95** 146802
[10] Moore J E and Balents L 2007 *Phys. Rev.* B **75** 121306(R)
[11] Bernevig B A, Hughes T L and Zhang S C 2006 *Science* **314** 1757
[12] Cheung C H, Fuh H R, Hsu M C, Lin Y C and Chang C R 2016 *Nanoscale Res. Lett.* **11** 459
[13] Fu L 2011 *Phys. Rev. Lett.* **106** 106802
[14] Hsieh T H *et al* 2012 *Nat. Commun.* **3** 982
[15] Slager R J, Mesaros A, Juričić V and Zaanen J 2013 *Nat. Phys.* **9** 98–102
[16] Kruthoff J, Boer J D, Wezel J V, Kane C L and Slager R J 2017 *Phys. Rev.* X **7** 041069
[17] Neupane M *et al* 2014 *Nat. Commun.* **5** 3786
[18] Uchida M *et al* 2017 *Nat. Commun.* **8** 2274
[19] Wang Z *et al* 2012 *Phys. Rev.* B **85** 195320
[20] Young S M and Kane C L 2015 *Phys. Rev. Lett.* **115** 126803
[21] Gyenis A *et al* 2016 *New J. Phys.* **18** 105003
[22] Murakami S 2007 *New J. Phys.* **9** 356
[23] Xu S Y *et al* 2015 *Science* **349** 6248
[24] Lv B Q *et al* 2015 *Phys. Rev.* X **5** 031013
[25] Li P *et al* 2017 *Nat. Commun.* **8** 2150
[26] Huang Z, Arovas1 D P and Balatsky A V 2013 *New J. Phys.* **15** 123019
[27] dos Reis R D *et al* 2016 *New J. Phys.* **18** 085006
[28] Yang H *et al* 2017 *New J. Phys.* **19** 015008
[29] Lepori L, Burrello M and Guadagnini E 2018 *J. High Energy Phys.* JHEP06(2018)110
[30] Lv B Q *et al* 2017 *Nature* **546** 627–31
[31] Bradlyn B *et al* 2016 *Science* **353** 6299
[32] Chang G *et al* 2017 *Sci. Rep.* **7** 1688
[33] Zhu Z *et al* 2016 *Phys. Rev.* X **6** 031003
[34] Weng H, Fang C, Fang Z and Dai X 2016 *Phys. Rev.* B **93** 241202(R)
[35] Weng H, Fang C, Fang Z and Dai X 2016 *Phys. Rev.* B **94** 165201
[36] Sun Y *et al* 2017 *Phys. Rev.* B **95** 235104
[37] Fulga I C and Stern A 2017 *Phys. Rev.* B **95** 241116(R)
[38] Sun J P, Zhang D and Chang K 2017 *Phys. Rev.* B **96** 045121
[39] Winkler G W *et al* 2016 *Phys. Rev. Lett.* **117** 076403
[40] Zaheer S *et al* 2013 *Phys. Rev.* B **87** 045202
[41] Yu J, Yan B and Liu C X 2017 *Phys. Rev.* B **95** 235158
[42] Heikkilä T T and Volovik G E 2015 *New J. Phys.* **17** 093019
[43] Wang Z *et al* 2013 *Phys. Rev.* B **88** 125427
[44] Chen C *et al* 2017 *Phys. Rev. Mater.* **1** 044201
[45] Bradley C J and Cracknell A P 1972 *The Mathematical Theory of Symmetry in Solids* (Oxford: Oxford University Press)
[46] Cheung C H *et al* 2017 arXiv:1709.07763
[47] Koster G F, Dimmock J D, Wheeler R G and Statz H 1963 *Properties of the Thirty-Two Point Groups* (Cambridge, MA: MIT Press)
[48] Xiao R C *et al* 2018 *J. Phys.: Condens. Matter* **30** 245502
[49] Soluyanov A A *et al* 2015 *Nature* **527** 495–8
[50] Curtarolo S *et al* 2012 *Comput. Mater. Sci.* **58** 218–26
[51] Kayhan M 2013 *Transition Metal Borides: Synthesis, Characterization and Superconducting Properties* Ph.D. ThesisTechnische Universität, Darmstadt
[52] Kresse G *et al* 1996 *Phys. Rev.* B **54** 11169
[53] Kresse G *et al* 1996 *Comput. Mater. Sci.* **6** 15
[54] Zhang K *et al* 2017 *Phys. Rev.* B **96** 125102
[55] Bradley C J and Davies B L 1968 *Rev. Mod. Phys.* **40** 2