Predicting topological materials: symmetry-based indicator theories and beyond

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Received 26 May 2021, revised 27 June 2021
Accepted for publication 13 July 2021
Published 27 July 2021

Abstract
Though symmetry-based indicators formulae are powerful in diagnosing topological states with a gapped band structure at/between any high-symmetry points, it fails in diagnosing topological degeneracies when the compatibility condition is violated. In such cases, we can only obtain information of whether there is a band degeneracy at some high-symmetry points or along some high-symmetry lines by the compatibility condition. Under the framework of symmetry-based indicator theories, we proposed an algorithm to diagnose the topological band crossings in the compatibility condition-violating systems to obtain the whole topological information, by using the symmetry-based indicator formulae of their subgroups. In this paper, we reinterpret the algorithm in a simpler way with two material examples preserving different topological states in spinless systems with time-reversal symmetry, discuss the limitation of the symmetry-based indicator theories, and make further discussions on the algorithm applying in spinful systems with time-reversal symmetry.

Keywords: symmetry-based indicator theories, topological band theory, topological materials, first-principle calculation

(Some figures may appear in colour only in the online journal)

1. Introduction
Symmetry-based indicator theories [1–5] greatly decrease the calculation to diagnose topological phases of a material, and tremendous progress has been made in effectively diagnosing topological materials in the past few years [6–8], such as symmetry-based indicator formulae for topological insulators [3, 5], topological crystalline insulators [3, 5], and topological semimetals [4]. However, on one hand, two conditions should be met before the application of those formulae: (a) the number of each irreducible representation at high-symmetry points (HSPs) should satisfy the compatibility condition, i.e. the band structure either has no band crossing at/between any of those HSPs or has band crossing along high-symmetry lines (HSLs) can be gapped out without making an additional band inversion at any HSPs, as shown in figures 1(b) and (c); (b) the system should preserve a nontrivial symmetry-based indicator group, which means that symmetry-based indicator formulae are restricted in limited space groups. On the other hand, as presented in our previous work [6], more than 62% (98%) materials are diagnosed to be a topological semimetal in the spinful (spinless) case. Among those topological semimetals, which are the majority of the diagnosed topological materials,
Figure 1. Three different kinds of band structure between two high-symmetry points, where the red and blue line represents the occupied and the unoccupied band, respectively. HSP1 and HSP2 are two different high-symmetry points in the Brillouin zone. (a) Band structure violating the compatibility condition. (b), (c) Two different band structures satisfying the compatibility condition. (d) Two cases where we cannot (case (A)) and can (case (B)) use the symmetry-based indicator formulae to diagnose topological information.

100% of them in the spinful case and 99% in the spinless case violate the condition (a), which means that we cannot use the symmetry-based indicator formulae to get further topological information with a simple calculation.

However, according to the algorithm proposed in our previous work [9], most of the topological semimetals can be further diagnosed by the symmetry-based indicator of their subgroups to obtain the whole topological information. Such algorithm requires one to ignore some crystalline symmetries of the system, so as to obtain a subgroup which meets both of condition (a) and condition (b) at the same time. Yet, still a minority of them cannot be diagnosed by the symmetry-based indicators under this algorithm, but only by the compatibility condition, and we will also discuss such cases in detail. Thus, such diagnosing algorithm is under the symmetry-based indicator theories, but also beyond them.

In this paper, we will first give a brief overview of the condition (a) and condition (b), which are two basic conditions before using the symmetry-based indicator formulae to diagnose topological phases. Second, two cases in different topological phases are analyzed by the symmetry-based indicator theories and beyond, and then followed by the restriction of the symmetry-based indicator theories. In the end, similar discussions for the algorithm applied in spinful systems with time-reversal symmetry (\( T \)) are outlined in the last section.

2. Compatibility condition and symmetry-based indicator group

Compatibility conditions restrict the number of symmetry data, i.e. a set of irreducible representations for the occupied bands at HSPs in the Brillouin zone (BZ). Since such condition only involves the symmetry data at HSPs, it can only tell the information of band inversion at HSPs rather than along HSLs, compared to the band structure of an atomic insulator [1, 2]. For example, band structure with a band inversion at a HSP in figure 1(a) does not satisfy the compatibility condition, while band structure with a band inversion along a HSL in figure 1(c) will satisfy the compatibility condition like figure 1(b), since such a band inversion can be gradually gapped out through by a perturbation without making a new band inversion at any HSPs. Thus, a topological semimetal like SrSi\(_2\) [10] with a band inversion along a HSL, like figure 1(c), will not be considered here due to the satisfaction of the compatibility condition and diagnosed as a trivial insulator by the symmetry-based indicator theories. Namely, it is a shortcoming of the compatibility condition that a band structure like figure 1(c) is diagnosed also as a ‘gapped’ phase. Thus, if the symmetry data of a system satisfies the compatibility condition, there will be no band crossings at any HSPs or along any HSLs, which corresponds to a ‘gapped’ band structure. Likewise, if the symmetry data of a system does not satisfy the compatibility condition, there will be a band crossing at some HSPs or along some HSLs, but the condition (a) can still be satisfied if we ignore some crystalline symmetries of the system.

Symmetry-based indicators are powerful in predicting topological materials, because we can tell the topological information of a material by just calculating the symmetry data at up to eight HSPs [1–8]. However, systems with certain space groups have a trivial symmetry-based indicator group [1], which means that the symmetry data only at HSPs is not enough to diagnose the topological states of such systems, but wavefunctions at other \( k \) points need to be calculated. In some cases, ignoring some crystalline symmetries may give rise to a nontrivial symmetry-based indicator group, which will still help us to diagnose the topological phases.

As we discussed in the section 1, symmetry-based indicator formulae cannot be used when either/both of conditions (a) and (b) are violated, and we call such situation case (A). In order to proceed to use the symmetry-based indicator formulæ for further diagnosis, we need to ignore some crystalline symmetries to make case (A) to case (B), where both of the conditions are satisfied, as shown in figure 1(d).

In the following, we will give two examples with case (A) in the Al class system (spinless system with \( T \)) [11–13], and show how to reach case (B) and to use symmetry-based indicator formulæ to obtain the topological information afterwards. One example is Weyl phonons in a noncentrosymmetric material ZrPdSn, which satisfies condition (a) but breaks condition (b); the other one is node-ring phonons in a centrosymmetric material Na\(_3\)BrO, which break both condition (a) and (b).

3. Diagnosis process for Weyl phonons in ZrPdSn

ZrPdSn is a narrow-band-gap semiconductor with half-Heusler crystal structure of space group \( F43m \) (#216) [14], as shown in figure 2(a). The compatibility condition is satisfied for the lowest 6 phonon bands according to the symmetry data at HSPs shown in table 1. However, the phonon spectra in figure 2(c) shows that the 6th band and the 7th band are very close to each other at around 5.4 THz, and such kind of band structure may bring out Weyl points composed of the 6th
Figure 2. (a) Crystal structure, (b) Brillouin zone and (c) phonon band structure of ZrPdSn. (d) Subgroups of #216. (e) Case (A) for #216 and case (B) for #82 after ignoring $C_{111}$ and $M_{110}$ symmetries. (f) One possible configuration of $z_2 = 0$ for #82. Red and green dots represent Weyl points with different chiralities. (g) Distribution of Weyl points for ZrPdSn with #216. (h) Surface arcs for 24 Weyl points on the [111] surface, where every pair of two Weyl points with opposite chirality will be projected onto one point.

Table 1. Irreducible representations for the lowest six bands of ZrPdSn at each high-symmetry momentum. The symmetry data for #216 satisfies the compatibility condition.

| ZrPdSn | k points | irreducible representations |
|--------|----------|-----------------------------|
| Γ      |          | $2Γ_4$                      |
| L      |          | $2L_1 + 2L_3$               |
| W      |          | $2W_1 + W_2 + 2W_3 + W_4$  |
| X      |          | $X_1 + X_3 + 2X_5$          |

4. Diagnosis process for node-ring phonons in Na$_3$BrO

Na$_3$BrO is also a narrow-gap insulator but with an anti-perovskite oxide structure of space group Pm-3 m (#221) [15], as shown in figure 3(a). From the phonon spectra in figure 3(c),...
Figure 3. (a) Crystal structure, (b) Brillouin zone and (c) phonon spectra for Na$_3$BrO. (d) Subgroups for #221. (e) Case (A) for #221 and case (B) for both subgroup #81 and #146 after ignoring different symmetries. (f) One of the possible configurations for subgroup #81 with $z_2z_2 = (00)$. (g) One of the possible configurations for subgroup #148 with $z_2z_4 = (03)$. (h) Nodal ring distribution for Na$_3$BrO by both symmetry-based indicator analysis and first-principle calculation. (i) Surface states for node-ring phonons in Na$_3$BrO on [001] surface at 5.76 THz.

Table 2. Irreducible representations for the lowest nine phonon bands of Na$_3$BrO at each high-symmetry momentum. The symmetry data for #221 breaks the compatibility condition.

| k points | irreducible representations |
|----------|-----------------------------|
| $\Gamma$ | $2\Gamma_4 - + \Gamma_5$ |
| M        | $M_2 + M_2 - + M_5 + M_5$  |
| R        | $2R_4 - + R_5$             |
| X        | $X_2 + X_2 + X_3 - + X_5$  |

one may notice that there are several band crossing along $\Gamma$–M, R–M and M–X directions around 5.8 THz, crossed by the 9th band and 10th band. Those band crossings along HSLs indicate the violation of condition (a) for the lowest nine bands, which is also confirmed by the symmetry data of Na$_3$BrO shown in table 2. Furthermore, #221 has a trivial symmetry-based indicator group $Z_2Z_2$ for subgroup #81, $Z_2Z_2$ for subgroup #148, all the $C_4$ symmetries, all the $C_2$ symmetries except for the $C_3$ symmetry are ignored. For subgroups, e.g. #148, after ignoring all the mirror symmetries and $C_4$ symmetries, each irrep from #221 can be mapped to #148. Then, we need to use the compatibility condition of the subgroup #148, which is different from #221, to check whether the mapped irreps satisfy the compatibility condition or not. Both of the subgroups satisfy the (a) compatibility condition and (b) nontrivial symmetry-based indicator group condition, and can alter Na$_3$BrO from case (A) to case (B), as shown in figure 3(e).

For subgroup #81, $S_4$ symmetry is the only generator. This group has a nontrivial indicator group $Z_2Z_2$ [1], and it takes a value of $z_2z_2 = (00)$ for the symmetry data of Na$_3$BrO. Such zero indicators of #81 tell us that there are 0 mod 8 band crossings both on $k_z = 0$ plane and on $k_z = \pi$ plane, and the number of band crossings on those two planes can be different. Figure 3(f) shows one possible configuration of the band crossings with $z_2z_2 = (00)$, i.e. eight band crossings on the $k_z = \pi$ plane and 0 band crossings on the $k_z = 0$ plane, where band crossings are marked by red crosses. Since both the $T$ and inversion symmetry are preserved in Na$_3$BrO, the band crossings may belong to nodal lines/rings instead of isolated Dirac points. Thus, only with the information given by the indicator of subgroup #81 we cannot get the whole topological configuration for Na$_3$BrO. Thus, we need to proceed to analyze the topological information given by the indicators of the other subgroup #148.
An indicator group for #148 is $\mathbb{Z}_2\mathbb{Z}_4$, which is actually equivalent to the indicator group of $\mathbb{Z}_2\mathbb{Z}_2\mathbb{Z}_2\mathbb{Z}_4$ for #2, with the first three indicators $\mathbb{Z}_2$ having the same value. In addition, for space groups with inversion symmetry, subgroup #2 is always a choice to turn the system from case (A) to case (B), because the compatibility condition for #2 is always satisfied for any symmetry data. Symmetry data of #148 (#2) gives rise to indic-

the compatibility condition for #2 is always satisfied for any choice to turn the system from case (A) to case (B), because

(1101)

topological band crossings of a system can be diagnosed by
turn the system from case (A) to case (B), i.e. not all the
gnose topological states even when the system is in case (A). However, not all the systems have a subgroup which can
turn the system from case (A) to case (B), because the position and number of surface states will change with dif-

ferent energies, since node-ring band crossings not related by

two node-ring band crossings, thus there will be two drumhead

surfaces of #143/146

marked in figure

pink and grey dots are the projection of nodal rings and also

those nodal rings along \( [001] \) direction at 5.76 THz, where the

node-ring band crossings along \( X-M \) direction in figure

(c). Since the projection of the grey dots along the surface boundary contains four

two node-ring band crossings, thus there will be two drumhead

system will be a combination of those three cases. If a system

the compatibility condition, it is easy to know that there is a pair of Weyl

points with opposite chirality locating along the \( C_3 \) axis,
as shown in figure 4. If a system only has a mirror symmetry

and the compatibility condition is violated, there will be node-

line/ring band crossings locating on the mirror plane, as shown in

Figure 4. Three cases where the topological degeneracies can be only
diagnosed by compatibility condition, but cannot by the

symmetry-based indicator. (a) System only with \( C_2 \) symmetry.
(b) System only with \( C_3 \) symmetry. (c) System with a single mirror

symmetry.

5. Topological states that cannot be diagnosed
by symmetry-based indicators

In the previous sections, we introduced the algorithm to use the

symmetry-based indicator formulae of subgroups to dia-
gnose topological states even when the system is in case (A). However, not all the systems have a subgroup which can
turn the system from case (A) to case (B), i.e. not all the
topological band crossings of a system can be diagnosed by

the indicators of its subgroups. In such cases, the subgroup

search will end up with #1 with no subgroups satisfying both

cases where topological degeneracies can be only dia-
gnosed by the compatibility condition, but not the symmetry-

based indicators. They are systems only with \( C_2 \) symmetry

e.g. #3 and #5), systems only with \( C_3 \) symmetry (e.g. #143

and #146) and systems with a single mirror symmetry (e.g. #6

and #8). We note that topological information for those cases

are still easy to be obtained since crystalline symmetries are

very simple. Other cases with more complex symmetries can

be treated as a combination of those three cases. If a system

only with \( C_2/C_3 \) symmetry but still violates the compatibil-

ity condition, it is easy to know that there is a pair of Weyl

points with opposite chirality locating along the \( C_3/C_1 \) axis,
as shown in figure 4. If a system only has a mirror symmetry

and the compatibility condition is violated, there will be node-

line/ring band crossings locating on the mirror plane, as shown in

Figure 4.

6. Diagnosing topological states by
symmetry-based indicator in class AI systems

The algorithm of diagnosing topological states by the indic-

ator of subgroups can also be used in other symmetry classes

with minor changes, such as class AI systems, i.e. spinful sys-

tems with \( T \). In class AI systems, the compatibility condi-

tion can help us to diagnose topological semimetals with band

crossings located at HSPs or along HSLs, but symmetry-based

indicators are used to diagnose gapped states like trivial insu-

lators, topological insulators (TIs) and topological crystalline

insulators (TCIs). Thus, by using the indicators of subgroups,
one can obtain the topological phase transition from a topolo-

gical semimetal to trivial insulator/TI/TCI when certain crys-

talline symmetries are broken by perturbations.
The algorithm for diagnosing the complete topological information of systems violates compatibility condition and/or nontrivial symmetry-based indicator group condition is under the framework of symmetry-based indicators, but it compensates for the shortcomings of symmetry-based indicators. We display how to diagnose topological information in systems either violating compatibility condition or having a nontrivial symmetry-based indicator group condition with two material examples in class AI systems, i.e. spinless system with $\mathcal{T}$, to show both the effectiveness and correctness of this algorithm. We also discuss the limitation of the symmetry-based indicator, which cannot diagnose all the topological states in all cases. But we can still get the whole topological information by the compatibility condition. Furthermore, the algorithm is also discussed in class AI systems, i.e. spinful systems with $\mathcal{T}$ to show the topological phase transition between topological semimetals and topological (trivial) gapped states. Similar discussion can also be made in other systems, like photons [16–19], phonons [20–34], and magnons [35, 36].

### Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

### Acknowledgments

We acknowledge the supports from JSPS KAKENHI Grant Nos. JP18H03678 and JP20H04633, Tokodai Institute for Element Strategy (TIES) funded by MEXT Elements Strategy Initiative to Form Core Research Center. T Z also acknowledge the support by Japan Society for the Promotion of Science (JSPS), KAKENHI Grant No. 21K13865

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