**qeirreps:** an open-source program for QUANTUM ESPRESSO to compute irreducible representations of Bloch wavefunctions

Akishi Matsugatani\textsuperscript{a}, Seishiro Ono\textsuperscript{a}, Yusuke Nomura\textsuperscript{b}, Haruki Watanabe\textsuperscript{a}

\textsuperscript{a}Department of Applied Physics, University of Tokyo, Tokyo 113-8656, Japan
\textsuperscript{b}RIKEN Center for Emergent Matter Science, 2-1 Hirosawa, Wako, Saitama 351-0198, Japan

**Abstract**

Bloch wavefunctions in solids form a representation of crystalline symmetries. Recent studies revealed that symmetry representations in band structure can be used to diagnose the topological properties of weakly interacting materials. In this work, we introduce an open-source program \textit{qeirreps} that computes the representations in a band structure based on the output file of QUANTUM ESPRESSO. Our program also calculates the $\mathbb{Z}_4$ index, i.e., the sum of inversion parities at all time-reversal invariant momenta, for materials with inversion symmetry. When combined with the symmetry indicator method, this program can be used to explore new topological materials.

**Keywords:** QUANTUM ESPRESSO; Irreducible representations; Non-symmorphic space groups.

**PROGRAM SUMMARY**

| Program title: | qeirreps |
|---------------|----------|
| Catalogue identifier: | |
| Licensing provisions: | GNU General Public Licence 3.0 |
| Programming language: | Fortran 90 |
| Computer: | any architecture with a Fortran 90 compiler |
| Operating system: | Unix, Linux |
| RAM: | Variable, depends on the complexity of the problem |
| External routines/libraries used: | |
| • BLAS (http://www.netlib.org/blas) |
| • LAPACK (http://www.netlib.org/lapack) |

**Nature of problem:** Irreducible representations of Bloch wavefunctions

**Solution method:** Linear algebra calculation for Bloch wavefunctions

**Running time:** 1 min - 1 h (strongly depends on the complexity of the problem)

1. **Introduction**

One of the main goals in condensed matter physics is to predict the properties of materials of our interest by solving the Schrödinger equation. In practice, this challenging problem is reduced to a manageable one in two ways. The first is to map the interacting system to a free (i.e., noninteracting) electronic system, as is done in the Kohn-Sham density functional theory (DFT) [1]. The other simplification utilizes the symmetry of the system. For example, the lattice translation symmetry of an ideal crystal that is free from impurities or disorders allows us to block-diagonalize the Hamiltonian by switching to the momentum space. The original problem of interacting electrons is thereby transformed into the one within the standard band theory. The
electronic structure of an enormous number of weakly interacting materials has been successfully computed in this way.

In addition to the lattice translation symmetry, a perfect crystal tends to have other symmetries such as a spatial inversion and a discrete rotation. The set of symmetry operations of a crystal forms a group, called space group. In three dimensions, there are 230 different space groups, and the spatial symmetry of the crystal at work falls into one of them. Crystalline symmetries help us to a better understanding on the electronic band structure. Bloch wavefunctions form a representation of the space group, and the representation puts constraints on how many energy bands degenerate at each momentum and how energy bands at different momenta connect with each other. Furthermore, there has been an increasing number of evidence that the space group representation also informs us of the topological aspects of the Bloch wavefunction.

Since the discovery of the $\mathbb{Z}_2$ topological insulator [2, 3], topological materials have attracted researchers around the world. In the early stage of the study of topological phases, the focus was on the phases protected by internal symmetries: the time-reversal, the particle-hole, and the chiral symmetry [4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18]. These pioneering studies were united into the celebrated topological periodic table [19, 20, 21]. They were followed by a large number of studies that take into account the various types of crystalline symmetries [22, 23, 24, 25, 26, 27, 28]. It turned out that there exist various novel topological phases protected by crystalline symmetries, such as mirror Chern insulators [29, 30], higher-order topological insulators [31, 32, 33, 34, 35, 36, 37], and topological semimetals of the Dirac [38] and Weyl [39] type. These topological materials host robust surface states and exhibits unique bulk responses, which could be leveraged for new low-power devices. Therefore, discovering new candidates of topological materials is one of the important tasks both for the fundamental physics and for the application.

At this moment, listing up the full set of topological invariants, for a given symmetry setting, that completely characterize all possible topological phases is still a pending problem. Furthermore, even if we know the mathematical definition of topological invariants, it is sometimes difficult to compute them directly using their definitions [40, 41, 42]. These issues can be resolved with the help of crystalline symmetries. By using the information of the representations of the Bloch wavefunctions at a set of crystalline momenta, it is sometimes possible to judge the topology encoded in the Bloch wavefunctions quite easily. The prototypical example is the Fu-Kane formula [9], which determines the $\mathbb{Z}_2$ invariant based on the inversion parities. Recently, this idea has been extended to a wider class of topological (crystalline) insulators and semimetals in all 230 space groups [43]. The usefulness of this extended method, called “symmetry indicators,” in the search for realistic topological materials was clearly demonstrated by the recent comprehensive survey of topological materials among existing databases of inorganic substances [44, 45, 46, 47, 48]. As a result of this survey, thousands of candidates of topological (crystalline) insulators and semimetals have been identified. The theory of symmetry indicators has also been extended to magnetic space groups [49] and superconductors [50, 51, 52, 53, 54, 55], and further investigation of topological magnetic materials and superconductors is awaiting us.

Having in mind these applications, it is evidently important to make it possible to automatically compute irreducible representations of Bloch wavefunctions by using DFT. Although the authors of Refs. [44, 45, 46, 47, 48, 56] implemented this function for WIEN2k [57] and VASP [58], these softwares require paid licenses. In contrast, for the QUANTUM ESPRESSO [59, 60], which is a free, open-source package, the existing program can handle only one type of space groups, called “symmorphic” space groups, and does not work for the other type, called “non-symmorphic.” Given this situation, we develop an open-source code, named qeirreps, that works equally for symmorphic and non-symmorphic space groups. This would allow everyone to compute the band structure and determine the irreducible representations by themselves, and when combined with the method of symmetry-indicator, would accelerate our search of novel topological materials like topological superconductors.

The rest of this paper is organized as follows. In Sec. 2, we briefly review the theoretical background of space groups and their representations. In Sec. 3, we explain the installation and usage of qeirreps. After providing some examples: bismuth, silicon, and PbPt$_3$ in Sec. 4, we conclude in Sec. 5.
2. Theoretical background

We start with reviewing the basics of space groups and their representations.

2.1. Space group action on the real and momentum space

Let us consider a space group \( G \). An element \( g \in G \) moves \( x \in \mathbb{R}^3 \) to
\[
g(x) = p_g x + t_g, \quad (1)
\]
where \( p_g \in \text{O}(3) \) represents the point group part and \( t_g \in \mathbb{R}^3 \) represents the translation part of \( g \). The product of two elements \( g, g' \in G \) is defined by
\[
p_{gg'} = p_g p_{g'}, \quad t_{gg'} = p_g t_{g'} + t_g. \quad (2)
\]
In general, \( t_g \) is not necessarily a lattice vector. If we can choose the origin of \( x \) in such a way that \( t_g \) becomes a lattice vector simultaneously for all \( \forall g \in G \), the space group is symmorphic; otherwise, it is nonsymmorphic. Nonsymmorphic space groups typically contain either screw axes or glide planes.

A space group \( G \) always has a subgroup \( T \) composed of lattice translations. An element \( T_{\mathbf{R}} \) of \( T \) can be characterized by a lattice vector \( \mathbf{R} \). We introduce the wavevector \( k \) through the representation of \( T_{\mathbf{R}} \):
\[
U_k(T_{\mathbf{R}}) = e^{-i k \cdot \mathbf{R}}. \quad (3)
\]
An element \( g \in G \) changes \( k \) to \( g(k) = p_g k \). We say \( k \) is invariant under \( g \) when \( g(k) = k + G \), with a reciprocal lattice vector \( G \). For each \( k \), the set of \( g \in G \) that leaves \( k \) invariant, i.e., \( \{ h \in G \mid h(k) = k + G \} \), forms a subgroup of \( G \) called the little group \( G_k \).

2.2. Crystalline symmetries of band structures

Suppose that the single-particle Hamiltonian in momentum space satisfies
\[
U_k(g) H_k = H_{p_g k} U_k(g). \quad (4)
\]
Here unitary matrices \( U_k(g) \) form a projective representation of \( G \). That is, they satisfy
\[
U_{g'k}(g') U_k(g) = \omega^{gp}(g,g') U_k(gg'), \quad (5)
\]
where \( \omega^{gp}(g,g') = \pm 1 \) is the projective factor originated from the spin of electrons. For spin-rotation invariant systems, \( \omega^{gp}(g,g') \) can be chosen 1 by neglecting the spin degree of freedom.

The single-particle Hamiltonian \( H_k \) can be diagonalized as
\[
H_k = \Psi_k \begin{pmatrix}
\epsilon_{k1} \mathbb{1}_{\alpha_1} & 0 & \cdots & 0 \\
0 & \epsilon_{k2} \mathbb{1}_{\alpha_2} & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & \epsilon_{kM} \mathbb{1}_{\alpha_{M_k}}
\end{pmatrix} \Psi_k^\dagger, \quad (6)
\]
where \( \epsilon_{kn} \) is the \( n \)-th eigenenergy of \( H_k \), and \( \Psi_k \) is composed of all eigenvectors of \( H_k \). When \( h \) is an element of \( G_k \), \( U_k(h) \) can also be block-diagonalized by \( \Psi_k \) into irreducible representations \( U_k^\alpha(h) \):
\[
U_k(h) = \Psi_k \begin{pmatrix}
U_{k1}^{\alpha_1}(h) & 0 & \cdots & 0 \\
0 & U_{k2}^{\alpha_2}(h) & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & U_{kM_k}^{\alpha_{M_k}}(h)
\end{pmatrix} \Psi_k^\dagger \quad (\forall h \in G_k), \quad (7)
\]
Although the specific representation $U_k^{\alpha}(h)$ depends on the detailed choice of $\Psi_k$, its character
\[ \chi_k^{\alpha}(h) = \text{tr}[U_k^{\alpha}(h)] \] (8)
is basis independent. The output of our program is the list of characters $\chi_k^{\alpha}(h)$ for each the energy level $\epsilon_{kn}$ and high-symmetry point $k$.

Since $G_k$ is an infinite group due to its translation subgroup $T$, sometimes the finite group $G_k/T$, called “little co-group [61],” is discussed instead. Irreducible representations of $G_k/T$ and $G_k$ are related to each other by a simple rule, and one can convert one to the other easily. Note that the output of our program is the character of representations of $G_k$, not $G_k/T$, and one should not confuse them.

2.3. Application to symmetry indicators

The characters $\chi_k^{\alpha}(h)$ in the output of our program can be converted to integers $\{n_k^{\alpha}\}$ that count irreducible representations $U_k^{\alpha}(h)$ appearing in the occupied bands at each high-symmetry point $k$. These integers are used, for example, to diagnose the topological indices of band insulators through the method of symmetry indicators [43, 62]. Formulas of topological indices in terms of $\{n_k^{\alpha}\}$ are provided in Refs. [63, 64, 65, 50].

For the user’s convenience, we implemented the function that automatically computes the $Z_4$ index as the sum of the inversion parities of all occupied bands at all the time-reversal invariant momenta (TRIMs). The $Z_4$ index can detect not only strong topological insulators but also topological crystalline insulators such as mirror Chern insulators or higher-order topological insulators [64, 65]. See Sec. 4.1 for an example.

Other symmetry indicators can also be computed in the same way using the output of our program. We discuss several examples in Sec. 4.3.

2.4. Conventions

Let us summarize our conventions that are necessary to compare the output of our program with that of others. There are three sources of ambiguities that affect the $U(1)$ phase of the representation $U_k^{\alpha}(h)$: (i) the choice of representatives of $G$, (ii) the choice of the coordinates, and (iii) the choice of spin rotation matrices. Readers not interested in the details can skip to Sec. 3.

2.4.1. The choice of representatives of $G$

Although the number of elements of $G$ is infinite because of its translation subgroup, in the actual calculation, it is sufficient to discuss a finite number of elements by choosing one $g \in G$ for each $p_g$. This is because, if $g'$ differs from $g$ by its translation part (i.e., $p_{g'} = p_g$ and $t_{g'} = t_g + R$ for a lattice vector $R$), the little-group representation of $g'$ is simply given by $U_k(g') = U_k(g)e^{-ik\cdot R}$. The choice of $g$’s is not unique, and in our program, they are automatically selected by QUANTUM ESPRESSO based on the input file. The chosen elements of $G$ are stored in our output files: the list of $p_g$’s is in $pg.dat$ and the list of the corresponding $t_g$’s is in $tg.dat$.

2.4.2. The choice of the coordinates

When using QUANTUM ESPRESSO, one needs to prepare an input file that contains the information of the coordinates of atomic positions. In QUANTUM ESPRESSO, the fixed point of point group symmetries is always set to $(0,0,0)$, and the input file must be carefully prepared. For a given material, even after fixing the symmetry operation, there can still be multiple choices of the coordinates, and the irreducible representations can in general be affected by this choice. In our examples discussed in Sec. 4, the information of the chosen coordinates is stored in the input file named $\.scf.in$.

To see this subtlety through a simple example, let us consider the inversion symmetric 1D system illustrated in Fig. 1. In this model, there are two atoms $A$ and $B$ in a unit cell. In the panel (a), the atom $A$ is placed at the origin and the coordinate of the atom $B$ is $x = \frac{1}{2}$. In the panel (b), the atom $B$ is placed at the origin and the coordinate of the atom $A$ is $x = \frac{1}{2}$. This is the ambiguity of the coordinates mentioned above. In both cases, the inversion symmetry is about the origin $x = 0$, but the atom at the fixed point is different. This means that the inversion in (a) and that in (b) are physically different operations. As a consequence, their representations are not the same and are related by $U_k^{\alpha}(I)^{(a)} = e^{ikx}U_k^{\alpha}(I)^{(b)}$. 

4
2.4.3. The choice of the spin rotation

As is well-known, the correspondence between a point group $p_g \in O(3)$ and the spin rotation $p^{sp}_g \in SU(2)$ has a sign ambiguity. Namely, when $p^{sp}_g$ denotes a spin rotation corresponding to the point group $p_g$, $-p^{sp}_g$ is also an equally valid choice of the spin rotation. For a given choice of $p^{sp}_g$ for all $p_g$'s, the projective factor in Eq. (5) is determined by

$$p^{sp}_g p^{sp}_{g'} = \omega^{sp}(g, g')p^{sp}_{g'}.$$  \hspace{1cm} (9)

In our program, the information of $p^{sp}_g$ and $\omega^{sp}(g, g')$ are stored, respectively, in srg.dat and factor_system_spin.dat.

3. Installation and usage

Here we explain how to install and use qeirreps. The flowchart of the calculations is shown in Fig. 2.

3.1. Compiling environment for qeirreps

A Fortran 90 compiler, BLAS, and LAPACK libraries are required for the installation of qeirreps. Quantum ESPRESSO must also be installed in advance. The version of Quantum ESPRESSO must be qe-6.3 or before. \footnote{This is because qe2respack does not support the later version of Quantum ESPRESSO. In future updates, we will propose our own interface between Quantum ESPRESSO and qeirreps instead of qe2respack to solve this limitation.} To obtain old-formatted output files, Quantum ESPRESSO must be compiled with the following option:

\$ ./configure --enable-xml=no \.

In addition, the program qe2respack \cite{66} \footnote{This program qe2respack is the part of the program package RESPACK \cite{66}. For the latest version of RESPACK, qe2respack does not support DFT calculations with spin-orbit coupling. For the usage of qeirreps, the specific version should be obtained as described in this section.} is required, which can be downloaded or cloned from the branch of respack “maxime2” in the GitHub repository (https://github.com/mnmpdadish/respackDev/). The program qe2respack is in the directory util/qe2respack. For installation, the file Makefile must be edited to specify the compiler, libraries, and the location of Quantum ESPRESSO in your compiling environment. By typing \$ make in the directory util/qe2respack, the executable binary qe2respack is compiled.
3.2. Installation of qeirreps

Our program qeirreps is released at GitHub (https://github.com/qeirreps/qeirreps). The program files which contain source files, documents, and examples can be cloned or downloaded from this repository. The file qeirreps/src/Makefile must be edited to specify the compiler and libraries in your compiling environment. By typing $ make in the source directory qeirreps/src/, the executable binary qeirreps.x is compiled.

3.3. Preparing input files of qeirreps

Our program qeirreps works based on the output of QUANTUM ESPRESSO. To prepare input files of qeirreps, the following three steps are needed to be done one by one:

1. Self-consistent first-principles (scf) calculation of a target material.
2. Non-self-consistent first-principles (nscf) calculation of the material for each high-symmetry momentum.
3. Data conversion from QUANTUM ESPRESSO output files to qeirreps input files.

The first two steps can be carried out by the standard functions of QUANTUM ESPRESSO. The result of the scf calculation is used in the successive nscf calculation. We refer to the directory that stores the wavefunction data computed by the nscf calculation OUTDIR/PREFIX.save below. For the moment, qeirreps requires norm-conserving calculations. Pseudo-potentials must be optimized for norm-conserving calculations [67] is available in PseudoDojo (http://www.pseudo-dojo.org) [68] and the option wf_collect should be set .TRUE. in the input files for DFT calculations.

The output files in OUTDIR/PREFIX.save must be converted by qe2respack into the form of input files of qeirreps. To do this, a directory named dir-wfn must be created in advance in the work directory. The work directory is referred to as DIRECTORY_NAME here. Then, type the following in the work directory:

```
$ PATH_OF_qe2respack/qe2respack OUTDIR/PREFIX.save
```

where PATH_OF_qe2respack is the path to the directory util/qe2respack. qeirreps reads the files produced by qe2respack in the dir-wfn directory.

3.4. Running qeirreps

To run qeirreps, a directory named output must be created in the directory DIRECTORY_NAME above. Then type

```
$ PATH_OF_qeirreps/qeirreps.x DIRECTORY_NAME
```

where PATH_OF_qeirreps is the path to the directory qeirreps/src. There should be ten output files in output. Five of them named *.dat contain the following information: (i) the list of the point group part p\_g in pg.dat, (ii) the list of the translation part t\_g in tg.dat, (iii) the list of the spin rotation part p\_sp\_g in srg.dat, (iv) the factor system \( \omega^{sp}(g,g') \) associated with the electronic spin in factor\_system\_spin.dat, and (v) the character tables of irreducible representations of Bloch wavefunctions in character.dat. Five of them named \_import.txt are the corresponding files for Mathematica usage. The standard output that appears during this calculation shows the lattice vectors, reciprocal lattice vectors, operation type of each symmetry operators, and so on.

For materials with inversion symmetry, qeirreps also implements the automatic evaluation of the \( Z_4 \) index. To do this, an option of filling should be added to the command as

```
$ PATH_OF_qeirreps/qeirreps.x DIRECTORY_NAME FILLING
```

Here, FILLING is the number of electrons per unit cell of the target material and is shown in the standard output of scf calculation by QUANTUM ESPRESSO as “number of electrons = FILLING.” Then, the program should generate an additional output named z4.dat that contains the value of the \( Z_4 \) index.
4. Examples

In this section, we discuss several examples to demonstrate the usage of qeirreps. We also explain how to compute topological indices based on the output of qeirreps.

4.1. Bismuth

Our first example is bismuth. The space group $R\bar{3}m$ (No.166) contains the inversion symmetry $I$. We obtain the crystal structure data of bismuth [Fig. 3 (a)] from Material Project [69] and converted it into the form of an input file for QUANTUM ESPRESSO (included in Appendix A.1) by SeeK-path [70, 71].

We compute the irreducible representations of wavefunctions by qeirreps, taking into account the spin-orbit coupling. Our results are shown in the band structure in Fig. 3 (b). The correspondence between the labels and characters of irreducible representations is included in Appendix B.1. These results are consistent with previous studies [47, 72].

---

3In this particular example, we manually shifted positions of atoms in the primitive unit cell so that we can compare our results with the one in Ref. [47]
We also compute the $Z_4$ index [64, 65] using the option explained in Sec. 3.4. The output (z4.dat) shows

\[
\text{sum of parities for 8 k-points:} \\
-7.99999999999963 \\
z4 \text{ index:} \\
2
\]

Namely, the $Z_4$ index for bismuth with the significant spin-orbit coupling is 2, indicating that this material is a higher-order topological insulator [73, 48, 47, 74]. The sample input files for bismuth are available in the directory qeirreps/example.

4.2. Silicon

To demonstrate that qeirreps equally works for nonsymmorphic space groups, let us discuss silicon. Its space group is $Fd\overline{3}m$ (No. 227), which also contains the inversion symmetry $I$. The calculation procedure is completely the same as those for bismuth in Sec. 4.1. Our results of irreducible representations are in Fig. 4 (b). The $Z_4$ index is found to be zero. These results are consistent with the previous study in Ref. [47]. Sample programs for silicon are also in the directory qeirreps/example.
Figure 3: (a) The crystal structure [69] and the Brillouin zone [70, 71] of bismuth. (b) The band structure of bismuth with spin-orbit coupling. $\bar{K}_\alpha(m)$ denotes a $m$-dimensional irreducible representation $U^\alpha_K$ at a high-symmetry point $K$. The correspondence between these labels and representation characters is included in Appendix B.1. The color of dots represents the inversion parity: when $K_{\alpha}(m)$ is marked red (blue), all $m$ levels have the even (odd) parity.

$^5$“H0” and “H2” are distinct momenta (i.e., their difference is not a reciprocal lattice vector) but they are related by a symmetry operation. The same is true for “S0” and “S2”.

---

\[ \text{Euler equation:} \quad \mathbf{K} \cdot \mathbf{E} = \mathbf{0} \]
Figure 4: (a) The crystal structure [69] and the Brillouin zone [70, 71] of silicon. (b) The band structure of silicon with spin-orbit coupling. $\bar{K}_\alpha(m)$ denotes a $m$-dimensional irreducible representation $U^\alpha_K$ at a high-symmetry point $K$. The correspondence between these labels and representation characters is included in Appendix B.3. The color of dots represents the inversion parity: when $\bar{K}_\alpha(m)$ is marked red (blue), all $m$ levels have the even (odd) parity, and when it is black, the half of them are even and the other half is odd. The little group at $W$ does not have the inversion symmetry and open circles represent the absence of the inversion symmetry.

4.3. $\text{PbPt}_3$

As our third example, let us discuss $\text{PbPt}_3$, whose space group $Pm\bar{3}m$ (No. 221). This space group contains various elements such as the inversion ($I$), the rotoinversion about the $z$-axis ($S^4_1$), and the mirror symmetries. We also assume the time-reversal symmetry. Our results of irreducible representations in the presence of the spin-orbit coupling are in Fig. 5 (b).

In this symmetry settings, we can define a $\mathbb{Z}_4$ index (other than the sum of the inversion parities) and a
Z_8 index by \[75, 64, 65\]

\[ z_4 = \frac{3}{2}n_R + \frac{1}{2}n_R + n_6^R + n_8^R - n_8^R + \frac{3}{2}n_X + \frac{3}{2}n_X - \frac{1}{2}n_X + \frac{1}{2}n_X \]

\[ z_8 = \frac{1}{4} \sum_{K \in \text{TRIMs}} \sum_{\alpha_K} \chi_K^{\alpha_K}(I)n_K^{\alpha_K} - \frac{1}{\sqrt{2}} \sum_{K' \in K_4} \sum_{\alpha_{K'}} \chi_{K'}^{\alpha_{K'}}(S_z^+ n_{K'}^{\alpha_{K'}} \mod 8, \quad (11) \]

where $n_{K'}^{\alpha_{K'}}$ represents the number of occupied states that have irreducible representations $U_{K'}^{\alpha_{K'}}$ of $G_K$, and the set of $\{n_{K'}^{\alpha_{K'}}\}$ is included in Appendix B.6. $K_4$ denotes four momenta invariant under the $S_z^+$. Although our program \texttt{qeirreps} does not offer an automated calculation of these indices, one can compute them manually using the output of our program. In this example, we find $(z_4, z_8) = (3, 6)$, which is consistent with Ref. [47]. According to Ref. [64, 65], these values indicate nontrivial mirror Chern numbers. Sample programs for PbPt$_3$ are included in \texttt{qeirreps/example}. 

11
5. Conclusions

In conclusion, we developed a new open-source code `qeirreps` for computing irreducible representations in band structures based on the output of Quantum ESPRESSO. We explained the installation of the program and demonstrated its usage through examples. When combined with the symmetry indicator method, the output of this program can be used to diagnose the topological property of weakly interacting materials. Since Quantum ESPRESSO is a free, widely-used software, `qeirreps` should accelerate the exploration of new topological materials.

Acknowledgement

We would like to thank Ryotaro Arita and Motoaki Hirayama for fruitful discussions. All DFT calculations in this work has been done using the facilities of the Supercomputer Center, the Institute for Solid
Appendix A. Samples of Quantum ESPRESSO input

Appendix A.1. For the scf calculation of bismuth

```espresso
&CONTROL
  calculation = 'scf',
  restart_mode = 'from_scratch',
  prefix = 'Bi',
  pseudo_dir = '/.../pseudo/soc/',
  outdir = './work/scf/',
  tstress = .true.,
  tprnfor = .true.,
  wf_collect = .true.,
/
&SYSTEM
  ibrav = 0
  nat = 2
  ntyp = 1
  ecutwfc = 100.
  occupations = 'smearing'
  smearing = 'm-p'
  degauss = 0.01
  use_all_frac = .true.,
  lspinorb = .true.,
  noncolin = .true.,
/
&ELECTRONS
  mixing_beta = 0.3
  conv_thr = 1.0d-8
/
ATOMIC_SPECIES
  Bi  208.9804 Bi.upf
ATOMIC_POSITIONS angstrom
  Bi  2.30479336 1.330673067 1.153637296
  Bi -0.00000000 -0.00000000 2.838187257
K_POINTS automatic
  8 8 8 0 0 0
CELL_PARAMETERS angstrom
  2.3047933600 1.3306730668 3.9918245533
  -2.3047933600 1.3306730668 3.9918245533
  0.0000000000 -2.6613461336 3.9918245533
```

Appendix A.2. For the nscf calculation of bismuth

```espresso
&CONTROL
  calculation = 'bands',
  restart_mode = 'from_scratch',
  prefix = 'Bi',
  pseudo_dir = '/.../pseudo/soc/',
  outdir = './work/rep/',
  tstress = .true.,
  tprnfor = .true.,
  wf_collect = .true.,
/
&SYSTEM
  ibrav = 0
  nat = 2
```

State Physics, the University of Tokyo. The work of AM and SO is supported by Materials Education program for the future leaders in Research, Industry, and Technology (MERIT). SO is also supported by the ANRI Fellowship and JSPS KAKENHI Grant No. JP20J21692. The work of YN is supported by JSPS KAKENHI Grant No. 16H06345, 17K14336, 18H01158, 20K14423. The work of HW is supported by JSPS KAKENHI Grant No. JP17K17678 and by JST PRESTO Grant No. JPMJPR18LA.
Appendix A.3. For the scf calculation of silicon

&CONTROL
   calculation = 'scf',
   restart_mode = 'from_scratch',
   prefix = 'Si',
   pseudo_dir = 'pseudo/scf',
   outdir = '/work/scf',
   tstress = true,
   tprnfor = true,
   wf_collect = true.
/
&SYSTEM
   ibrav = 0
   nat = 2
   ntyp = 1
   ecutwfc = 100.
   occupations = 'smearing'
   smearing = 'm-p'
   degauss = 0.01
   use_all_frac = true,
   lspinorb = true,
   noncolin = true.
/
&ELECTRONS
   mixing_beta = 0.3
   conv_thr = 1.0d-8
/
ATOMIC_SPECIES
   Si 28.0855 Si.upf
ATOMIC_POSITIONS crystal
   Si 0.625 0.625 0.625
Si 0.375 0.375 0.375
K_POINTS automatic
8 8 8 0 0 0
CELL_PARAMETERS angstrom
0.0000000000 2.7347724300 2.7347724300
2.7347724300 0.0000000000 2.7347724300
2.7347724300 2.7347724300 0.0000000000

Appendix A.4. For the nscf calculation of silicon

&CONTROL
  calculation = 'bands',
  restart_mode = 'from_scratch',
  prefix = 'Si',
  pseudo_dir = '/.../pseudo/soc',
  outdir = '/work/rep/',
  tstress = true,
  tprnfor = true,
  wf_collect = true.
/
&SYSTEM
  ibrav = 0
  nat = 2
  ntyp = 1
  ecutwfc = 100.
  occupations = 'smearing'
  smearing = 'm-p'
  degauss = 0.01
  use_all_frac = true,
  lspinorb = true,
  noncolin = true.
/
&ELECTRONS
  mixing_beta = 0.3
  conv_thr = 1.0d-8
/
ATOMIC_SPECIES
Si 28.0855 Si.upf
ATOMIC_POSITIONS crystal
Si 0.625 0.625 0.625
Si 0.375 0.375 0.375
K_POINTS crystal
8
0.0 0.0 0.0 1
0.5 0.0 0.0 1
0.0 0.5 0.0 1
0.0 0.0 0.5 1
0.0 0.5 0.5 1
0.5 0.0 0.5 1
0.5 0.5 0.0 1
0.5 0.5 0.5 1
CELL_PARAMETERS angstrom
0.0000000000 2.7347724300 2.7347724300
2.7347724300 0.0000000000 2.7347724300
2.7347724300 2.7347724300 0.0000000000

Appendix A.5. For the scf calculation of PbPt₃

&CONTROL
  calculation = 'scf',
  restart_mode = 'from_scratch',
  prefix = 'PbPt3',
  pseudo_dir = '/.../pseudo/soc/',
  outdir = '/work/scf/',
  tstress = true,
  tprnfor = true.
/

Appendix A.6. For the nscf calculation of PbPt$_3$

&CONTROL
  calculation = 'bands',
  restart_mode = 'from_scratch',
  prefix = 'PbPt3',
  pseudo_dir = '/.../pseudo/soc/',
  outdir = '/work/rep',
  tstress = .true.,
  tprnfor = .true.,
  wf_collect = .true.
/
&SYSTEM
  ibrav = 0
  nat = 4
  ntyp = 2
  ecutwfc = 100.
  occupations = 'smearing'
  smearing = 'm-p'
  degauss = 0.01
  use_all_frac = .true.
  lspinorb = .true.
  noncolin = .true.
/
&ELECTRONS
  mixing_beta = 0.3
  conv_thr = 1.0d-8
/
ATOMIC_SPECIES
  Pt 195.084 Pt.upf
  Pb 207.2 Pb.upf
/
ATOMIC_POSITIONS angstrom
  Pt 0.0000000000 2.0660527150 2.0660527150
  Pt 2.0660527150 0.0000000000 2.0660527150
  Pt 2.0660527150 2.0660527150 0.0000000000
  Pb 0.0000000000 0.0000000000 0.0000000000
/
CELL_PARAMETERS angstrom
  4.1321054300 0.0000000000 0.0000000000
  0.0000000000 4.1321054300 0.0000000000
  0.0000000000 0.0000000000 4.1321054300
Appendix A.6. For the nscf calculation of PbPt$_3$
Appendix B. Information of irreducible representations

Appendix B.1. Character tables for bismuth

|   | \(\Gamma_4\) | \(\Gamma_5\) | \(\Gamma_6\) | \(\Gamma_7\) | \(\Gamma_8\) | \(\Gamma_9\) |
|---|---|---|---|---|---|---|
| 1 | 1 | 1 | 1 | 1 | 2 | 2 |
| \(3_{001}\) | -1 | -1 | -1 | -1 | 1 | 1 |
| \(3_{001}\) | -1 | -1 | -1 | -1 | 1 | 1 |
| \(2_{110}\) | -i | i | -i | i | 0 | 0 |
| \(2_{100}\) | i | -i | i | -i | 0 | 0 |
| \(2_{010}\) | -i | i | -i | i | 0 | 0 |
| \(I\) | 1 | 1 | -1 | -1 | 2 | -2 |
| \(I\) | 1 | 1 | -1 | -1 | 2 | -2 |

|   | \(L_3\) | \(L_4\) | \(L_5\) | \(L_6\) |
|---|---|---|---|---|
| 1 | 1 | 1 | 1 | 1 |
| \(2_{110}\) | -i | i | -i | i |
| \(I\) | 1 | 1 | -1 | -1 |
| \(2_{110}\) | -i | i | -i | -i |

|   | \(F_3\) | \(F_4\) | \(F_5\) | \(F_6\) |
|---|---|---|---|---|
| 1 | 1 | 1 | 1 | 1 |
| \(2_{110}\) | -i | i | -i | i |
| \(I\) | 1 | 1 | -1 | -1 |
| \(2_{110}\) | -i | i | i | -i |
\[
\begin{array}{ccccccc}
T_4 & T_5 & T_6 & T_7 & T_8 & T_9 \\
1 & 1 & 1 & 1 & 2 & 2 \\
3_{001} & -1 & -1 & -1 & -1 & 1 & 1 \\
3_{001} & -1 & -1 & -1 & -1 & 1 & 1 \\
2_{110} & -i & i & -i & i & 0 & 0 \\
2_{100} & i & -i & i & -i & 0 & 0 \\
2_{010} & -i & i & -i & i & 0 & 0 \\
I & 1 & 1 & -1 & -1 & 2 & -2 \\
I_{3_{001}} & -1 & -1 & 1 & 1 & 1 & -1 \\
I_{3_{001}} & -1 & -1 & 1 & 1 & 1 & -1 \\
I_{2_{110}} & -i & i & -i & 0 & 0 \\
I_{2_{100}} & i & -i & -i & i & 0 & 0 \\
I_{2_{010}} & -i & i & -i & 0 & 0 \\
\end{array}
\]

\[
\begin{array}{cc}
H_3 & H_4 \\
1 & 1 \\
2_{110} & -i & i \\
\end{array}
\]

\[
\begin{array}{cc}
M_3 & M_4 \\
1 & 1 \\
m_{110} & -i & i \\
\end{array}
\]

\[
\begin{array}{cc}
S_3 & S_4 \\
1 & 1 \\
2_{110} & -i & i \\
\end{array}
\]
### Appendix B.2. The number of irreducible representations for bismuth

| $\nu$ | 30 |
|-------|----|
| $n_{1\Gamma}$ | 3 |
| $n_{1\Sigma}$ | 3 |
| $n_{2\Sigma}$ | 2 |
| $n_{3\Sigma}$ | 2 |
| $n_{6\Gamma}$ | 6 |
| $n_{7\Gamma}$ | 4 |
| $n_{7\Sigma}$ | 7 |
| $n_{8\Sigma}$ | 8 |
| $n_{8\Pi}$ | 8 |
| $n_{9\Pi}$ | 8 |
| $n_{9\Sigma}$ | 8 |
| $n_{10\Sigma}$ | 2 |
| $n_{10\Pi}$ | 2 |
| $n_{11\Pi}$ | 3 |
| $n_{11\Sigma}$ | 3 |
| $n_{12\Gamma}$ | 5 |
| $n_{12\Pi}$ | 5 |
Appendix B.3. Character tables for silicon

| \{\Gamma_0, \Gamma_7\} | \Gamma_5 | \Gamma_8 | \Gamma_9 | \Gamma_{10} | \Gamma_{11} |
|----------------------|---------|---------|---------|-----------|-----------|
| \{1,0,0\}            | 2       | 2       | 2       | 2         | 4         |
| \{200,0,0,0\}        | 0       | 0       | 0       | 0         | 0         |
| \{200,0,0,0\}        | 0       | 0       | 0       | 0         | 0         |
| \{200,0,0,0\}        | 0       | 0       | 0       | 0         | 0         |
| \{312,0,0\}          | 1       | 1       | 1       | 1         | -1 -1     |
| \{312,0,0,0\}        | 1       | 1       | 1       | 1         | -1 -1     |
| \{312,0,0,0\}        | 1       | 1       | 1       | 1         | -1 -1     |
| \{312,0,0,0\}        | 1       | 1       | 1       | 1         | -1 -1     |
| \{312,0,0,0\}        | 1       | 1       | 1       | 1         | -1 -1     |
| \{312,0,0,0\}        | 1       | 1       | 1       | 1         | -1 -1     |
| \{312,0,0,0\}        | 1       | 1       | 1       | 1         | -1 -1     |
| \{210,0,0,0\}        | 0       | 0       | 0       | 0         | 0         |
| \{210,0,0,0\}        | 0       | 0       | 0       | 0         | 0         |
| \{210,0,0,0\}        | 0       | 0       | 0       | 0         | 0         |
| \{400,0,0,0\}        | \sqrt{2} | -\sqrt{2} | \sqrt{2} | -\sqrt{2} | 0         |
| \{400,0,0,0\}        | \sqrt{2} | -\sqrt{2} | \sqrt{2} | -\sqrt{2} | 0         |
| \{400,0,0,0\}        | \sqrt{2} | -\sqrt{2} | \sqrt{2} | -\sqrt{2} | 0         |
| \{400,0,0,0\}        | \sqrt{2} | -\sqrt{2} | \sqrt{2} | -\sqrt{2} | 0         |
| \{400,0,0,0\}        | \sqrt{2} | -\sqrt{2} | \sqrt{2} | -\sqrt{2} | 0         |
| \{400,0,0,0\}        | \sqrt{2} | -\sqrt{2} | \sqrt{2} | -\sqrt{2} | 0         |
| \{400,0,0,0\}        | \sqrt{2} | -\sqrt{2} | \sqrt{2} | -\sqrt{2} | 0         |
| \{210,0,0,0\}        | 0       | 0       | 0       | 0         | 0         |
| \{210,0,0,0\}        | 0       | 0       | 0       | 0         | 0         |
| \{210,0,0,0\}        | 0       | 0       | 0       | 0         | 0         |
| \{400,0,0,0\}        | \sqrt{2} | -\sqrt{2} | \sqrt{2} | -\sqrt{2} | 0         |
| \{400,0,0,0\}        | \sqrt{2} | -\sqrt{2} | \sqrt{2} | -\sqrt{2} | 0         |
| \{400,0,0,0\}        | \sqrt{2} | -\sqrt{2} | \sqrt{2} | -\sqrt{2} | 0         |
| \{400,0,0,0\}        | \sqrt{2} | -\sqrt{2} | \sqrt{2} | -\sqrt{2} | 0         |
| \{400,0,0,0\}        | \sqrt{2} | -\sqrt{2} | \sqrt{2} | -\sqrt{2} | 0         |
| \{400,0,0,0\}        | \sqrt{2} | -\sqrt{2} | \sqrt{2} | -\sqrt{2} | 0         |
| \{400,0,0,0\}        | \sqrt{2} | -\sqrt{2} | \sqrt{2} | -\sqrt{2} | 0         |
\[ \begin{array}{cccccc}
| & L_4 & L_5 & L_6 & L_7 & L_8 & L_9 \\
\{1|0,0,0\} & 1 & 1 & 1 & 1 & 2 & 2 \\
\{3|_{111}\} & -1 & -1 & -1 & -1 & 1 & 1 \\
\{3|_{111}\} & -1 & -1 & -1 & -1 & 1 & 1 \\
\{2|_{110}\} & -i & i & -i & i & 0 & 0 \\
\{2|_{011}\} & -i & i & -i & i & 0 & 0 \\
\{2|_{011}\} & -i & i & -i & i & 0 & 0 \\
\{I|0,0,0\} & 1 & 1 & -1 & -1 & 2 & -2 \\
\{I|3_{111}\} & -1 & -1 & 1 & 1 & 1 & -1 \\
\{I|3_{111}\} & -1 & -1 & 1 & 1 & 1 & -1 \\
\{I|2_{110}\} & -i & i & -i & 0 & 0 \\
\{I|2_{011}\} & -i & i & -i & 0 & 0 \\
\{I|2_{011}\} & -i & i & -i & 0 & 0 \\
\end{array} \]

\[ \begin{array}{c}
\chi_5 \\
| & 4 \\
\{1|0,0,0\} & 4 \\
\{2|_{010}\} & 0 \\
\{2|_{010}\} & 0 \\
\{2|_{100}\} & 0 \\
\{4|_{010}\} & 0 \\
\{4|_{010}\} & 0 \\
\{4|_{010}\} & 0 \\
\{4|_{010}\} & 0 \\
\{4|_{010}\} & 0 \\
\{I|0,0,0\} & 0 \\
\{I|2_{010}\} & 0 \\
\{I|2_{010}\} & 0 \\
\{I|2_{010}\} & 0 \\
\{I|2_{010}\} & 0 \\
\{I|2_{010}\} & 0 \\
\{I|2_{010}\} & 0 \\
\end{array} \]

\[ \begin{array}{cccccc}
| & W_3 & W_4 & W_5 & W_6 & W_7 \\
\{1|0,0,0\} & 1 & 1 & 1 & 1 & 2 \\
\{2|_{100} - 1/2,0,0\} & -i & -i & -i & -i & 2i \\
\{2|_{101} 1/2,0,0\} & i & -i & i & -i & 0 \\
\{2|_{011} 0,0,0\} & e^{i\pi/4} & e^{-i\pi/4} & e^{-i\pi/4} & e^{i\pi/4} & 0 \\
\{I|2_{001} 0,0,1/2\} & e^{-i\pi/4} & e^{i\pi/4} & e^{i\pi/4} & e^{-i\pi/4} & 0 \\
\{I|2_{010} 1/2,0,0\} & e^{-i\pi/4} & e^{i\pi/4} & e^{i\pi/4} & e^{-i\pi/4} & 0 \\
\{I|2_{001} 0,0,-1/2\} & e^{i3\pi/4} & e^{-i\pi/4} & e^{-i\pi/4} & 0 \\
\{I|2_{001} 0,0,-1/2\} & e^{-i3\pi/4} & e^{i\pi/4} & e^{i\pi/4} & 0 \\
\{I|2_{001} 0,0,-1/2\} & e^{-i3\pi/4} & e^{i\pi/4} & e^{i\pi/4} & 0 \\
\end{array} \]
### Appendix B.4. Irreducible representations of silicon

| \( \nu \) | 8 |
|---|---|
| \( n_{\mathbb{G}}^8 \) | 1 |
| \( n_{\mathbb{L}}^8 \) | 1 |
| \( n_{\pi}^8 \) | 0 |
| \( n_{\mathbb{W}}^8 \) | 0 |
| \( n_{\pi}^0 \) | 1 |
| \( n_{\pi}^1 \) | 0 |
| \( n_{\mathbb{G}}^0 \) | 1 |
| \( n_{\mathbb{L}}^0 \) | 1 |
| \( n_{\pi}^0 \) | 0 |
| \( n_{\mathbb{W}}^0 \) | 0 |
| \( n_{\pi}^2 \) | 2 |
| \( n_{\pi}^4 \) | 1 |
| \( n_{\mathbb{W}}^2 \) | 1 |
| \( n_{\mathbb{W}}^1 \) | 1 |
| \( n_{\mathbb{W}}^1 \) | 1 |
| \( n_{\mathbb{W}}^1 \) | 1 |
| \( n_{\mathbb{W}}^2 \) | 2 |
### Appendix B.5. Character table for PbPt$_3$

|   | $\Gamma_6$ | $\Gamma_7$ | $\Gamma_8$ | $\Gamma_9$ | $\Gamma_{10}$ | $\Gamma_{11}$ |
|---|------------|------------|------------|------------|--------------|--------------|
| 1 | 1          | 1          | 2          | 2          | 2            | 4            |
| 2001 | 0          | 0          | 0          | 0          | 0            | 0            |
| 2010 | 0          | 0          | 0          | 0          | 0            | 0            |
| 2100 | 0          | 0          | 0          | 0          | 0            | 0            |
| 2110 | 1          | 1          | 1          | 1          | 1            | 1            |
| 3111 | 1          | 1          | 1          | 1          | 1            | 1            |
| 3111 | 1          | 1          | 1          | 1          | 1            | 1            |
| 3111 | 1          | 1          | 1          | 1          | 1            | 1            |
| 3111 | 1          | 1          | 1          | 1          | 1            | 1            |
| 2110 | 0          | 0          | 0          | 0          | 0            | 0            |
| 2100 | 0          | 0          | 0          | 0          | 0            | 0            |
| 4001 | $\sqrt{2}$ | $-\sqrt{2}$ | $\sqrt{2}$ | $-\sqrt{2}$ | 0            | 0            |
| 4010 | $\sqrt{2}$ | $-\sqrt{2}$ | $\sqrt{2}$ | $-\sqrt{2}$ | 0            | 0            |
| 4100 | $\sqrt{2}$ | $-\sqrt{2}$ | $\sqrt{2}$ | $-\sqrt{2}$ | 0            | 0            |
| 2011 | 0          | 0          | 0          | 0          | 0            | 0            |
| 2011 | 0          | 0          | 0          | 0          | 0            | 0            |
| 4100 | $\sqrt{2}$ | $-\sqrt{2}$ | $\sqrt{2}$ | $-\sqrt{2}$ | 0            | 0            |
| 4010 | $\sqrt{2}$ | $-\sqrt{2}$ | $\sqrt{2}$ | $-\sqrt{2}$ | 0            | 0            |
| 2100 | 0          | 0          | 0          | 0          | 0            | 0            |
| 2010 | 0          | 0          | 0          | 0          | 0            | 0            |
| $T$ | 2          | 2          | $-2$       | $-2$       | 4            | 4            |
| 12001 | 0          | 0          | 0          | 0          | 0            | 0            |
| 12001 | 0          | 0          | 0          | 0          | 0            | 0            |
| 13110 | 0          | 0          | 0          | 0          | 0            | 0            |
| 13110 | 1          | 1          | $-1$       | $-1$       | $-1$         | $-1$         |
| 13110 | 1          | 1          | $-1$       | $-1$       | $-1$         | $-1$         |
| 13110 | 1          | 1          | $-1$       | $-1$       | $-1$         | $-1$         |
| 13110 | 1          | 1          | $-1$       | $-1$       | $-1$         | $-1$         |
| 13110 | 1          | 1          | $-1$       | $-1$       | $-1$         | $-1$         |
| 13110 | 1          | 1          | $-1$       | $-1$       | $-1$         | $-1$         |
| 12110 | 0          | 0          | 0          | 0          | 0            | 0            |
| 12110 | 0          | 0          | 0          | 0          | 0            | 0            |
| 14001 | $\sqrt{2}$ | $-\sqrt{2}$ | $-\sqrt{2}$ | $\sqrt{2}$ | 0            | 0            |
| 14001 | $\sqrt{2}$ | $-\sqrt{2}$ | $-\sqrt{2}$ | $\sqrt{2}$ | 0            | 0            |
| 14001 | $\sqrt{2}$ | $-\sqrt{2}$ | $-\sqrt{2}$ | $\sqrt{2}$ | 0            | 0            |
| 12011 | 0          | 0          | 0          | 0          | 0            | 0            |
| 13011 | 0          | 0          | 0          | 0          | 0            | 0            |
| 14001 | $\sqrt{2}$ | $-\sqrt{2}$ | $-\sqrt{2}$ | $\sqrt{2}$ | 0            | 0            |
| 14001 | $\sqrt{2}$ | $-\sqrt{2}$ | $-\sqrt{2}$ | $\sqrt{2}$ | 0            | 0            |
| 14001 | $\sqrt{2}$ | $-\sqrt{2}$ | $-\sqrt{2}$ | $\sqrt{2}$ | 0            | 0            |
| 12011 | 0          | 0          | 0          | 0          | 0            | 0            |
| 13011 | 0          | 0          | 0          | 0          | 0            | 0            |
| 12011 | 0          | 0          | 0          | 0          | 0            | 0            |
| 13011 | 0          | 0          | 0          | 0          | 0            | 0            |
| 12011 | 0          | 0          | 0          | 0          | 0            | 0            |
| 13011 | 0          | 0          | 0          | 0          | 0            | 0            |
|     | $M_6$ | $M_7$ | $M_8$ | $M_9$ |
|-----|-------|-------|-------|-------|
| 1   | 2     | 2     | 2     | 2     |
| $2_{001}$ | 0     | 0     | 0     | 0     |
| $2_{010}$ | 0     | 0     | 0     | 0     |
| $2_{100}$ | 0     | 0     | 0     | 0     |
| $2_{110}$ | 0     | 0     | 0     | 0     |
| $4_{001}$ | $-\sqrt{2}$ | $\sqrt{2}$ | $-\sqrt{2}$ | $\sqrt{2}$ |
| $4_{001}$ | $-\sqrt{2}$ | $\sqrt{2}$ | $-\sqrt{2}$ | $\sqrt{2}$ |
| $I$ | 2     | 2     | $-2$  | $-2$  |
| $I_{2001}$ | 0     | 0     | 0     | 0     |
| $I_{2010}$ | 0     | 0     | 0     | 0     |
| $I_{2100}$ | 0     | 0     | 0     | 0     |
| $I_{2110}$ | 0     | 0     | 0     | 0     |
| $I_{4001}$ | $-\sqrt{2}$ | $\sqrt{2}$ | $\sqrt{2}$ | $-\sqrt{2}$ |
| $I_{4001}$ | $-\sqrt{2}$ | $\sqrt{2}$ | $\sqrt{2}$ | $-\sqrt{2}$ |
|    | $R_6$ | $R_7$ | $R_8$ | $R_9$ | $R_{10}$ | $R_{11}$ |
|----|------|------|------|------|--------|--------|
| 1  | 2    | 2    | 2    | 2    | 4      | 4      |
| $2_{001}$ | 0  | 0    | 0    | 0    | 0      | 0      |
| $2_{010}$ | 0  | 0    | 0    | 0    | 0      | 0      |
| $2_{100}$ | 0  | 0    | 0    | 0    | 0      | 0      |
| $3_{111}$ | 1  | 1    | 1    | 1    | -1     | -1     |
| $3_{111}^+$ | 1  | 1    | 1    | 1    | -1     | -1     |
| $3_{111}^+$ | 1  | 1    | 1    | 1    | -1     | -1     |
| $3_{111}^+$ | 1  | 1    | 1    | 1    | -1     | -1     |
| $3_{111}^+$ | 1  | 1    | 1    | 1    | -1     | -1     |
| $3_{111}^+$ | 1  | 1    | 1    | 1    | -1     | -1     |
| $3_{111}^+$ | 1  | 1    | 1    | 1    | -1     | -1     |
| $3_{111}^+$ | 1  | 1    | 1    | 1    | -1     | -1     |
| $3_{111}^+$ | 1  | 1    | 1    | 1    | -1     | -1     |
| $2_{101}$ | 0  | 0    | 0    | 0    | 0      | 0      |
| $2_{110}$ | 0  | 0    | 0    | 0    | 0      | 0      |
| $4_{001}$ | $\sqrt{2}$ | $-\sqrt{2}$ | $\sqrt{2}$ | $-\sqrt{2}$ | 0      | 0      |
| $4_{001}^+$ | $\sqrt{2}$ | $-\sqrt{2}$ | $\sqrt{2}$ | $-\sqrt{2}$ | 0      | 0      |
| $4_{001}^+$ | $\sqrt{2}$ | $-\sqrt{2}$ | $\sqrt{2}$ | $-\sqrt{2}$ | 0      | 0      |
| $4_{010}$ | $\sqrt{2}$ | $-\sqrt{2}$ | $\sqrt{2}$ | $-\sqrt{2}$ | 0      | 0      |
| $2_{011}$ | 0  | 0    | 0    | 0    | 0      | 0      |
| $2_{011}$ | 0  | 0    | 0    | 0    | 0      | 0      |
| $4_{010}$ | $\sqrt{2}$ | $-\sqrt{2}$ | $\sqrt{2}$ | $-\sqrt{2}$ | 0      | 0      |
| $4_{010}$ | $\sqrt{2}$ | $-\sqrt{2}$ | $\sqrt{2}$ | $-\sqrt{2}$ | 0      | 0      |
| $2_{101}$ | 0  | 0    | 0    | 0    | 0      | 0      |
| $2_{101}$ | 0  | 0    | 0    | 0    | 0      | 0      |
| $T_{2001}$ | 0  | 0    | 0    | 0    | 0      | 0      |
| $T_{2010}$ | 0  | 0    | 0    | 0    | 0      | 0      |
| $T_{2100}$ | 0  | 0    | 0    | 0    | 0      | 0      |
| $1_{3111}$ | 1  | 1    | -1   | -1   | -1     | 1      |
| $1_{3111}^+$ | 1  | 1    | -1   | -1   | -1     | 1      |
| $1_{3111}^+$ | 1  | 1    | -1   | -1   | -1     | 1      |
| $1_{3111}^+$ | 1  | 1    | -1   | -1   | -1     | 1      |
| $1_{3111}^+$ | 1  | 1    | -1   | -1   | -1     | 1      |
| $1_{3111}$ | 1  | 1    | -1   | -1   | -1     | 1      |
| $1_{3111}^+$ | 1  | 1    | -1   | -1   | -1     | 1      |
| $1_{3111}^+$ | 1  | 1    | -1   | -1   | -1     | 1      |
| $1_{3111}^+$ | 1  | 1    | -1   | -1   | -1     | 1      |
| $1_{3111}^+$ | 1  | 1    | -1   | -1   | -1     | 1      |
| $1_{3111}$ | 1  | 1    | -1   | -1   | -1     | 1      |
| $T_{2110}$ | 0  | 0    | 0    | 0    | 0      | 0      |
| $T_{2110}$ | 0  | 0    | 0    | 0    | 0      | 0      |
| $I_{3001}$ | $\sqrt{2}$ | $\sqrt{2}$ | $\sqrt{2}$ | $\sqrt{2}$ | 0      | 0      |
| $I_{3001}^+$ | $\sqrt{2}$ | $\sqrt{2}$ | $\sqrt{2}$ | $\sqrt{2}$ | 0      | 0      |
| $I_{3001}^+$ | $\sqrt{2}$ | $\sqrt{2}$ | $\sqrt{2}$ | $\sqrt{2}$ | 0      | 0      |
| $I_{3001}^+$ | $\sqrt{2}$ | $\sqrt{2}$ | $\sqrt{2}$ | $\sqrt{2}$ | 0      | 0      |
| $I_{3011}$ | 0  | 0    | 0    | 0    | 0      | 0      |
| $I_{3011}$ | 0  | 0    | 0    | 0    | 0      | 0      |
| $I_{4001}$ | $\sqrt{2}$ | $-\sqrt{2}$ | $\sqrt{2}$ | $-\sqrt{2}$ | 0      | 0      |
| $I_{4001}$ | $\sqrt{2}$ | $-\sqrt{2}$ | $\sqrt{2}$ | $-\sqrt{2}$ | 0      | 0      |
| $I_{4001}$ | $\sqrt{2}$ | $-\sqrt{2}$ | $\sqrt{2}$ | $-\sqrt{2}$ | 0      | 0      |
| $I_{4010}$ | $\sqrt{2}$ | $-\sqrt{2}$ | $\sqrt{2}$ | $-\sqrt{2}$ | 0      | 0      |
| $I_{4010}$ | $\sqrt{2}$ | $-\sqrt{2}$ | $\sqrt{2}$ | $-\sqrt{2}$ | 0      | 0      |
| $I_{4010}$ | $\sqrt{2}$ | $-\sqrt{2}$ | $\sqrt{2}$ | $-\sqrt{2}$ | 0      | 0      |
| $I_{4010}$ | $\sqrt{2}$ | $-\sqrt{2}$ | $\sqrt{2}$ | $-\sqrt{2}$ | 0      | 0      |
| $I_{4010}$ | $\sqrt{2}$ | $-\sqrt{2}$ | $\sqrt{2}$ | $-\sqrt{2}$ | 0      | 0      |
Appendix B.6. Irreducible representations of PbPt$_3$

| $\nu$ | 68 |
|-------|---|
| $n^g_x$ | 4 |
| $n^g_y$ | 4 |
| $n^g_z$ | 3 |
| $n^g_{\bar{z}}$ | 1 |
| $n^g_{\bar{x}}$ | 7 |
| $n^g_{\bar{y}}$ | 4 |
| $n^e_M$ | 10 |
| $n^e_R$ | 9 |
| $n^e_{\bar{R}}$ | 8 |
| $n^e_{\bar{M}}$ | 7 |
| $n^e_{\bar{X}}$ | 3 |
| $n^e_{\bar{Y}}$ | 4 |
| $n^e_{\bar{Z}}$ | 2 |
| $n^e_{\bar{Y}}$ | 3 |
| $n^e_{\bar{Z}}$ | 7 |
| $n^e_{\bar{Y}}$ | 4 |
| $n^e_X$ | 9 |
| $n^e_Y$ | 9 |
| $n^e_Z$ | 7 |

References

[1] W. Kohn and L. J. Sham, Phys. Rev. 140, A1133 (1965).
[2] C. L. Kane and E. J. Mele, Phys. Rev. Lett. 95, 146802 (2005).
[3] C. L. Kane and E. J. Mele, Phys. Rev. Lett. 95, 226801 (2005).
[4] B. A. Bernevig, T. L. Hughes, and S.-C. Zhang, Science 314, 1757 (2006).
5. M. König, S. Wiedmann, C. Brüne, A. Roth, H. Buhmann, L. W. Molenkamp, X.-L. Qi, and S.-C. Zhang, Science 318, 766 (2007).
6. L. Fu and C. L. Kane, Phys. Rev. B 74, 195312 (2006).
7. L. Fu, C. L. Kane, and E. J. Mele, Phys. Rev. Lett. 98, 106803 (2007).
8. J. E. Moore and L. Balents, Phys. Rev. B 75, 121306 (2007).
9. L. Fu and C. L. Kane, Phys. Rev. B 76, 045302 (2007).
10. D. Hsieh, D. Qian, L. Wray, Y. Xia, Y. S. Hor, R. J. Cava, and M. Z. Hasan, Nature 452, 970 (2008).
11. C. Liu, T. L. Hughes, X.-L. Qi, K. Wang, and S.-C. Zhang, Phys. Rev. Lett. 100, 236601 (2008).
12. X.-L. Qi, T. L. Hughes, and S.-C. Zhang, Phys. Rev. B 78, 195424 (2008).
13. D. Hsieh, Y. Xia, D. Qian, L. Wray, J. H. Dil, F. Meier, J. Osterwalder, L. Patthey, J. G. Checkelsky, N. P. Ong, A. V. Fedorov, H. Lin, A. Bansil, D. Grauer, Y. S. Hor, R. J. Cava, and M. Z. Hasan, Nature 460, 1101 (2009).
14. Y. Xia, D. Qian, D. Hsieh, L. Wray, A. Pal, H. Lin, A. Bansil, D. Grauer, Y. S. Hor, R. J. Cava, and M. Z. Hasan, Nature Physics 5, 598 (2009).
15. R. Roy, Phys. Rev. B 79, 195322 (2009).
16. R. Yu, W. Zhang, H.-J. Zhang, S.-C. Zhang, X. Dai, and Z. Fang, Science 329, 61 (2010).
17. I. Knez, R.-R. Du, and G. Sullivan, Phys. Rev. Lett. 107, 136603 (2011).
18. C.-Z. Chang, J. Zhang, X. Feng, J. Shen, Z. Zhang, M. Guo, K. Li, Y. Ou, P. Wei, L.-L. Wang, Z.-Q. Ji, Y. Feng, S. Ji, X. Chen, J. Jia, X. Dai, Z. Fang, S.-C. Zhang, K. He, Y. Wang, L. Lu, X.-C. Ma, and Q.-K. Xue, Science 340, 167 (2013).
19. A. P. Schnyder, S. Ryu, A. Furusaki, and A. W. W. Ludwig, Phys. Rev. B 78, 195125 (2008).
20. A. Kitaev, AIP Conference Proceedings 1134, 22 (2009).
21. S. Ryu, A. P. Schnyder, A. Furusaki, and A. W. W. Ludwig, New Journal of Physics 12, 065010 (2010).
22. D. S. Freed and G. W. Moore, Annales Henri Poincaré 14, 1927 (2013).
23. H. Song, S.-J. Huang, L. Fu, and M. Hermele, Phys. Rev. X 7, 011020 (2017).
24. J. Kruthoff, J. de Boer, J. van Wezel, C. L. Kane, and R.-J. Slager, Phys. Rev. X 7, 041069 (2017).
25. R. Thorngreen and D. V. Else, Phys. Rev. X 8, 011040 (2018).
26. S.-J. Huang, H. Song, X.-P. Huang, and M. Hermele, Phys. Rev. B 96, 205106 (2017).
27. K. Shiozaki, M. Sato, and K. Gomi, arXiv:1802.06894.
28. Z. Song, S.-J. Huang, Y. Qi, C. Fang, and M. Hermele, arXiv:1810.02330.
29. Y. Tanaka, Z. Ren, T. Sato, K. Nakayama, S. Souma, T. Takahashi, K. Segawa, and Y. Ando, Nature Physics 8, 800 (2012).
30. T. H. Hsieh, H. Lin, J. Liu, W. Duan, A. Bansil, and L. Fu, Nature Communications 3, 982 (2012).
31. F. Schindler, A. M. Cook, M. G. Vergniory, Z. Wang, S. S. P. Parkin, B. A. Bernevig, and T. Neupert, Science Advances 4, eaat0346 (2018).
32. Z. Song, Z. Fang, and C. Fang, Phys. Rev. Lett. 119, 246402 (2017).
33. W. A. Benalcazar, B. A. Bernevig, and T. L. Hughes, Science 357, 61 (2017).
34. W. A. Benalcazar, B. A. Bernevig, and T. L. Hughes, Phys. Rev. B 96, 245115 (2017).
35. A. Matsugatani and H. Watanabe, Phys. Rev. B 98, 205129 (2018).
36. L. Trifunovic and P. W. Brouwer, Phys. Rev. X 9, 011012 (2019).
37. C. Fang and L. Fu, Science Advances 5, eaat2374 (2019).
38. S. M. Young, S. Zaheer, J. C. Y. Teo, C. L. Kane, E. J. Mele, and A. M. Rappe, Phys. Rev. Lett. 108, 140405 (2012).
39. X. Wan, A. M. Turner, A. Vishwanath, and S. Y. Savrasov, Phys. Rev. B 83, 205101 (2011).
40. Z. Wang, A. Alexandradinata, R. J. Cava, and B. A. Bernevig, Nature 532, 189 (2016).
41. K. Shiozaki, M. Sato, and K. Gomi, Phys. Rev. B 91, 155120 (2015).
42. C. Fang and L. Fu, Phys. Rev. B 91, 161105 (2015).
43. H. C. Po, A. Vishwanath, and H. Watanabe, Nat. Commun. 8, 50 (2017).
44. F. Tang, H. C. Po, A. Vishwanath, and X. Wan, Nat. Phys. 15, 470 (2019).
45. F. Tang, H. C. Po, A. Vishwanath, and X. Wan, Sci. Adv. 5 (2019).
46. T. Zhang, Y. Jiang, Z. Song, H. Huang, Y. He, Z. Fang, H. Weng, and C. Fang, Nature 566, 475 (2019).
47. M. G. Vergniory, L. Elcoro, C. Felser, N. Regnault, B. A. Bernevig, and Z. Wang, Nature 566, 486 (2019).
48. H. Watanabe, H. C. Po, and A. Vishwanath, Sci. Adv. 4, eaat8685 (2018).
49. S. Ono and H. Watanabe, Phys. Rev. B 98, 115150 (2018).
50. S. Ono, Y. Yanase, and H. Watanabe, Phys. Rev. Res. 1, 013012 (2019).
51. A. Skurativskia, T. Neupert, and M. H. Fischer, Phys. Rev. Research 2, 013064 (2020).
52. K. Shiozaki, arXiv:1907.13632.
53. A. Ono, and H. Watanabe, Science Advances 6, eaaz3676 (2020).
54. M. Geier, P. W. Brouwer, and L. Trifunovic, (2019), arXiv:1910.11271.
55. J. Gao, Q. Wu, C. Persson, and Z. Wang, “It’s possible to get irreducible representations of electronic states in the VASP,” (2020), arXiv:2002.04302.
56. P. Blaha, K. Schwarz, G. K. H. Madsen, D. Kvasnicka, and J. Luitz, WIEN2K, An Augmented Plane Wave + Local Orbitals Program for Calculating Crystal Properties (Karlheinz Schwarz, Techn. Universität Wien, Austria, 2001).
57. G. Kresse and J. Furthmüller, Phys. Rev. B 54, 11169 (1996).
58. P. Giannozzi, S. Baroni, N. Bonini, M. Calandra, R. Car, C. Cavazzoni, D. Ceresoli, G. L. Chiarotti, M. Cococcioni, I. Dabo, A. D. Corso, S. de Gironcoli, S. Fabris, G. Fratesi, R. Gebauer, U. Gerstmann, C. Gougoussis, A. Kokalj, M. Lazzeri,
