Irvsp: to obtain irreducible representations of electronic states in the VASP

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We present an open-source program “irvsp”, to compute irreducible representations of electronic states for all 230 space groups with an interface to the Vienna ab-initio Simulation Package. This code is fed with plane-wave-based wavefunctions (e.g. WAVECAR) and space group operators (listed in OUTCAR), which are generated by the VASP package. This program computes the traces of matrix presentations and determines the corresponding irreducible representations for all energy bands and all the k-points in the three-dimensional Brillouin zone. It also works with spin-orbit coupling (SOC), i.e., for double groups. It is in particular useful to analyze energy bands, their connectivities, and band topology, after the establishment of the theory of topological quantum chemistry. In addition, the code has been also extended to (Wannier-based) tight-binding Hamiltonians. A sister program “ir2tb” is presented as well.

I. INTRODUCTION

Topological states [1–9] have been intensively studied in the past decades. During the period, lots of materials have theoretically been proposed to be topological insulators and topological semimetals, based on calculations within the density-functional theory (DFT) [10–16]. Many of them are verified in experiments, and substantially intrigue much interest in theories and experiments, such as three-dimensional (3D) topological insulator Bi2Se3 [17–19], Dirac semimetals Na3Bi [20, 21] and Cd3As2 [22, 23], Weyl semimetal TaAs [24–27], topological crystalline insulator SnTe [28, 29] and hourglass material KHgSb [30, 31] et al. To some extent, these topological electron bands are related to a band-inversion feature. Explicitly, there must be a band inversion happened between different irreducible representations (IRs) of the little groups at k-points in the 3D Brillouin zone (BZ) [32]. In the situation of Dirac semimetals or symmetry-protected nodal-line semimetals, it happens on a high-symmetry line or in a high-symmetry plane with different IRs.

Very recently, new insights about band theory have been used to classify all the nontrivial electron band topologies compatible with a given crystal structure [10–12]. In particular, based on the theory of topological quantum chemistry (TQC) [33–36], the topology of a set of isolated electron bands is relied on IRs at the maximal high-symmetry k-points (HSK), as the compatibility relations are solved in Ref. [37], and open accessible on the Bilbao Crystallographic Server (BCS) [38, 39]. The set of maximal HSK points can be found by using the BCS. The determination of the IRs of electron bands at maximal HSK points is of great interest, for which the program – vasp2trace – was developed [12]. However, it is not suitable for any non-maximal HSK points.

Generally speaking, in order to obtain the IRs for electron energy bands in crystals, two ingredients are necessary: a) wave-functions (WFs) at k-points and b) character tables (CRTs) for k-little groups. Different versions of the codes can be developed based on the different types of the WFs and conventions of the CRTs. The program irrep in the WIEN2k package [40, 41] is a precursor in determining the IRs, which is based on the plane-wave (PW) basis (the part of the WFs outside muffin-tin spheres) and the CRTs of 32 point groups (PNGs). There is an advantage of describing the IRs in terms of the more well-known PNG symmetries, however, the disadvantage is that in many cases k-points on the BZ surface cannot be classified with PNGs for nonsymmorphic crystals. In this paper, the program – irvsp – is developed based on the CRTs on the BCS for the VASP package [42]. It originates from the WIEN2k irrep code [40, 41] that considers both single- and double groups, analyses of time-reversal symmetry, and

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The codes are available in the repository: https://github.com/zjwang11/irvsp/.
handles accidental degeneracies. The present code inherits those features but it has been extended to also be able to determine IRs of those special $k$-points for nonsymmorphic crystals. Hence, the code labels the IRs according to the convention of the BCS notation [39] for all 230 space groups. In fact, it considers both type-I and type-II magnetic space groups. In addition, the code has been also extended to (Wannier-based) tight-binding (TB) Hamiltonians. A sister program – $ir2tb$ – is developed also.

This paper is organized as follows. In Section II, we present some basic derivations to compute the traces of matrix presentations in different bases. In Section III, we introduce the general process of the code. In Section IV, we introduce the capabilities of this package. In Section V, we introduce the installation and basic usages. In Section VI, we introduce some examples in order to show how to use $irvsp$ to determine the IRs and further explore the topology.

II. METHODS

Space-group symmetry operations, $O_s = \{R_s|v_s\}$, are consist of two parts: a rotation part $R_s$ and a translation part $v_s$. The product of two operations is defined as $\{R_s|v_s\}\{R_t|v_t\} = \{R_sR_t|R_s v_t + v_s\}$. An operator acting on a function in real space is expressed by $O_{f}(r) = f(O^{-1}r) = f(R^{-1}r - R^{-1}v)$. (There is a typo in Section A of the supplementary information of Ref. [12]). The matrix presentations (MPs), $O_{mn}^s$, can be obtained in the basis of the Bloch wavefunctions $|\psi_{nk}\rangle$: $O_{mn}^s = \langle \psi_{mk}|O_s|\psi_{nk}\rangle$. The traces of the obtained MPs are the characters, and they are essential to determine the corresponding IRs of the little group (LG) of $k$. The LG of $k$ [$LG(k)$] is defined as a set of space-group operations (SGOs): $LG(k) : \{O_s|R_s k = k + G\}$, with $G = l g_1 + m g_2 + n g_3$, $l, m, n \in \mathbb{N}$ (1)

Here, $G$ could be any integer reciprocal lattice translation ($g_1, g_2, g_3$ are primitive reciprocal lattice vectors). The traces of MPs of SGOs are defined as: $\text{Tr}[O_s] = \sum_n O_{mn}^s$ with $O_{mn}^s = \langle \psi_{mk}|O_s|\psi_{nk}\rangle$, $O_s \in LG(k)$.

(2)

Here, the WFs have to be normalized, $\langle \psi_{nk}|\psi_{nk}\rangle = 1$.

Under different bases, the WFs can be expressed in different ways, and the derivations of Eq. (2) are different. Here, we have derived the expressions in two bases: i) PW basis and ii) TB basis. In what follows, symbols in the bold text are vectors, and common bracket notations are employed:

$\langle r|A \rangle \equiv A(r)$

$\langle A|B \rangle \equiv \int dr A^*(r)B(r)$

$\langle r|k \rangle \equiv e^{ik \cdot r}$

To be convenient, we present the derivations in the cases without the spin degree of freedom. However, the derivations can be easily extended to the cases including SOC, by substituting $R_s \otimes SU_s(2)$ for $R_s$, where the bases are doubled by the direct product: $\{\text{real basis}\} \otimes \{\uparrow, \downarrow\}$. In fact, the code has been designed for both single- and double groups.

A. Plane-wave basis

In a PW basis, wavefunctions/eigenstates are expressed in the basis of plane waves:

$\psi_{nk}(r) = \sum_j C_{k,j} e^{i(k+G_j) \cdot r}$ with $\langle k + G_i|k + G_j\rangle = \delta_{ij}$ (3)
The coefficients \((C_{k,j})\) are usually computed in the \textit{ab-initio} calculations and output by the DFT package (e.g. VASP). The SGOs acting on WFs are derived as:

\[
\mathcal{O}_s \psi_{nk}(r) = \sum_j C_{k,j} e^{i (k+G_j) \cdot (R_s^{-1} r - R_s^{-1} v_s)} = \sum_j C_{k,j} e^{i R_s (k+G_j) \cdot (r - v_s)}
\]

with \(k + G_j \equiv R_s (k + G_j)\)

\[
= e^{-ik \cdot v_s} \sum_j C_{k,j} e^{-i (G_j' \cdot v_s)} e^{i (k+G_j') \cdot r} \quad \text{with} \quad G_j' \equiv R_s (k + G_j) - k
\]

Then, Eq. (2) can be written as:

\[
\langle \psi_{nk} | \mathcal{O}_s | \psi_{nk} \rangle = e^{-ik \cdot v_s} \sum_j C^*_{k,j} C_{k,j} e^{-i (G_j' \cdot v_s)} \quad \text{with} \quad G_j' \equiv R_s (k + G_j) - k
\] (4)

The program “irvsp” is developed based on the above derivations with the interface to VASP. However, it should work for any PW-based code, once a proper interface is made.

**B. Tight-binding basis**

In a TB Hamiltonian, WFs are expressed in the basis of localized (Wannier) orbitals:

\[
|0, \mu \alpha \rangle \equiv \phi^\mu_\alpha (r) \equiv \phi^\alpha_{\mu} (r - \tau_{\mu})
\]

and \(|L_j, \mu \alpha \rangle \equiv \phi^\alpha_{\mu} (r - L_j - \tau_{\mu})\), where \(\mu\) label the atoms, \(\alpha\) label the orbitals, \(L_j\) label the lattice vectors in 3D crystals, and \(\tau_{\mu}\) label the positions of atoms in a home unit cell. At a given \(k\)-point, WFs are given as:

\[
\psi_{nk}(r) = \sum_{\mu \alpha} C^n_{\mu \alpha, k} \phi^\mu_{\alpha k} (r) \quad \text{where} \quad n \text{ is a band index},
\] (5)

\[
\phi^\mu_{\alpha k} (r) = \sum_{\beta} \phi^\alpha_{\mu} (r - \tau_{\mu} - L_j) e^{i k \cdot (L_j + \tau_{\mu})}, \quad \langle \phi^\mu_{\beta k} | \phi^\mu_{\alpha k} \rangle = \delta_{\mu \mu'} \delta_{\alpha \beta}
\] (6)

The states \(\phi^\mu_{\alpha k} (r)\) are the Fourier transformations of the local orbitals \(\phi^\alpha_{\mu} (r)\), as shown in Eq. (6). The coefficients are obtained as the eigenvectors of the TB Hamiltonian: \(H_{\mu' \beta, \mu \alpha} (k) = \sum_j e^{i k \cdot (L_j + \tau_{\mu} - \tau_{\mu'})} \langle 0, \mu' \beta | \hat{H} | L_j, \mu \alpha \rangle\). The rotational symmetries \(R_s\) acting on the local orbitals \(|\phi^\alpha_{\mu} (r)\rangle\) of the \(\mu\) site are given as:

\[
\hat{R}_s \phi^\alpha_{\mu} (r) \equiv R_s \phi^\alpha_{\mu} (r) = \sum_{\beta} \phi^\beta (r) D^s_{\beta \alpha}
\] (7)

These \(D\)-matrices are explicitly given in Table S3 in the Appendix. Under the basis of real spherical harmonic functions with different total angular momenta (integer \(l\)), these \(D\)-matrices are real.
The SGOs acting on the states $\phi^\mu_{nk}(r)$ are given below:

$$
\mathcal{O}_s \phi^\mu_{nk}(r) = \phi^\mu_{nk}(R_{s}^{-1}r - R_{s}^{-1}v_s)
= \sum_j \phi_\alpha(R_{s}^{-1}r - R_{s}^{-1}v_s - \tau_\mu - L_j) e^{i\mathbf{k} \cdot (L_j + \tau_\mu)}
= \sum_j \phi_\alpha(R_{s}^{-1}r - v_s - R_s\tau_\mu - R_sL_j)e^{i\mathbf{k} \cdot (L_j + \tau_\mu)}
= \sum_j \tilde{R}_{s}\phi_\alpha[r - v_s - R_s\tau_\mu - R_sL_j]e^{i(\mathbf{R}_s \cdot \mathbf{k}) \cdot (\mathbf{L}_j + \tau_\mu)}
\equiv \sum_\beta \phi_\beta(r) D^s_{\beta\alpha}
= e^{-i(R_s \cdot \mathbf{k}) \cdot \mathbf{r}} \sum_j \tilde{R}_{s}\phi_\alpha[r - (v_s + R_s\tau_\mu) - R_sL_j]e^{i(\mathbf{R}_s \cdot \mathbf{k}) \cdot (\mathbf{L}_j + (R_s \tau_\mu + v_s))}
= e^{-i(R_s \cdot \mathbf{k}) \cdot \mathbf{r}} \sum_j \tilde{R}_{s}\phi_\alpha[r - \tau_\mu' - \mathbf{L}_j] e^{i(\mathbf{R}_s \cdot \mathbf{k}) \cdot (\mathbf{L}_j + (\tau_\mu' + v_s))}
\quad \text{with } \mathbf{v}_s + R_s\tau_\mu = \mathbf{L}_0 + \tau_\mu'.
$$

Thus, Eq. (2) is written as:

$$
\langle \psi_{nk} | \mathcal{O}_s | \psi_{nk} \rangle = e^{-i(R_s \cdot \mathbf{k}) \cdot \mathbf{r}} \sum_{\alpha\mu,\beta} C^n_{\mu'\beta} e^{i(R_s \cdot \mathbf{k}) \cdot \tau_\mu'} D^s_{\beta\alpha} C^m_{\mu\alpha} \quad \text{with } \mathbf{v}_s + R_s\tau_\mu = \mathbf{L}_0 + \tau_\mu'.
$$

In a matrix format,

$$
\langle \psi_{nk} | \mathcal{O}_s | \psi_{nk} \rangle = e^{-i(R_s \cdot \mathbf{k}) \cdot \mathbf{r}} \left[ \mathcal{V}(R_s \cdot \mathbf{k}) DC \right]_{nn}
$$

with

$$
\mathcal{V}(\mathbf{k})_{\mu',\mu,\alpha} = e^{i\mathbf{k} \cdot \tau_\mu} \delta_{\mu'\mu} \delta_{\alpha\beta}, \quad \mathcal{C}_{\mu\alpha,n} = C^m_{\mu\alpha}, \quad D^s_{\beta\alpha,n} = \begin{cases} D^s_{\beta\alpha} & \text{when } \mathbf{v}_s + R_s\tau_\mu = \mathbf{L}_0 + \tau_\mu' \vspace{1mm} \\ 0 & \text{otherwise.} \end{cases}
$$

Based on the above derivations, the code has been extended to the TB basis. The sister program is called “ir2tb”. Users must provide two files: case.jr.dat and.tbbox.in. The file called case.jr.dat, containing the TB parameters, may be generated by the software Wannier90 [43, 44] with symmetrization [45–47], or generated by users with a toy TB model, or generated from Slater-Koster method [48] or discretization of $k \cdot p$ model onto a lattice [49]. The other file tbbox.in is the master input file for “ir2tb”. It should be given consistently with the TB parameters in case.jr.dat. An example of tbbox.in is given for Bi$_2$Se$_3$ in the Appendix.

### III. GENERAL PROCESS OF THE CODE

In the main text, we are mainly focused on “irvsp”, which is based on the PW basis with an interface to the VASP package [42]. One can check more details for “ir2tb” in the Appendix.

#### A. Wavefunctions at $k$-points

In the VASP package, the all-electron wave-function is obtained by acting a linear operator $\mathcal{T}$ on the pseudo-wavefunction: $|\psi_{nk}\rangle = \mathcal{T} |\tilde{\psi}_{nk}\rangle$. The linear operator can be written explicitly as: $\mathcal{T} = \mathbf{1} + \sum_i (|\phi_i\rangle - |\tilde{\phi}_i\rangle) \langle p_i|$, where $|\phi_i\rangle$ ($|\tilde{\phi}_i\rangle$) is a set of all-electron (pseudo) partial waves around each atom and $|p_i\rangle$ is a set of corresponding projector functions on each atom within an augmentation region ($r < R_0$), where $R_0$ is the core part for each atom. The pseudo-wavefunction is expanded in the plane waves:

$$
\tilde{\psi}_{nk}(\mathbf{r}) = \sum_{\mathbf{g}} C_{n,\mathbf{k} + \mathbf{g}} e^{i(\mathbf{k} + \mathbf{g}) \cdot \mathbf{r}}
$$

(11)
where $\vec{G}$ vectors are determined by the condition $\frac{h^2}{2m_e}(\mathbf{k} + \vec{G})^2 < E_{\text{cutoff}}$ with a cutoff $E_{\text{cutoff}}$. It is worth noting that $\langle \tilde{\psi}_{nk} \rangle$ are sufficient for the calculations of the traces of MPs of SGOs.

Since the pseudo-wavefunctions $\langle \tilde{\psi}_{nk} \rangle$ are usually not normalized, they have to be renormalized before their traces can be computed via Eq. (2). The coefficients ($C_{\mathbf{k}+\vec{G},j}$) are output in WAVECAR by VASP. In the program, they are read by the subroutine: `wave_data.f90`. In the SOC case, the $C_{\mathbf{k}+\vec{G},j}$, and $C_{\mathbf{k}+\vec{G},j}$, are stored in the complex variables `coeffa(:)` and `coeffb(:)`. In the case without SOC, the $C_{\mathbf{k}+\vec{G},j}$ are stored in `coeffa(:)`, while `coeffb(:)` are invalid (set to be zero).

\begin{table}[h]
\centering
\caption{A brief summary of key subroutines}
\begin{tabular}{lll}
\hline
\textbf{File} & \textbf{Description} & \textbf{Input} \\
\textit{wave\_data.f90} & reading the coefficients. & WAVECAR \\
\textit{init.f90} & reading lattice vectors and space group operators, and setting up the $Z$ and $Z^{-1}$ matrices. & OUTCAR \\
\textit{kgroup.f90} & determining the $\mathbf{k}$-little groups. & \\
\textit{nonsymm.f90} & retrieving the character tables from the BCS & \\
\textit{chrt.f90} & computing the traces through the Eq. (4), and determining the IRs & \\
\hline
\end{tabular}
\end{table}

**B. Symmetry operators of a crystal**

Instead of generating space group operators from a crystal structure (i.e., POSCAR), the program reads the SGOs directly from the standard output of VASP (i.e., OUTCAR), which is done by the subroutine: `init.f90`. In other words, the SGOs are generated by the VASP package (e.g. with ISYM = 1 or 2 in INCAR for vasp.5.3.3), which are listed below the line of ‘Space group operators’ in OUTCAR. Fig. 1 shows an example of Bi$_2$Se$_3$ for the SGOs of space group (SG) 166. They are given by $\text{Det} \cdot e^{-i \omega \langle \vec{n} \cdot \vec{L} \rangle}$, $L_x = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}$, $L_y = \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix}$, $L_z = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$; (12)

$S(\omega, \vec{n}) = e^{-i \omega \langle \vec{n} \cdot \vec{S} \rangle}$, $S_x = \frac{\sigma_x}{2} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $S_y = \frac{\sigma_y}{2} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, $S_z = \frac{\sigma_z}{2} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$.

\begin{table}[h]
\centering
\hline
\textbf{Space group operators:} & \textbf{det(S)} & \textbf{alpha} & \textbf{n.x} & \textbf{n.y} & \textbf{n.z} & \textbf{tau.x} & \textbf{tau.y} & \textbf{tau.z} \\
\hline
1 & 1.000000 & 0.000000 & 1.000000 & 0.000000 & 0.000000 & 0.000000 & 0.000000 & 0.000000 \\
2 & -1.000000 & 0.000000 & 1.000000 & 0.000000 & 0.000000 & 0.000000 & 0.000000 & 0.000000 \\
3 & 1.000000 & 180.000000 & 0.866025 & 0.500000 & 0.000000 & 0.000000 & 0.000000 & 0.000000 \\
4 & -1.000000 & 180.000000 & 0.866025 & 0.500000 & 0.000000 & 0.000000 & 0.000000 & 0.000000 \\
5 & 1.000000 & 120.000000 & 0.000000 & 0.000000 & 0.000000 & 0.000000 & 0.000000 & 0.000000 \\
6 & -1.000000 & 120.000000 & 0.000000 & 0.000000 & 0.000000 & 0.000000 & 0.000000 & 0.000000 \\
7 & 1.000000 & 179.999999 & 0.000000 & 1.000000 & 0.000000 & 0.000000 & 0.000000 & 0.000000 \\
8 & -1.000000 & 179.999999 & 0.000000 & 1.000000 & 0.000000 & 0.000000 & 0.000000 & 0.000000 \\
9 & 1.000000 & 120.000000 & 0.000000 & 0.000000 & 0.000000 & 1.000000 & 0.000000 & 0.000000 \\
10 & -1.000000 & 120.000000 & 0.000000 & 0.000000 & 0.000000 & 1.000000 & 0.000000 & 0.000000 \\
11 & 1.000000 & 180.000000 & 0.866025 & -0.500000 & 0.000000 & 0.000000 & 0.000000 & 0.000000 \\
12 & -1.000000 & 180.000000 & 0.866025 & -0.500000 & 0.000000 & 0.000000 & 0.000000 & 0.000000 \\
\hline
\end{tabular}
\end{table}

**FIG. 1:** Screenshot of OUTCAR, showing the space group operators of Bi$_2$Se$_3$ generated by VASP.
FIG. 2: Screenshot of OUTCAR, showing the lattice vectors and reciprocal lattice vectors of Bi$_2$Se$_3$ which are used in VASP.

In 3D crystals, it is more convenient to use matrix presentations in the lattices of ($t_1, t_2, t_3$) in real space and in reciprocal lattices of ($g_1, g_2, g_3$) in momentum space. They are given in the following convention:

$$
\vec{v} = t_1 v_1 + t_2 v_2 + t_3 v_3 = (t_1, t_2, t_3) \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix}, \quad (t_1, t_2, t_3) \equiv \begin{pmatrix} t_{1x} \\ t_{2x} \\ t_{3x} \\ t_{1y} \\ t_{2y} \\ t_{3y} \\ t_{1z} \\ t_{2z} \\ t_{3z} \end{pmatrix}; \quad (14)
$$

$$
\vec{k} = k_1 g_1 + k_2 g_2 + k_3 g_3 = (k_1, k_2, k_3) \begin{pmatrix} g_1 \\ g_2 \\ g_3 \end{pmatrix}, \quad (k_1, k_2, k_3) \equiv \begin{pmatrix} g_{1x} \\ g_{1y} \\ g_{1z} \\ g_{2x} \\ g_{2y} \\ g_{2z} \\ g_{3x} \\ g_{3y} \\ g_{3z} \end{pmatrix}. \quad (15)
$$

with \( \begin{pmatrix} g_1 \\ g_2 \\ g_3 \end{pmatrix} (t_1, t_2, t_3) = 2\pi I_{3 \times 3} \)

The rotational symmetry operators acting on the vectors are transformed as:

$$
R\vec{v} = (t_1, t_2, t_3) Z \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix}, \quad R\vec{k} = (k_1, k_2, k_3) Z^{-1} \begin{pmatrix} g_1 \\ g_2 \\ g_3 \end{pmatrix}; \quad (16)
$$

$$
R(t_1, t_2, t_3) = (t_1, t_2, t_3) Z, \quad (17)
$$

Thus, rotational matrix presentations in the lattice vectors are \( 3 \times 3 \) integer matrices \( (Z) \), which are defined in Eq. (17). Instead of the real \( R \)-matrices in Cartesian coordinates in Eq. (12), the integer matrices, \( Z \) and \( Z^{-1} \), are actually stored and used throughout the code, which are all set in the subroutine: \textit{init.f90}

If one wants to do some sub-space-group symmetry calculations, one can modify the SGOs in OUTCAR and give space group 2 to run \textit{irvsp}.

C. Little group of a certain \( k \)-point

The eigen-wavefunctions at a certain \( k \)-point only support the IRs of the little group of \( k \), \( LG(k) \). Therefore, for any given \( k \)-point, the program has to determine the \( k \)-little group \( LG(k) \) first. This is done in the subroutine: \textit{kgroup.f90}. The \( LG(k) \) are defined by Eq. (1). In the program, the integer matrices \( Z^{-1} \) and Eq. (16) in momentum space are used.

D. Character tables for \( k \)-little groups

Currently, there are two conventions of CRTs for \( k \)-little groups. In the first convention, the \( k \) points are labeled by the IRs of the PNGs, since IRs of the space group can be expressed as IRs of the corresponding point group multiplied by a phase factor. They are suitable either for symmorphic space groups, or the inner \( k \)-points (not on the BZ boundary/surface) for the non-symmorphic space groups. The CRTs of PNGs are given in the Ref. [50, 51], which have been implemented in the program \textit{irrep} of the WIEN2k package [40, 41]. In the second convention, all the CRTs for \( k \)-points of all 230 space groups are listed on the BCS [39]. To compare the computed traces with these characters, one do not need to distinguish symmorphic and nonsymmorphic space groups at all. Therefore, the program “irvsp” is valid for all 230 space groups. The CRTs are retrieved from the inputs of the BCS, which are done by the subroutine: \textit{nonsymn.f90}.

As an example, consider the \( \Gamma \) point of Bi$_2$Se$_3$. Fig. 3 shows the CRT of the point group \( D_{3d} \) in the PNG convention. Fig. 4 shows the CRT in the BCS convention. Both tables can be used to determine the IRs at \( \Gamma \) in SG 166. In the
table of Fig. 4, the first and two columns show the reality and the BCS labels of IRs, respectively. The following columns indicate the characters of different SGOs. The reality of an IR is given by the definition \[ \frac{1}{|G|} \sum_{j=1}^{|G|} \chi(G^2_j) = \begin{cases} 1 & \text{potentially real, case (a)} \\ 0 & \text{essentially complex, case (b)} \\ -1 & \text{pseudo-real, case (c)} \end{cases} \] (18)

where \( G_j \) is an element of a group \( G \), and \( |G| \) is the rank of the group \( G \). In case (a), the IR is equivalent to its complex representation, and also equivalent to a real representation. In case (b), the IR is not equivalent to its complex representation. In case (c), the IR is equivalent to its complex representation, but not to a real representation.

In the type-II magnetic space groups (MSGs), including pure time-reversal symmetry (TRS), the existence of anti-unitary SGOs in the \( k \)-little group is indicated at the beginning of the character table (Fig. 4). In the absence of SOC (integer spin), TRS doubles the degeneracy of IRs in cases (b) and (c); while in the presence of SOC (half-integer spin), it doubles the degeneracy of the IRs in cases (a) and (b).

\[ \frac{1}{|G|} \sum_{j=1}^{|G|} \chi(G^2_j) = \begin{cases} 1 & \text{potentially real, case (a)} \\ 0 & \text{essentially complex, case (b)} \\ -1 & \text{pseudo-real, case (c)} \end{cases} \] (18)

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\[ \frac{1}{|G|} \sum_{j=1}^{|G|} \chi(G^2_j) = \begin{cases} 1 & \text{potentially real, case (a)} \\ 0 & \text{essentially complex, case (b)} \\ -1 & \text{pseudo-real, case (c)} \end{cases} \] (18)

where \( G_j \) is an element of a group \( G \), and \( |G| \) is the rank of the group \( G \). In case (a), the IR is equivalent to its complex representation, and also equivalent to a real representation. In case (b), the IR is not equivalent to its complex representation. In case (c), the IR is equivalent to its complex representation, but not to a real representation.

In the type-II magnetic space groups (MSGs), including pure time-reversal symmetry (TRS), the existence of anti-unitary SGOs in the \( k \)-little group is indicated at the beginning of the character table (Fig. 4). In the absence of SOC (integer spin), TRS doubles the degeneracy of IRs in cases (b) and (c); while in the presence of SOC (half-integer spin), it doubles the degeneracy of the IRs in cases (a) and (b).

\[ \frac{1}{|G|} \sum_{j=1}^{|G|} \chi(G^2_j) = \begin{cases} 1 & \text{potentially real, case (a)} \\ 0 & \text{essentially complex, case (b)} \\ -1 & \text{pseudo-real, case (c)} \end{cases} \] (18)

where \( G_j \) is an element of a group \( G \), and \( |G| \) is the rank of the group \( G \). In case (a), the IR is equivalent to its complex representation, and also equivalent to a real representation. In case (b), the IR is not equivalent to its complex representation. In case (c), the IR is equivalent to its complex representation, but not to a real representation.

In the type-II magnetic space groups (MSGs), including pure time-reversal symmetry (TRS), the existence of anti-unitary SGOs in the \( k \)-little group is indicated at the beginning of the character table (Fig. 4). In the absence of SOC (integer spin), TRS doubles the degeneracy of IRs in cases (b) and (c); while in the presence of SOC (half-integer spin), it doubles the degeneracy of the IRs in cases (a) and (b).

\[ \frac{1}{|G|} \sum_{j=1}^{|G|} \chi(G^2_j) = \begin{cases} 1 & \text{potentially real, case (a)} \\ 0 & \text{essentially complex, case (b)} \\ -1 & \text{pseudo-real, case (c)} \end{cases} \] (18)

where \( G_j \) is an element of a group \( G \), and \( |G| \) is the rank of the group \( G \). In case (a), the IR is equivalent to its complex representation, and also equivalent to a real representation. In case (b), the IR is not equivalent to its complex representation. In case (c), the IR is equivalent to its complex representation, but not to a real representation.

In the type-II magnetic space groups (MSGs), including pure time-reversal symmetry (TRS), the existence of anti-unitary SGOs in the \( k \)-little group is indicated at the beginning of the character table (Fig. 4). In the absence of SOC (integer spin), TRS doubles the degeneracy of IRs in cases (b) and (c); while in the presence of SOC (half-integer spin), it doubles the degeneracy of the IRs in cases (a) and (b).
TABLE II: Four versions of “irvsp” are implemented. The first column indicates the version number, the second column shows the convention of reference CRTs, and the brief description is followed in the last column.

| Version | CRTs      | Brief description                                                                 |
|---------|-----------|-----------------------------------------------------------------------------------|
| version I | PNG       | It resembles an analogue of the program \texttt{irrep} in the WIEN2k package.      |
| version II | BCS      | It works for the \(-k\)-points, where version I does not work.                    |
| version III | PNG&BCS  | It combines version I and version II.                                             |
| version IV | BCS       | It works for all the \(-k\)-points and all 230 space groups, including nonsymmorphic space groups. All the IRs are labeled in the convention of the BCS notation. |

IV. CAPABILITIES OF “IRVSP”

In the study of the property of a material, the determination of IRs of computed electron bands is of great interest to diagnose the band crossing/anti-crossing, degeneracy and band topology. The program is aimed to get the IRs for all the bands at all the \(-k\)-points for all 230 space group. In particular, it also works for the \(-k\)-points on the boundary of the 3D BZ in nonsymmorphic space groups. Four versions of “irvsp” are implemented, as shown in Table II. Version I works similarly (using some subroutines directly) as \texttt{irrep} in the WIEN2k package (using some subroutines directly) and presents the IRs with PNG symmetries. This version can thus not classify the special \(-k\)-points on the boundary of the Brillouin zone of nonsymmorphic crystals, that is, when \(\exp[-ik(R_s v_t + v_s)] \neq 1\) for some \(O_s\) and \(O_t\) in LG\((-k\)).

Version II has been extended to classify the IRs at also all BZ surface \(-k\)-points for nonsymmorphic space groups. Version III combines version I and II. In the (default) version IV, it works for all the \(-k\)-points and all 230 space groups (\(i.e.,\) both type-I and type-II MSGs). Without additional information, the program “irvsp” refers to version IV throughout the work. All the IRs are labeled in the convention of the BCS notation. The obtained IRs at the maximal HSK points can be directly compared with the elementary band representations (EBRs) of the TQC theory, to further check the topology of a set of bands in materials.

V. INSTALLATION AND USAGE

In this section, we will show how to install and use the “irvsp” software package. This program is an open source free software package. It is released on Github under the Standard CPC licence, \url{http://cpc.cs.qub.ac.uk/licence/licence.html}, and it can be downloaded directly from the public code repository: \url{https://github.com/zjwang11/irvsp/blob/master/src_irvsp_v2.tar.gz}.

To build and install “irvsp”, only a Fortran 90 compiler is needed. The downloaded “irvsp” software package is likely a compressed file with a zip or tar.gz suffix. One should uncompress it first, then move into the src\_irvsp\_v2 folder. After setting up the Fortran compiler in the ‘Makefile’ file, the executable binary \texttt{irvsp} will be compiled by typing the following command in the current directory (src\_irvsp\_v2):

\$ make

Before running \texttt{irvsp}, the user must provide two consistent files: WAVECAR and OUTCAR. The two files are generated by the VASP package in fixed format. It is designed to be simple and user friendly. After a running of VASP with WAVECAR and OUTCAR output, the program \texttt{irvsp} can be run immediately in the same folder. Giving a correct space group number \((sgn \in [1,230])\) and a version number \((nv \in \{1,2,3,4\})\), the program can be executed by the following command:

\$ irvsp -sgn sgn [-v nv] > outir &

VI. EXAMPLES

In the WIEN2k package, the program \texttt{irrep} classifies the IRs in PNG symmetries, which then excludes the possibility to describe certain BZ surface \(-k\)-points for nonsymmorphic crystals. Very recently, the codes \texttt{vasp2trace} and \texttt{CheckTopologicalMat}, designed for TQC in the Ref. [12], have been used (tested) in all 230 space groups and uncover thousands of new materials with topological electron bands. However, they are not suitable for non-maximal HSK points. Therefore, the demand to determine the IRs for all the \(-k\)-point and all 230 space groups is still unsatisfied. With the CRTs from the BCS, the program – \texttt{irvsp} – is developed to meet this demand. In this work, we take
topological materials PdSb$_2$ and Bismuth as examples to show how to study topological properties of new materials with “irvsp”.

FIG. 5: Electronic band structures of PdSb$_2$ without strain, with 0.3% (b) and 0.62% tensile strains. Panels (d), (e), and (f) are the zoom-in plots of (a) (b) (c) near the R point. In our calculations, the total number of electrons is 80. Therefore, the first 80 bands are regarded as valence bands (red-colored), while the other energetically higher bands are considered as conduction bands (blue-colored).

A. PdSb$_2$

PdSb$_2$ was predicted to be a candidate hosting sixfold-degenerate fermions because of the nonsymmorphic symmetry [52, 53]. The crystal of PdSb$_2$ is a cubic structure of SG 205. We adopt the experimental lattice constant $a$ [54–56] and fully relax the coordinate of inner atom positions. In the obtained band structure (BS) of Fig. 5(a) along the high-symmetry lines, we note that there is a tiny gap ($\sim$ 10 meV) between two sixfold degeneracies at R. Then, we want to know the corresponding IRs of two sixfold degeneracies and how they are going to evolve under strains. For this purpose, we performed the calculations with different tensile strains (i.e., $\Delta a/a$ = 0.3% and $\Delta a/a$ = 0.62%). Their electronic band structures are shown in Figs. 5(b) and (c), respectively. Comparing with the strain-free BS in Fig. 5(a), we find that the overall BS doesn’t change much, except for the R point. The zoom-in plots around

![Graphs showing band structures with strain](image)

FIG. 6: The IRs at R are determined by the program “irvsp”. The CRT of the R-little group is shown in Fig. S1 in the appendix. The first three columns stands for the band indices, degeneracies, and the energies (without subtracting the Fermi energy $E_F$). The following columns indicates the traces (characters) of the corresponding space group operators (listed as “E, 2, ..., 24”). The assigned IR labels are output to the right of the equality sign “=”. The (a), (b), (c) panels are the results of the three crystal structures, respectively.
FIG. 7: The calculated band representations of \( k \)-point \( P(a) \) and \( Q(b) \) as marked in Fig. 5(f). The number of total electrons is 80 in PdSb\(_2\).

The IRs at all the maximal HSK points can be computed directly by \textit{irvsp} (which can also generate the trace file – “trace.txt”). By directly comparing these obtained IRs with the EBRs of the TQC theory (released on the BCS) and solving the compatibility relations, we can find that it is a topological insulating phase without strain, while it’s a symmetry-enforced semimetallic phase with tiny tensile strains.

To further obtain the crossing points in the system, we computed the IRs along the R–X line (named S \([u,0.5,u] \) in the units of reciprocal lattice vectors). These points are also non-symmorphic, which are on the boundary of the 3D BZ for SG 205. The CRT for the S point is listed in Fig. S2. For the P and Q points in Fig. 5(f) of the strained crystal, we show the results of obtained IRs in Fig. 7. At the P point, the 79–80 degenerate bands are assigned to \("S3+S3"\), while 81–82 degenerate bands are assigned to \("S4+S4"\). However, at the Q point, the results are in the opposite way. Without doing further calculations with a denser \( k \)-mesh between P and Q points, we can still conclude that it’s a real 4-fold crossing along R–X on the BZ boundary, which is robust against SOC. The double degeneracy is due to the presence of TRS. The symmetry \#15 is the operator \( g_y \equiv \{M_y | 0 1 2 \ 1 2 1 \} \). Therefore, the doubly-degenerate bands have the same \( g_y \) eigenvalue (\( \{S3, S3\} \) or \( \{S4, S4\} \)), and the 4-fold crossing point along R–X is protected by \( g_y \) symmetry. As a result, the crossing 4-fold points actually form a Dirac nodal ring on the BZ boundary. Considering the full symmetry of SG 205, we conclude that there are three Dirac nodal rings in PdSb\(_2\) with tiny strains, which can be further checked in experiments in the future.

**B. Bismuth**

As aforementioned, with the IRs at maximal HSK points obtained by \textit{irvsp}, we can further check the topology by comparing them with the EBRs of the TQC theory. Here, we will take Bi as an example to briefly introduce the process. The element Bismuth has the rhombohedral structure of SG 166. The maximum HSK points of SG 166 are listed on the BCS, as \( \Gamma(GM), T, F, L \). After performing the \textit{ab-initio} calculations to obtain the eigen-wavefunctions at maximal HSK points, the obtained IRs of the occupied bands are given in Table III. From the TQC and BCS, the EBRs of SG 166 are obtained, as shown in Fig. 8. As there are only six valence bands, we can find that they are not belonging to any EBR induced form the 9\( d \) or 9\( e \) Wyckoff position. In the EBRs induced from the 3\( a \) and 3\( b \) Wyckoff

![Figure 8: A complete list of the EBRs of space group 166 in the presence of SOC. Each EBR is defined by a Maximal Wyckoff site (\( nx \)) and an IR of its site-symmetry group, which are indicated by the first and second rows, respectively. Then, the following rows present the IRs at the Maximal HSK points.](image)
positions, we can find that the number of the pairs of F5F6 at F has to be the same as the total number of the IRs GM9 and GM6GM7 at Γ. In Bismuth, the obtained IRs have three IRs of F5F6, but neither GM9 nor GM6GM7. In conclusion, the set of occupied bands in Bismuth can not be expressed as any sum of EBRs in SG 166. In other words, it has to be topological [7].

**TABLE III:** The IRs at maximal HSK points obtained by *irvsp* in Bismuth. “(n)” indicates the degeneracy of the bands, while “[m]” indicates the total number of the computed bands at the k-point.

| HSK   | six valence bands |
|-------|-------------------|
| GM    | GM5 (2); GM8 (2); GM4 GM5 (2); [6] |
| T     | T9 (2); T8 (2); T6 T7 (2); [6] |
| F     | F3 F4 (2); F5 F6 (2); F5 F6 (2); [6] |
| L     | L3 L4 (2); L5 L6 (2); L5 L6 (2); [6] |

**VII. CONCLUSIONS**

In summary, we presented an open-source software package called “irvsp” that determines the IRs of electronics states. It is very user-friendly and is written in Fortran 90/77, showing a powerful function to analyze the IRs for all the k-points in all 230 space groups. Thus, that also can classify BZ surface points for nonsymmorphic crystals. We showed how to use it to identify IRs and further get the topological property for a new material. As an example, we explored a new topological material PdSb$_2$, whose topology is very sensitive to the lattice parameter. Under tiny strains, it was identified as a four-fold Dirac nodal-line metal.

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[1] B. A. Bernevig, T. L. Hughes, and S.-C. Zhang, Science **314**, 1757 (2006).
[2] M. König, S. Wiedmann, C. Brüne, A. Roth, H. Buhmann, L. W. Molenkamp, X.-L. Qi, and S.-C. Zhang, Science **318**, 766 (2007).
[3] C. L. Kane and E. J. Mele, Physical review letters **95**, 226801 (2005).
[4] B. A. Bernevig and S.-C. Zhang, Physical review letters **96**, 106802 (2006).
[5] C. Kane and M. Hasan, Rev. Mod. Phys **82**, 3045 (2010).
[6] X.-L. Qi and S.-C. Zhang, Reviews of Modern Physics **83**, 1057 (2011).
[7] F. Schindler, A. M. Cook, M. G. Vergniory, Z. Wang, S. S. Parkin, B. A. Bernevig, and T. Neupert, Science advances **4**, eaat0346 (2018).
[8] X. Wan, A. M. Turner, A. Vishwanath, and S. Y. Savrasov, Physical Review B **83**, 205101 (2011).
[9] B. J. Wieder, B. Bradlyn, Z. Wang, C. Cano, Y. Kim, H.-S. D. Kim, A. M. Rappe, C. Kane, and B. A. Bernevig, Science **361**, 246 (2018).
[10] F. Tang, H. C. Po, A. Vishwanath, and X. Wan, arXiv preprint arXiv:1807.09744 (2018).
[11] T. Zhang, Y. Jiang, Z. Song, H. Huang, Y. He, Z. Fang, H. Weng, and C. Fang, Nature **566**, 475 (2019).
[12] M. Vergniory, L. Elcoro, C. Felser, N. Regnault, B. A. Bernevig, and Z. Wang, Nature **566**, 480 (2019).
[13] Y. Xu, Z. Song, Z. Wang, H. Weng, and X. Dai, Phys. Rev. Lett. **122**, 256402 (2019), URL https://link.aps.org/doi/10.1103/PhysRevLett.122.256402.
[14] G. Li, B. Yan, Z. Wang, and K. Held, Phys. Rev. B **95**, 035102 (2017), URL https://link.aps.org/doi/10.1103/PhysRevB.95.035102.
[15] S. Nie, L. Xing, R. Jin, W. Xie, Z. Wang, and F. B. Prinz, Phys. Rev. B **98**, 125143 (2018), URL https://link.aps.org/doi/10.1103/PhysRevB.98.125143.
[16] Y. Qian, S. Nie, C. Yi, L. Kong, C. Fang, T. Qian, H. Ding, Y. Shi, Z. Wang, H. Weng, et al., npj Computational Materials **5**, 121 (2019), URL https://doi.org/10.1038/s41524-019-0260-6.
[17] H. Zhang, C.-X. Liu, X.-L. Qi, X. Dai, Z. Fang, and S.-C. Zhang, Nature physics **5**, 438 (2009).
[18] Y. Xia, D. Qian, D. Hsieh, L. Wray, A. Pal, H. Lin, A. Bansil, D. Grauer, Y. S. Hor, R. J. Cava, et al., Nature physics **5**, 398 (2009).
Y. Chen, J. G. Analytis, J.-H. Chu, Z. Liu, S.-K. Mo, X.-L. Qi, H. Zhang, D. Lu, X. Dai, Z. Fang, et al., science 325, 178 (2009).

Z. Wang, Y. Sun, X.-Q. Chen, C. Franchini, G. Xu, H. Weng, X. Dai, and Z. Fang, Physical Review B 85, 195320 (2012).

Z. Liu, B. Zhou, Y. Zhang, Z. Wang, H. Weng, D. Prabhakaran, S.-K. Mo, Z. Shen, Z. Fang, X. Dai, et al., Science 343, 864 (2014).

Z. Wang, H. Weng, Q. Wu, X. Dai, and Z. Fang, Phys. Rev. B 88, 125427 (2013), URL https://link.aps.org/doi/10.1103/PhysRevB.88.125427.

Z. Liu, J. Jiang, B. Zhou, Z. Wang, Y. Zhang, H. Weng, D. Prabhakaran, S. Mo, H. Peng, P. Dudin, et al., Nature materials 13, 677 (2014).

H. Weng, C. Fang, Z. Fang, B. A. Bernevig, and X. Dai, Physical Review X 5, 011029 (2015).

S.-M. Huang, S.-Y. Xu, I. Belopolski, C.-C. Lee, G. Chang, B. Wang, N. Alidoust, G. Bian, M. Neupane, C. Zhang, et al., Nature communications 6, 7373 (2015).

B. Lv, H. Weng, B. Fu, X. Wang, H. Miao, J. Ma, P. Richard, X. Huang, L. Zhao, G. Chen, et al., Physical Review X 5, 031013 (2015).

S.-Y. Xu, I. Belopolski, N. Alidoust, M. Neupane, G. Bian, C. Zhang, R. Sankar, G. Chang, Z. Yuan, C.-C. Lee, et al., Science 349, 613 (2015).

T. H. Hsieh, H. Lin, J. Liu, W. Duan, A. Bansil, and L. Fu, Nature communications 3, 982 (2012).

Y. Yanaka, Z. Ren, T. N. K. Nahayama, S. Souma, T. Takahashi, K. Segawa, and Y. Ando, Nature Physics 8, 800 (2012).

Z. Wang, A. Alexandradinata, R. J. Cava, and B. A. Bernevig, Nature 532, 189 (2016).

J. Ma, C. Yi, B. Lv, Z. Wang, S. Nie, L. Wang, L. Kong, Y. Huang, P. Richard, P. Zhang, et al., Science advances 3, e1602415 (2017).

Z. Zhu, Y. Cheng, and U. Schwingenschl"ogl, Physical Review B 85, 235401 (2012).

B. Bradlyn, L. Elcoro, J. Cano, M. Vergniory, Z. Wang, C. Felser, M. Aroyo, and B. A. Bernevig, Nature 547, 298 (2017).

J. Cano, B. Bradlyn, Z. Wang, L. Elcoro, M. Vergniory, C. Felser, M. Aroyo, and B. A. Bernevig, Physical Review B 97, 035139 (2018).

M. Vergniory, L. Elcoro, Z. Wang, J. Cano, C. Felser, M. Aroyo, B. A. Bernevig, and B. Bradlyn, Physical Review E 96, 023310 (2017).

J. Cano, B. Bradlyn, Z. Wang, L. Elcoro, M. Vergniory, C. Felser, M. Aroyo, and B. A. Bernevig, Physical review letters 120, 266401 (2018).

L. Elcoro, B. Bradlyn, Z. Wang, M. G. Vergniory, J. Cano, C. Felser, B. A. Bernevig, D. Orobenoa, G. Flor, and M. I. Aroyo, Journal of Applied Crystallography 50, 1457 (2017).

M. I. Aroyo, J. Perez-Mato, D. Orobenoa, E. Tasci, G. De La Flor, and A. Kirov, Bulg. Chem. Commun 43, 183 (2011).

H. T. Stokes, B. J. Campbell, and R. Cordes, Acta Crystallographica Section A: Foundations of Crystallography 69, 388 (2013).

P. Blaha, K. Schwarz, G. K. Madsen, D. Kvasnicka, and J. Luitz, An augmented plane wave+ local orbitals program for calculating crystal properties (2001).

C. Persson, Electronic structure of intrinsic and doped silicon carbide and silicon, PhD thesis, ISBN 91-7219-442-1 (1999).

G. Kresse and J. Furthm"uller, Phys. Rev. B 54, 169 (1996).

N. Marzari, A. A. Mostofi, J. R. Yates, I. Souza, and D. Vanderbilt, Rev. Mod. Phys. 84, 1419 (2012), URL https://link.aps.org/doi/10.1103/RevModPhys.84.1419.

A. A. Mostofi, J. R. Yates, G. Pirzi, Y.-S. Lee, I. Souza, D. Vanderbilt, and N. Marzari, Computer Physics Communications 185, 2309 (2014).

Q. Wu, S. Zhang, H.-F. Song, M. Troyer, and A. A. Soluyanov, Computer Physics Communications 224, 405 (2018), ISSN 0010-4655, URL http://www.sciencedirect.com/science/article/pii/S0010465517303442.

C. Yue, Symmetrization of wannier tight-binding models, https://github.com/quanshengwu/wannier_tools/tree/master/wannhr_symm.

D. Gresch, Q. Wu, G. W. Winkler, R. H"auselmann, M. Troyer, and A. A. Soluyanov, Physical Review Materials 2, 103805 (2018).

J. C. Slater and G. F. Koster, Phys. Rev. 94, 1498 (1954), URL https://link.aps.org/doi/10.1103/PhysRev.94.1498.

M. Willatzen and L. L. Y. Voon, The kp Method-Electronic Properties of Semiconductors, vol. 53 (SpringerBerlinHeidelberg, Berlin,Heidelberg, 2009).

J. F. Cornwell, Group Theory in Physics [Vol. 1-2]. (Academic Press, 1984).

H.-W. Streitwolf, Group theory in solid-state physics (Macdonald and Co., 1971).

B. Bradlyn, J. Cano, Z. Wang, M. Vergniory, C. Felser, R. J. Cava, and B. A. Bernevig, Science 353, aaf5037 (2016).

R. Chapai, Y. Jia, W. Shelton, R. Nepal, M. Saghayezhian, J. DiTusa, E. Plummer, C. Jin, and R. Jin, Physical Review B 99, 161110 (2019).

J. Pratt, K. Myles, J. Darby Jr, and M. Mueller, Journal of the Less Common Metals 14, 427 (1968).

S. Furuseth, K. Selte, A. Kjekshus, P. Nielsen, B. Sj"oberg, and E. Larsen, Acta Chem. Scand B 19 (1965).

N. E. Brese and H. G. von Schnering, Zeitschrift für anorganische und allgemeine Chemie 620, 393 (1994).
APPENDIX

1. tbbox.in for Bi$_2$Se$_3$

case = soc ! lda or soc

proj:
orbit = 2
ntau = 5
0.39900000 0.39900000 0.39900000 1 3 ! x1, x2, x3, itau, iorbit
0.60100000 0.60100000 0.60100000 1 3
0.20600000 0.20600000 0.20600000 2 3
0.79400000 0.79400000 0.79400000 2 3
0.00000000 0.00000000 0.00000000 2 3
end projections

kpoint:
kmesh = 10
Nk = 3
0.00000000 0.00000000 0.00000000 ! k0: y1,y2,y3
0.50000000 0.50000000 0.50000000 ! k1
0.50000000 0.50000000 0.00000000 ! k2
0.00000000 0.50000000 0.00000000 ! k3
end kpoint

unit_cell:
1.194537707 -2.069000000 9.546666657 0.139523990 -0.241662639 0.034916201 ! b1x b1y b1z; g1x g1y g1z
1.194537707 2.069000000 9.546666657 0.139523990 0.241662639 0.034916201
-2.389075414 0.000000000 9.546666657 -0.279047979 0.000000000 0.034916201
1 1.000000 0.000000 1.000000 0.000000 0.000000 0.000000 ! SN,Det,omega,nx,ny,nz,v1,v2,v3
2 -1.000000 0.000000 1.000000 0.000000 0.000000 0.000000
3 1.000000 180.000000 0.866025 0.500000 0.000000 0.000000
4 -1.000000 180.000000 0.866025 0.500000 0.000000 0.000000
5 1.000000 120.000000 0.000000 0.000000 -1.000000 0.000000
6 -1.000000 120.000000 0.000000 0.000000 -1.000000 0.000000
7 1.000000 179.999999 0.000000 1.000000 0.000000 0.000000
8 -1.000000 179.999999 0.000000 1.000000 0.000000 0.000000
9 1.000000 120.000000 0.000000 0.000000 1.000000 0.000000
10 -1.000000 120.000000 0.000000 0.000000 1.000000 0.000000
11 1.000000 180.000000 0.866025 -0.500000 0.000000 0.000000
12 -1.000000 180.000000 0.866025 -0.500000 0.000000 0.000000
end unit_cell

TABLE S1: A list of codes are available in the repository: https://github.com/zjwang11/irvsp/. Different
versions of the codes can be developed based on the different types of the WFs and conventions of the CRTs. Besides
the src_irvsp_v2.tar.gz code mainly discussed in the main text, there are more codes developed.

| WFs  | CRTs      | PNG        | BCS        |
|------|-----------|------------|------------|
| PW   | src_irvsp_v1.tar.gz | src_irvsp_v1.tar.gz | src_irvsp_v2.tar.gz |
| TB   | src_ir2tb_v1.tar.gz | src_ir2tb_v1.tar.gz | src_ir2tb_v2.tar.gz |
2. The brief description of inputs for “ir2tb”

Based on the different types of the WFs and the codes of the CRTs, different versions of the codes are developed, as shown in Table S1. The program “ir2tb” is based on the TB WFs. BLAS and LAPACK linear algebra libraries are needed to diagonalize the TB Hamiltonian. It needs two input files: `bbox.in` and `case.hr.dat`.

The `case.hr.dat` file, containing the TB parameters in Wannier90 format [43], may be generated by the software Wannier90 [44] with symmetrization [47], or generated by users with a toy TB model, or generated from Slater-Koster method [48] or a discretization of $k \cdot p$ model onto a lattice [49].

The `bbox.in` file provides detailed information about the TB Hamiltonian (i.e., the `case.hr.dat` file), which is an essential input for the program “ir2tb”. The tag `case = lda` (case = soc) indicates that the TB Hamiltonian does not (does) have the SOC effect. The `lda/soc.hr.dat` is needed accordingly. In the “proj” block, “orbt=1 or 2” indicates the convention of the local basis ordering on each atom. The local orbitals in convention 1 are listed in Table S3, while those in convention 2 are in the order as implemented in Wannier90. “ntau” indicates the total number of the atoms in the TB Hamiltonian, which also means how many lines follow in this block. The local orbitals of the TB Hamiltonian are provided by: ‘x1,x2,x3, itau, iorbit’. ‘x1,x2,x3’ stand for the positions of atoms: $\tau = (x_1 t_1, x_2 t_2, x_3 t_3)$; “itau” stand for the kinds of atoms; and “iorbit” stand for the total number of local orbitals on each atom. So far, “iorbit” is limited to the values of [1,3,5,4,6,7,8,9], whose detailed orbital informations are provided in Table S3. In the case of `case = soc`, the local orbitals will be doubled automatically: the first half are spin-up and the second half are spin-down. In the “kpoint” block, the $k$-path is given as $k_0 - k_1 - \ldots - k_N$ with $k_{mesh}$ on each segment. The “unit_cell” block gives the lattice vectors and reciprocal lattice vectors in first three lines, followed by space group operators of the system we considered. They are the same lines as the program “irvsp” reads in OUTCAR file.

### TABLE S2: A brief summary of `bbox.in`

| Comments | Descriptions |
|----------|--------------|
| ! lda or soc | lda: nspin=1 (without SOC); soc: nspin=2 (with SOC) |
| ! x1,x2,x3, itau, iorbit | defining $\tau = (x_1 t_1, x_2 t_2, x_3 t_3)$, iorbit $\in \{1, 3, 4, 5, 6, 7, 8, 9\}$ |
| ! k0: y1,y2,y3 | defining $k_0 = (y_1 g_1, y_2 g_2, y_3 g_3)$; kpath is along $k_0 - k_1 - \ldots - k_n$. |
| ! b1x bly b1z; g1x gly g1z | defining $t_1 = (b_1 x, b_1 y, b_1 z)$; $g_1 = 2\pi (g_1 x, g_1 y, g_1 z)$ |
| ! SN, Det, omega, nx, ny, nz, v1, v2, v3 | defining $O = \{R(v)\}$ with $R = \text{Det} \cdot e^{i \omega (R, L)}$ and $v = (v_1 t_1, v_2 t_2, v_3 t_3)$. SN stands for the sequential number. |

### TABLE S3: The local orbitals in convention 1 (orbt=1) are given in the table.

| iorbit | Local orbitals | $D_{\text{rep. in Eq. (7)}}$ |
|--------|---------------|------------------|
| 1      | $s$           | $D^1$            |
| 3      | $p_x, p_y, p_z$ | $D^3 = \text{Det} \cdot e^{i \omega (R, L)}$ |
| 5      | $d_{xy}, d_{yz}, d_{zx}, d_{x^2-y^2}, d_{x^2-z^2}$ | $D^5 = e^{-i \omega (R, F)}$ |
| 7      | $s, p_x, p_y, p_z$ | $D^4 = D^1 \oplus D^3$ |
| 9      | $s, d_{xy}, d_{yz}, d_{zx}, d_{x^2-y^2}, d_{x^2-z^2}$ | $D^6 = D^2 \oplus D^3$ |
| 11     | $s, p_x, p_y, p_z, d_{xy}, d_{yz}, d_{zx}, d_{x^2-y^2}$ | $D^7 = D^3 \oplus D^5 \oplus D^7$ |
| 13     | $f_{xy}, f_{x^2-y^2}, f_{y^2-z^2}$ | $D^{12} = D^3 \oplus D^5 \oplus D^7$ |

$$P_x = \begin{pmatrix} 0 & 0 & -i & 0 & 0 \\ 0 & 0 & 0 & -i & -i \sqrt{3} \\ 0 & i & 0 & 0 & 0 \\ 0 & i & 0 & 0 & 0 \\ 0 & i \sqrt{3} & 0 & 0 & 0 \end{pmatrix}; P_y = \begin{pmatrix} 0 & i & 0 & 0 & 0 \\ -i & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -i & i \sqrt{3} \\ 0 & 0 & i & 0 & 0 \\ 0 & 0 & -i \sqrt{3} & 0 & 0 \end{pmatrix}; P_z = \begin{pmatrix} 0 & 0 & 0 & 2i & 0 \\ 0 & 0 & 0 & -i & 0 \\ 0 & 0 & -i & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ -2i & 0 & 0 & 0 & 0 \end{pmatrix}$$
\[
F_x = \begin{pmatrix}
0 & 0 & 0 & 0 & 2i & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \frac{3i}{2} & 0 & 0 & i\sqrt{\frac{15}{2}} \\
0 & 0 & -\frac{3i}{2} & 0 & 0 & i\sqrt{\frac{15}{2}} & 0 \\
-2i & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -\frac{i\sqrt{15}}{2} & 0 & 0 & -\frac{i}{2} \\
0 & 0 & -\frac{i\sqrt{15}}{2} & 0 & 0 & \frac{i}{2} & 0
\end{pmatrix}
\]

(19)

\[
F_y = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 2i & 0 \\
0 & 0 & 0 & -\frac{3i}{2} & 0 & 0 & i\sqrt{\frac{15}{2}} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \frac{3i}{2} & 0 & 0 & i\sqrt{\frac{15}{2}} & 0 & 0 \\
-2i & 0 & 0 & 0 & 0 & 0 & \frac{i}{2} \\
0 & 0 & 0 & 0 & 0 & -\frac{i}{2} & 0
\end{pmatrix}
\]

(20)

\[
F_z = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 & 2i \\
0 & 0 & \frac{3i}{2} & 0 & 0 & \frac{i\sqrt{15}}{2} & 0 \\
0 & -\frac{3i}{2} & 0 & 0 & i\sqrt{\frac{15}{2}} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -\frac{i\sqrt{15}}{2} & 0 & 0 & -\frac{i}{2} & 0 \\
-2i & 0 & 0 & 0 & 0 & \frac{i}{2} & 0
\end{pmatrix}
\]

(21)

3. The transformation from the standard conventional unit to the primitive unit cell

The maximal HSK points from the BCS are given in the convention reciprocal lattice vectors, while the lattice vectors in VASP usually are given in the primitive cell. The transformation depends on the type of the lattice. There are only seven different types of lattices, i.e. P, C, B, A, R, F and I. In the X type, the primitive lattices \((\vec{p}_1, \vec{p}_2, \vec{p}_3)\) are defined by a transformation matrix \(M_X\).

\[
(\vec{p}_1 \; \vec{p}_2 \; \vec{p}_3) = (\vec{c}_1 \; \vec{c}_2 \; \vec{c}_3) \cdot M_X
\]

(22)

where \(\vec{c}_1, \vec{c}_2\) and \(\vec{c}_3\) are the standard conventional lattices. In the program, all the matrices \(M_X\) are given as follows:

\[
M_P = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} ;
M_C = \begin{pmatrix} 0.5 & 0.5 & 0 \\ -0.5 & 0.5 & 0 \\ 0 & 0 & 1 \end{pmatrix} ;
M_B = \begin{pmatrix} 0.5 & 0 & -0.5 \\ 0 & 1 & 0 \\ 0.5 & 0 & 0.5 \end{pmatrix} ;
M_A = \begin{pmatrix} 1 & 0 & 0 \\ 0.5 & -0.5 & 0 \\ 0 & 0.5 & 0.5 \end{pmatrix} ;
\]

\[
M_R = \begin{pmatrix} 2/3 & -1/3 & -1/3 \\ 1/3 & 1/3 & -2/3 \\ 1/3 & 1/3 & 1/3 \end{pmatrix} ;
M_F = \begin{pmatrix} 0 & 0.5 & 0.5 \\ 0.5 & 0.5 & 0 \\ 0.5 & 0 & 0.5 \end{pmatrix} ;
M_I = \begin{pmatrix} -0.5 & 0.5 & 0.5 \\ 0.5 & -0.5 & 0.5 \\ 0.5 & 0.5 & -0.5 \end{pmatrix} .
\]
4. The character tables for $R$-little group and $S$-little group

Figs. S1 and S2 show the character tables for $R$-little group and $S$-little group, respectively. At the $k$-point $[(u, v, w)]$ given in the conventional reciprocal basis, the block $\begin{bmatrix} x + iy \\ a & b & c \end{bmatrix}$ corresponds to a complex value of $(x + iy) \cdot \exp[i\pi(au + bv + cw)]$.

**FIG. S1:** The CRT of $R$-little group in the BCS convention.

**FIG. S2:** The CRT of $S$-little group in the BCS convention.