High-throughput screening for Weyl Semimetals with $S_4$ Symmetry

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Abstract

Based on irreducible representations (or symmetry eigenvalues) and compatibility relations, a material can be predicted to be a topological/trivial insulator [satisfying compatibility relations] or a topological semimetal [violating compatibility relations]. However, Weyl semimetals usually go beyond this symmetry-based strategy. In other words, the Weyl nodes could emerge in a material, no matter if its occupied bands satisfy compatibility relations, or if the symmetry indicators are zero. In this work, we propose a new topological invariant $\chi$ for the systems with $S_4$ symmetry, which can be used to diagnose the Weyl semimetal phase. It can be easily computed through the one-dimensional Wilson-loop technique. By applying it in the high-throughput screening in first-principles calculations, we predict a lot of Weyl semimetals in both nonmagnetic and magnetic compounds.

I. INTRODUCTION

In the last few years, the understanding of topological phases has been greatly improved due to the significant progress in theoretical algorithms, such as symmetry classifications [1–3], topological quantum chemistry (TQC) [4–8], and symmetry indicators (SIs) [9, 10]. It turns out that these theories are very similar in identifying topological phases in three-dimensional (3D) crystals except for the fragile phases [11–13], which can be only diagnosed by the TQC. In principle, they all rely on the symmetry-based strategy, in which two ingredients are needed. The first one is the computed irreducible representations (irreps) of the occupied states in a material, which can be computed with an open-source code irvsp [14–16]. The second one is the compatible relations in 230 space groups (SGs), which are released for the first time within the work of TQC [4] and open-accessible on the Bilbao Crystallographic Server (BCS) [15–17]. With the code –CheckTopologicalMat– on the BCS [18], the topology of a material can be “automatically” diagnosed based on the occupied states at several maximal high-symmetry $k$-points in the 3D Brillouin zone (BZ). Recently, the high-throughput screening of topological materials has been performed straightforwardly [18–20].

Generally speaking, if the occupied bands of a material satisfy compatibility relations, it could be classified as an insulator. Otherwise, it is classified as a symmetry-enforced semimetal. However, it’s well known that the Weyl nodes [21–29] do not need any symmetry protections (but the lattice translations), making the appearance of Weyl nodes completely beyond the symmetry-based strategy. In other words, no matter if its occupied bands satisfy the compatibility relations, or if the SIs are zero, Weyl nodes can still emerge. Two conjectures are implied explicitly: i) the “topological” materials predicted by the nonzero SIs could be Weyl semimetals (WSMs) [18–20]; ii) the “trivial” materials classified by the symmetry-based strategy (i.e., all SIs are zero) could also be WSMs [30].

Here, we present an effective method to diagnose the WSM phase in the systems with $S_4$ symmetry, no matter whether time-reversal symmetry (TRS) is respected or not. A topological invariant $\chi$ is defined as the integral of the Berry curvature on a certain surface in the 3D BZ. By employing the one-dimension (1D) Wilson-loop technique, $\chi$ can be easily computed by tracing the evolution of the average Wannier charge centers. We have demonstrated that a nonzero $\chi$ guarantees the existence of Weyl nodes in the systems. By applying it in our first-principles calculations on the materials of twenty SGs, whose symmetry operators contain $S_4$ symmetry but no inversion symmetry (IS), we predict a lot of WSMs in both nonmagnetic and magnetic compounds, which can be further checked in future experiments.

II. THE DEFINITION AND PHYSICAL MEANING OF THE TOPOLOGICAL INDEX $\chi$

A. Systems with only $S_4$ symmetry

In a general case, we consider only $S_4$ symmetry in a system. In order to determine the existence of Weyl nodes in an $S_4$-symmetric system, one could compute the net topological charge (NTC) enclosed in a quarter BZ, reshaped as a triangular prism (spanned by the $z$ $(k_z)$ axis and a $xy$-plane $(k_x,k_y$-plane) triangle $\tilde{M}'\tilde{\Gamma}\tilde{M}$–$\tilde{M}'$, which can be expressed as

$$2\pi \times NTC = \int_{S'} \Omega d\mathbf{S}' + \int_{\mathbf{S}} \Omega d\mathbf{S} + \int_{S_{\mathbf{3}}} \Omega d\mathbf{S}_{\mathbf{3}}$$

(1)
Here, $\Omega$ is the Berry curvature, which is a vector and has three components in 3D momentum space. In Fig. 1(a), the two surfaces ($S$ and $S'$) of the prism are colored in orange and cyan respectively, while the $S_4$ surface spanned by the $z$ axis and $M-M'$ segment is not shadowed. Their normal vectors are pointing from inside to outside of the surface. In the presence of $C_{2z}$ symmetry ($C_{2z} = [S_4]^2$), the first integral on $S_4$ surface has to be zero, since $C_{2z}$ symmetry reverses the normal vector of this surface.

To reveal the relationship between the first and the second terms under $S_4$ symmetry, we introduce an intermediate surface $S''$ [colored in yellow in Fig. 1(a)]. The $C_{4z}$ symmetry and IS yield the following equations

$$\int S \Omega dS = \int_{S''} \Omega dS'' = \int_{S'} \Omega dS', $$

where the normal vector of $S''$ surface is depicted in Fig. 1(a). The first equation is because of $C_{4z}$ symmetry, and the second equation is because IS makes $\Omega(k) = \Omega(-k)$. Therefore, under the combined symmetry $S_4$, the first integral is equal to the third one in the right-hand part of Eq. (1). Note that neither $C_{4z}$ nor IS is preserved in these systems.

Then, we define a topological invariant

$$\chi \equiv \frac{1}{\pi} \int S \Omega dS$$

Substituting Eq. (2) into Eq. (1), the NTC can be simply expressed as $NTC = \chi$. It’s worth noting that the topological invariant $\chi$ is an integer, which indicates the net topological charge in a quarter of BZ [i.e., the prism in Fig. 1(a)]. A proof with the Wilson-loop technique will be given later.

**B. $S_4$-invariant systems with $C_{2,110}$ symmetry**

In 230 SGs, we find that there are twenty SGs, which have $S_4$ symmetry, but neither four-fold rotational symmetry nor IS. These $S_4$-invariant SGs are listed in Table I. The topological charge in a quarter of BZ [i.e., the prism in Fig. 1(a)]. The first equation is because of $S_4$ symmetry ($S_4 = [S_4]^2$), and the second equation is because IS makes $\Omega(k) = \Omega(-k)$. Therefore, under the combined symmetry $S_4$, the first integral is equal to the third one in the right-hand part of Eq. (1). Note that neither $C_{4z}$ nor IS is preserved in these systems.

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**C. 1D Wilson-loop technique**

To compute the integral for the topological invariant $\chi$, one can employ the 1D Wilson-loop technique. The average Wannier charge centers $[\Theta(k_x, k_y)]$ of the $k_z$-directed Wilson loops $[(k_x, k_y, 0) \rightarrow (k_x, k_y, 2\pi)]$ are defined as follows

$$\Theta(k_x, k_y) = \int_{(k_x, k_y, 0)}^{(k_x, k_y, 2\pi)} Tr[\vec{A}(k)] dl,$$

$$e^{i\Theta(k_x, k_y)} = Det(W(k_x, k_y)),$$

$$W_{mn}(k_x, k_y) \equiv \langle u_m(k_x, k_y, 2\pi) \prod_{k_z} P(k) | u_n(k_x, k_y, 0) \rangle,$$
where $\vec{A}(k) = i \langle u_m(k)| \partial_k | u_m(k) \rangle$, and $| u_m(k) \rangle$ are the Bloch eigenstates of the Hamiltonian $H(k)$ of the system. The indices $m, n$ run over its occupied bands, and $P(k) = | u_m(k) \rangle \langle u_m(k) |$ is the projector on the subspace of occupied bands at momentum $k$. It’s also known as $\Theta(k_x, k_y) = \sum_{j} \theta_j(k_x, k_y)$, with $\theta_j(k_x, k_y)$ representing the phase of the $j$th eigenvalue of the Wilson matrix $W(k_x, k_y)$ on occupied Bloch bands.

By plotting the average Wannier charge centers $\Theta(k_x, k_y)$ [or individual phases $\theta_j(k_x, k_y)$] as a function of the $xy$-plane path (called “Wilson bands” for short), the Eq. (2) can be rewritten as

$$\chi = \frac{1}{\pi} \int_{\vec{Γ} - \vec{M}} \text{or} \int_{\vec{Γ} - \vec{K} - \vec{M}} d\Theta(k_x, k_y)$$  \hspace{1cm} (4)

The $xy$-plane paths for the $S_4$-invariant SGs are given in Table 1. Thus, regardless of which one is the $xy$-plane path of the Wilson loops (WLP), the $\chi$ can be easily obtained in a Wilson-band plot, by counting the number of the positively-sloped lines crossing two horizontal reference lines [$\theta = 2\pi \delta$ and $\theta = 2\pi (1 - \delta)$ with $\delta \neq 0$ or $1/2$], and subtracting from it the number of negatively-sloped crossing ones (see examples in Fig. 2).

There are two particular paths at $\vec{Γ}$ and $\vec{M}$ [i.e., $W(\alpha, \alpha)$ with $\alpha = 0/\pi$], since they are the starting and ending loops, respectively. In the presence of $S_4$ symmetry, $W(\alpha, \alpha) = W^\dagger(\alpha, \alpha)$ because $S_4$ symmetry flips the direction of the 1D Wilson loops. This implies $\Theta(\alpha, \alpha) = -\Theta(\alpha, \alpha) \mod 2\pi$, resulting in $\Theta(\alpha, \alpha) = n\pi$. Substituting it into Eq. (4), one can conclude that $\chi$ has to be an integer. Here, we define a new $S_4$ SI in the absence of TRS as

$$s_4 = |\Theta(0, 0) + \Theta(\pi, \pi)|/\pi \mod 2,$$  \hspace{1cm} (5)

$n^0_K$ indicates the number of occupied states with $S_4$ eigenvalue $\lambda_\alpha = e^{i \pi n^0_K}$ ($\alpha = 0, 1, 2, 3$) at the $S_4$ invariant momentum (SIM) $K$ (See more details in the SM). Since $s_4 = 1$ implies $\chi = 2n + 1$ (nonzero), a magnetic WSM phase can be indicated by $s_4 = 1$.

### D. $S_4$-invariant systems with TRS

Once imposing TRS in the systems, both $S_4$ symmetry and TRS are preserved on the two particular $k_z$-directed loops. More importantly, each $k$-point on the loops respects $C_{2z}$ symmetry, which makes the two Wilson matrices $[W(\alpha, \alpha), \alpha = 0, \pi]$ block-diagonal by the $C_{2z}$ eigenvalues $\pm i$. TRS sends the states in the $+i$ subspace to those in the $-i$ subspace, while $S_4$ symmetry relates them in the same subspace. Considering $2N$ occupied bands, TRS makes the eigenvalues of the two Wilson matrices in the form of \(\{e^{i\theta_2}, e^{i\theta_2}, e^{i\theta_4}, e^{i\theta_4}, \ldots, e^{i\theta_{2N}}, e^{i\theta_{2N}}\}\). On the other hand, in one subspace (e.g. $C_{2z}$ eigenvalue $+i$), $S_4$ symmetry yields the constraint: $\phi(\alpha) = -\phi(\alpha) \mod 2\pi$ with $e^{i\phi(\alpha)} = \prod_{j=1}^{N} e^{i\theta_{2j}}(\alpha, \alpha)$ resulting in $\phi(\alpha) = n\pi$.

Considering the other subspace related by TRS, one concludes that $\Theta(\alpha, \alpha) = 2\phi(\alpha) = 2n\pi$, leading that the invariant $\chi$ has to be an even number ($\chi = 2n$) for the systems with TRS and $S_4$ symmetry. It’s notable that the $S_4$ SI $s_2$ can be easily defined as $s_2 = [\phi(0) + \phi(\pi)]/\pi \mod 2$ in the Wilson-loop calculations (see more details in the SM).

### III. HIGH-THROUGHPUT SCREENING OF WSMs

A nonzero $\chi$ indicates the existence of the Weyl nodes in the $S_4$-invariant systems. By computing the topological invariant $\chi$, one can easily diagnose the WSM phase in a material. Therefore, we compute the Wannier charge centers in $k_z$-directed Wilson loops in our first-principles calculations with spin-orbit coupling (SOC), to search for WSMs. In twenty SGs with $S_4$ symmetry, we discover many WSMs with both trivial and nontrivial SIs [1, 9], even though they satisfy the compatibility relations.

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**FIG. 3:** (Color online) (a) The Wilson bands of the $xy$-plane path for Hg$_2$SnSe$_4$. (b) The band structure with SOC. (c,d) The evolution of Wannier charge centers in the $k_z = 0$ and $k_z = \pi$ planes. (e,f) The (001) and (100) surface states of Hg$_2$SnSe$_4$. Filled squares and circles stand for the projections of Weyl points of different chirality.
A nonzero invariant $\chi$ suggests that some materials, previously predicted to be trivial insulators according to the $S_4$ indicator $z_2 = 0$, turn out to be WSMs [30]. Here, we choose Hg$_2$SnSe$_4$ and Cu$_2$Te$_2$Br$_2$O$_5$ as two examples of this kind of materials. The SOC band structure of Hg$_2$SnSe$_4$ with SG 82 is shown in Fig. 3(b), exhibiting a direct band gap along the high-symmetry lines. The occupied bands satisfy the compatibility relations and have a trivial SI ($i.e., z_2 = 0$). Therefore, Hg$_2$SnSe$_4$ is generally classified as a trivial insulator in the previous literatures [18, 20]. However, our 1D Wilson-loop calculations along $\Gamma$–$M$ in Fig. 3(a) show that the topological invariant $\chi$ is $-2$, indicating the existence of Weyl nodes in Hg$_2$SnSe$_4$. This result also can be checked with the criterion $\eta \neq z_2$, as defined in Ref. [30] for the systems with both $S_4$ symmetry and TRS. Here, $\eta$ is defined as $(-1)^{\nu}(-1)^{\nu_1}$ with $\nu_1$ and $\nu_2$ the time-reversal $Z_2$ invariants in $k_z = 0$ and $k_z = \pi$ planes, respectively. Wilson bands for the two planes are plotted in Figs. 3(c) and (d), respectively. One can find that $\nu_1 = 1$ and $\nu_2 = 0$, resulting in $\eta = 1$. Moreover, the $S_4$ $z_2$ is computed to be zero [19, 20]. So the criterion of $\eta \neq z_2$ still works in the WSM Hg$_2$SnSe$_4$.

After carefully checking the energy gap, we do find eight Weyl nodes with topological charge $|C| = 1$ in the full BZ, as shown in Table II, which are all related by symmetries in the material. As a hallmark of WSMs,
TABLE II: Distribution of Weyl points and associated topological charge in a quarter of the 3D BZ for Hg$_2$SnSe$_4$, Cu$_2$Te$_2$Br$_2$O$_5$, Zr$_3$Sb and Ta$_3$Ge. The positions of Weyl points are given in Cartesian coordinates.

| WSMs      | Positions ($k_x, k_y, k_z$) [in units of 1/Å] | Charge | $E - E_F$ [eV] | Multiplicity |
|-----------|-----------------------------------------------|--------|---------------|--------------|
| Hg$_2$SnSe$_4$ | (0.0028, 0.0181, 0.0737) | -1     | 0.0945        | 8            |
| Cu$_2$Te$_2$Br$_2$O$_5$ | (0.3674, 0.3901, 0.4846) | -1     | 0.1402        | 8            |
|           | (0.2952, 0.3460, 0.2522) | -1     | 0.0084        | 8            |
|           | (-0.0947, 0.1980, 0.4937) | 1      | 0.0989        | 4            |
|           | (-0.0497, 0.2040, 0.4937) | 1      | 0.1140        | 4            |
| Zr$_3$Sb | (0.1943, 0.2129, 0.4411) | -1     | 0.0906        | 8            |
|           | (0.0192, 0.3871, 0.0000) | 1      | -0.0338       | 4            |
|           | (0.0493, 0.3975, 0.0000) | 1      | -0.0344       | 4            |
|           | (-0.1223, 0.3743, 0.2395) | -1     | -0.0473       | 8            |
|           | (-0.1228, 0.3640, 0.2358) | -1     | -0.0481       | 8            |
|           | (-0.0240, 0.2715, 0.2307) | -1     | -0.0520       | 8            |
|           | (-0.1585, 0.2538, 0.2368) | 1      | -0.0618       | 8            |
|           | (-0.0706, 0.2514, 0.2362) | -1     | -0.0673       | 8            |
| Ta$_3$Ge | (0.0107, 0.4512, 0.2281) | -1     | 0.0947        | 8            |
|           | (0.0679, 0.2533, 0.0798) | -1     | 0.0395        | 8            |
|           | (-0.0702, 0.1591, 0.5455) | -1     | 0.0351        | 8            |
|           | (0.0225, 0.5648, 0.1636) | -1     | 0.0243        | 8            |
|           | (0.0426, 0.0735, 0.3311) | -1     | 0.0139        | 8            |
|           | (0.2291, 0.2970, 0.4729) | 1      | 0.0026        | 8            |
|           | (-0.1229, 0.2080, 0.2910) | -1     | 0.0140        | 8            |

the nontrivial surface sates on the semi-infinite (001) and (100) surfaces are shown in Figs. 3(c) and (f), respectively. Guided by the projections of the Weyl points represented by the square and circle points, we can clearly see that the Fermi arc states connecting the projections of the Weyl points. In addition, two arc states have to go across the $k_z = 0$ line, because it’s the edge of the $k_z = 0$ plane with a nontrivial $Z_2$ invariant $\nu_1$.

Then, we present the obtained band structure of Cu$_2$Te$_2$Br$_2$O$_5$ in Fig. 4(b). Based on the irreps on the maximal high-symmetry $k$-point, its occupied bands satisfy the compatibility relations and have a trivial SI. However, the $\chi$ is calculated to be -2 [Fig. 4(a)]. Consequently, we also find Weyl points in its bulk states, as shown in Table II. The Fermi arc states on (100) surface are presented in Figs. 4(c) and (d).

2. WSMs with nontrivial SI

We can also find that there are some WSMs, which are previously classified as topological insulators, because they have nonzero SIs and satisfy the compatibility relations. We take Zr$_3$Sb and Ta$_3$Ge as examples for this kind of WSMs.

In the database [18–20] discovered by the symmetry-based strategy, the $S_4$ SIs $\zeta_2$ of Zr$_3$Sb and Ta$_3$Ge are computed to be 1, leading that Zr$_3$Sb and Ta$_3$Ge are classified as the topological insulating phase. Although there is a continuous direct band gap of the band structure along the high-symmetry lines in Fig. 5(b), the 1D Wilson-loop calculations reveal the nontrivial topological invariant $\chi = -6$ of Zr$_3$Sb and $\chi = -10$ of Ta$_3$Ge, as shown in Fig. 5(a) and Fig. S4(j), guaranteeing the appearance of Weyl nodes in these materials. The Fermi-arc states of Zr$_3$Sb on (100) plane are shown in Figs. 5(c) and (d) for two constant energies.
3. Magnetic WSMs with $s_4 = 1$

In contrast to the SIs in nonmagnetic systems, the new topological invariant $\chi$ can be used to find the magnetic WSMs. Here, we choose Fe$_2$AgGaTe$_4$ as an example for illustrating this kind of materials, which has $s_4 = 1$. The band structure of ferromagnetic Fe$_2$AgGaTe$_4$ with SOC and the Wannier charge centers of $k_z$-directed Wilson loops are shown in Figs. 6(b) and (a), respectively. In Fig. 6(c), we can see that this is a continuous direct band gap between the conduction bands (blue-colored) and valence bands (red-colored), although the SOC band gaps are very small. The nontrivial topological invariant ($\chi = -1$) is consistent with the indicator $s_4 = 1$, which can guarantee the existence of Weyl nodes in the ferromagnetic Fe$_2$AgGaTe$_4$.

IV. CONCLUSION

We propose a new topological invariant $\chi$ for the $S_4$-invariant systems, which can be easily computed through the Wilson-loop technique. Based on the calculated topological invariant $\chi$ in our first-principles calculations, we have performed high-throughput screening for WSMs in materials of twenty $S_4$-invariant SGs. A lot of WSMs are predicted theoretically and the Fermi-arc states are presented as well for some representatives. The method of the topological invariant $\chi$ is very efficient and can be widely used to predict more WSMs with $S_4$ symmetry in both magnetic and nonmagnetic materials.

Calculation methods Our first-principles calculations were performed with the VASP package [31, 32] based on the density functional theory (DFT) with the projector augmented wave (PAW) method [33, 34]. The generalized gradient approximation (GGA) with exchange-correlation functional of Perdew, Burke and Ernzerhof (PBE) for the exchange-correlation functional [35] was employed. The cut-off energy of plane wave basis set was set to be 125% ENMAX value in the pseudo-potential file. A $\Gamma$-centered Monkhorst-Pack grid with 30 k-points per 1/Å was used for the self-consistent calculations. The lattice and atomic parameters in the Inorganic Crystal Structure Database (ICSD) were employed in our calculations [36]. The electronic structures with SOC were carried out. The Wilson-loop technique [37] was used to calculate topological invariants and chiral charges [22, 24], which was homemade and implemented within the VASP package (i.e., vasp.5.3.3). The Fermi arc states were calculated based on the Green’s function method [38] of the semi-infinite systems, which were constructed by the maximally localized Wannier functions [39].

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