Systematic investigation of emergent particles in type-III magnetic space groups

Gui-Bin Liu,1,* Zeying Zhang,2,* Zhi-Ming Yu,1 Shengyuan A. Yang,3 and Yugui Yao1,†

1Centre for Quantum Physics, Key Laboratory of Advanced Optoelectronic Quantum Architecture and Measurement (MOE), School of Physics, Beijing Institute of Technology, Beijing 100081, China and Beijing Key Laboratory of Nanophotonics and Ultrafine Optoelectronic Systems, School of Physics, Beijing Institute of Technology, Beijing 100081, China
2College of Mathematics and Physics, Beijing University of Chemical Technology, Beijing 100029, China
3Research Laboratory for Quantum Materials, Singapore University of Technology and Design, Singapore 487372, Singapore

(Dated: February 16, 2022)

In three-dimensional (3D) crystals, emergent particles arise when two or multiple bands contact and form degeneracy (band crossing) in the Brillouin zone. Recently a complete classification of emergent particles in 3D nonmagnetic crystals, which described by the type-II magnetic space groups (MSGs), has been established. However, a systematic investigation of emergent particles in magnetic crystals has not yet been performed, due to the complexity of the symmetries of magnetically ordered structures. Here, we address this challenging task by exploring the possibilities of the emergent particles in the 674 type-III MSGs. Based on effective $k \cdot p$ Hamiltonian and our classification of emergent particles [Yu et al., Sci. Bull. 67, 375 (2002)], we identify all possible emergent particles, including spinful and spinless, essential and accidental particles in the type-III MSGs. We find that all emergent particles in type-III MSGs also exist in type-II MSGs, with only one exception, i.e. the combined quadratic nodal line and nodal surface (QNL/NS). Moreover, tabulations of the emergent particles in each of the 674 type-III MSGs, together with the symmetry operations, the small corepresentations, the effective $k \cdot p$ Hamiltonians, and the topological character of these particles, are explicitly presented. Remarkably, combining this work and our homemade SpaceGroupRep and MSGCorep packages will provide an efficient way to search topological magnetic materials with novel quasiparticles.

I. INTRODUCTION

Since the discovery of topological Weyl and Dirac semimetals, the investigation of emergent particles has experienced rapid development and been attracting a variety of interests in condensed matter physics [1–23]. Compared with the elementary particles in high-energy physics, the quasiparticles in solids have much more abundant species due to looser symmetry constraints and then embrace more rich physics [24–37]. Thus identifying and classifying all the possible emergent particles in solids becomes a fundamentally important but also a challenging work. Recently, in Ref. [38] we present a complete list of emergent particles in three-dimensional (3D) nonmagnetic crystals with $T$-symmetry. In this work, we establish such list for the 3D magnetic crystals belonging to type-III magnetic space groups (MSGs).

In three dimensions, the crystal structure of materials are described by the symmetry of space groups (SGs). By introducing magnetic order, the crystals exhibit one more degree of freedom and then should be described by MSGs. There are in total 1651 MSGs which are divided into four types. The type-I MSGs are just the ordinary SGs, and do not have any anti-unitary operation. In contrast, the general form of the other three types of MSGs can be written

$$M = S + AS$$

with $S$ a unitary subgroup with index 2 of the MSG $M$ and $A$ an anti-unitary operation. $M$ can be constructed from an ordinary SG $G$. When $S = G$, the MSGs can be further classified into two types by whether $A$ is time reversal symmetry $T$ (type II) or a combined operation of $T$ and a pure translation (type IV). One then knows that the type-II MSGs have $T$ symmetry and are applied to nonmagnetic crystals. In type-III MSGs, $S$ is an isorotational (translationengleiche) subgroup of $G$ with index 2 and $A$ is a combined operation containing $T$ and an unitary (spatial) operation in $G - S$, making $AS = T(G - S)$.

It is clear that the symmetry of the type-III MSGs is lower than that of the type-II MSGs and heretofore most studies on emergent particles are in systems with $T$ symmetry, i.e. the systems belonging to the type-II MSGs. However, it should be noted that the emergent particles also can appear in magnetic systems [1, 39–44]. Actually, the original candidate for topological Weyl semimetal is a magnetic material [1]. In Ref. [39], Tang et al. predicted orthorhombic antiferromagnet CuMnAs as a candidate of magnetic Dirac semimetal. Moreover, novel emergent particles in magnetic materials with higher-order dispersion or 1D manifold of degeneracy also has been unveiled in previous works [45–47]. However, people still lack an overall and systematic understanding about what types of emergent particles can exist in magnetic crystals with various MSGs.

Towards this goal, in this work we perform an exhaustive investigation of the emergent particles in type-III MSGs and compile an encyclopedia for them. This is done for each of the 674 type-III MSGs, and the lists of

* These two authors contribute equally to this work.
† ygyao@bit.edu.cn
all possible emergent particles along with the symmetry conditions, the effective $k \cdot p$ Hamiltonians, and the topological characters of these particles for each type-III MSG is presented in SM-SIII (Section SIII in the supplementary material [48]). The main results are summarized in Tabs. I, II and the Tables in SM-SI, corresponding to the list of all possible emergent particles in type-III MSGs and a quantitative mapping between the emergent particles and type-III MSGs, respectively. Our key findings are the following. (i) According to our classification, there exist total 18 types of spinless emergent particles and 19 types of spinful emergent particles, as shown Tab. I. All these emergent particles can be realized in nonmagnetic systems. (ii) The type-III MSGs can also host several kinds of complex emergent particles, which are constituted by two different types of particles (see Tab. II). Remarkably, one of the complex quasiparticles, namely QNL/NS [combined quadratic nodal line (QNL) and nodal surface (NS)], only exists in magnetic systems. (iii) This encyclopedia provides a platform for systematic research on emergent particles by scanning all type-III MSGs. Compared with case-by-case study, the systematic research can usually provide comprehensive knowledge, complete inspection, and deep insights. Much important information can be and only can be inferred from our work. For example, only with our classification, one knows that in type-III MSGs the largest topological charge (Chern number) for the nodal point is $|C| = 3$ and the largest order of energy splitting for nodal line is quadratic. For comparison, the former is $|C| = 4$ and the latter is cubic in type-II MSGs [5, 49]. At last, for the complex particle QNL/NS, we also construct concrete lattice model to demonstrate its existence and study its surface state.

Our work not only presents a complete classification and detailed analysis of the emergent particles in type-III MSGs but also is useful for searching novel topological magnetic materials with desired emergent particles. For example, for a given magnetic crystals, when the first-principles band structure are obtained, one can use our homemade MSGCorep package [50] to calculate the small corepresentations (coreps) of the degenerate bands. Then the species of the degeneracy can be directly identified by looking up the tables in this encyclopedia.

II. RATIONALE

The approach to obtain the results in this work is similar to that in Ref. [38]. We first calculate the small coreps at all high-symmetry k-points and k-lines in the Brillouin zone (BZ) of each of the 674 type-III MSGs based on our homemade package SpaceGrouprep [51] and MSGCorep [50]. Both single-valued [for spinless systems, without spin-orbit coupling (SOC)] and double-valued coreps [for spinful systems, with SOC] are considered. Consider a type-III MSG $M$, which can be written as $M = S + T(G - S)$ [52]. For a wave vector $k$ in the BZ, its magnetic little group (MLG), denoted by $M_k$, is the subgroup of $M$ which is composed of the elements whose point parts leave $k$ invariant, i.e. $M_k = \{ Q \in M \land P(Q)k = k \}$, in which $P(Q)$ means the point part of $Q$ and $\doteq$ means two wave vectors differ by a reciprocal lattice vector. Note that $T k = -k$, $P(Q) = R$ if $Q = \{ R | t \}$, and $P(Q) = T R$ if $Q = T \{ R | t \}$. The MLG $M_k$ relates to the little group of $k$ in $S$, denoted by $S_k$, in two ways: (i) $M_k = S_k$, in this case there is no element $\{ R | t \}$ in $G - S$ which satisfies $R k = -k$ and hence $M_k$ is unitary; (ii) $M_k = S_k + A$, in this case $S_k$ is the unitary subgroup of $M_k$ and all elements in $A$ are anti-unitary with $S_k = |A|$. Then the small coreps of $M_k$ can be calculated according to the small representations of $S_k$ [50–52]. Here, we adopt the convention used in the book [52] to describe MSG. The book uses the BNS notation [53, 54] for MSG, but some MSGs are mistaken by the authors, which is also mentioned in [55]. We has corrected the MSGs which are not compatible with the BNS definition [50].

With the coreps information, we identify all the possible degeneracies including both essential and accidental degeneracies. For each degeneracy (at a certain high-symmetry wave vector $k_0$), we construct the $k \cdot p$ Hamiltonians according to the symmetry constraints

\[
\begin{align*}
\mathcal{D}(Q)H(k)\mathcal{D}(Q)^{-1} &= H(Rk), \quad \text{if } Q = \{ R | t \} \\
\mathcal{D}(Q)H^*(k)\mathcal{D}(Q)^{-1} &= H(-Rk), \quad \text{if } Q = T \{ R | t \}
\end{align*}
\]

where $\mathcal{D}(Q)$ is the unitary corep matrix of $Q$ for each $Q \in M_{k_0}$ and $\mathcal{D}(Q)$ can be either irreducible (for essential degeneracy) or reducible (for accidental degeneracy). Using the iteratively simplifying algorithm, $H(k)$ can be obtained up to any specified order of $k$ [56]. Here we use the lowest order of $k$ that is essential to make correct classification of emergent particles. Most of the physical properties of the degeneracies, such as energy dispersion and topological charge can be directly inferred from the constructed effective Hamiltonian. Finally, we classify all the band crossings by the standard of the classification established in [38] and the results are shown in Tabs. I (refer to the SM of [38] for the details of each notation in Tab. I), II, and the tables in SM. It should be pointed out that Weyl points at general k-points only need translation symmetries to protect them and hence they are not involved in our classification, as stated in [38].

In Tab. I, for each emergent particle, we explicitly list its occurrence number at the high-symmetry momenta of all type-III MSGs and also list the number of the type-III MSGs hosting it. For both counting number, four cases are listed separately: spinless essential particle, spinless accidental particle, spinful essential particle, and spinful accidental particle. These data can tell us which emergent particles are common and which ones are rare. As can be seen: (i) C-1 WP (Charge-1 Weyl point) is very common and WP becomes more and more rare as $|C|$ increases. Statistics further shows that C-2 WP only exists in tetragonal and hexagonal systems,
Table I. Classification and statistics of emergent particles in type-III MSGs. Similar to ref. [38], Abbr is the abbreviation for the notation of emergent particle, \(d_m\) is the dimension of the degeneracy manifold, \(d\) is the degree of degeneracy of the band crossing, \(L_d\) is the leading order of the band splitting near the crossing, and \(|\mathcal{C}|\) is the topological charge (Chern number for nodal point or Berry phase for nodal line) of the emergent particles. \(N_{\text{ess}}\) (\(N_{\text{acc}}\)) is the spinless particle’s occurrence number in SM-SIIIA (SM-SIIIB) for essential (accidental) degeneracy, and \(N^\text{SOC}_{\text{ess}}\) (\(N^\text{SOC}_{\text{acc}}\)) is similar but for spinful particles in SM-SIIIC (SM-SIIID). The number in the parentheses is the number of MSGs that host the particle.

| Notation                                    | Abbr       | \(d_m\) | \(d\) | \(|\mathcal{C}|\) | \(N_{\text{ess}}\) | \(N_{\text{acc}}\) | \(N^\text{SOC}_{\text{ess}}\) | \(N^\text{SOC}_{\text{acc}}\) |
|---------------------------------------------|------------|---------|-------|----------------|-------------------|----------------|----------------|----------------|
| Charge-1 Weyl point                          | C-1 WP     | 0 2     | (111) | 1              | 130 (59)          | 1448 (321)     | 218 (76)       | 1448 (321)     |
| Charge-2 Weyl point                          | C-2 WP     | 0 2     | (122) | 2              | 83 (37)           | 228 (56)       | 29 (21)        | 228 (56)       |
| Charge-3 Weyl point                          | C-3 WP     | 0 2     | (133) | 3              | \(\times\)       | 42 (14)        | \(\times\)     | 42 (14)        |
| Charge-4 Weyl point                          | C-4 WP     | 0 2     | (223) | 4              | \(\times\)       | \(\times\)      | \(\times\)     | \(\times\)     |
| Triple point                                 | TP         | 0 3     | (111) | \(\times\)     | 47 (18)           | 748 (222)      | \(\times\)     | 67 (27)        |
| Charge-2 triple point                        | C-2 TP     | 0 3     | (111) | 2              | 15 (10)           | \(\times\)      | 5 (5)          | \(\times\)     |
| Quadratic triple point                       | QTP        | 0 3     | (122) | \(\times\)     | 28 (10)           | \(\times\)      | \(\times\)     | \(\times\)     |
| Quadratic contact triple point               | QCTP       | 0 3     | (222) | 0              | 60 (26)           | \(\times\)      | \(\times\)     | \(\times\)     |
| Dirac point                                 | DP         | 0 4     | (111) | 0              | 83 (59)           | 173 (102)      | 349 (161)      | 565 (236)      |
| Charge-2 Dirac point                         | C-2 DP     | 0 4     | (111) | 2              | 2 (2)             | 30 (30)        | 6 (4)          | 30 (30)        |
| Charge-4 Dirac point                         | C-4 DP     | 0 4     | (111) | 4              | \(\times\)       | \(\times\)      | \(\times\)     | \(\times\)     |
| Quadratic Dirac point                        | QDP        | 0 4     | (122) | 0              | 42 (30)           | 18 (18)        | 9 (7)          | 10 (10)        |
| Charge-4 quadratic Dirac point               | C-4 QDP    | 0 4     | (122) | 4              | \(\times\)       | \(\times\)      | \(\times\)     | \(\times\)     |
| Quadratic contact Dirac point                | QCDP       | 0 4     | (222) | 0              | \(\times\)       | \(\times\)      | 13 (10)        | \(\times\)     |
| Cubic Dirac point                            | CDP        | 0 4     | (133) | 0              | \(\times\)       | \(\times\)      | 1 (1)          | \(\times\)     |
| Cubic crossing Dirac point                   | CCDP       | 0 4     | (223) | 0              | 3 (3)             | \(\times\)      | \(\times\)     | \(\times\)     |
| Sextuple point                               | SP         | 0 6     | (111) | 0              | 8 (8)             | \(\times\)      | 4 (4)          | \(\times\)     |
| Charge-4 sextuple point                      | C-4 SP     | 0 6     | (111) | 4              | \(\times\)       | \(\times\)      | \(\times\)     | \(\times\)     |
| Quadratic contact sextuple point             | QCSP       | 0 6     | (222) | 0              | \(\times\)       | \(\times\)      | \(\times\)     | \(\times\)     |
| Octuple point                                | OP         | 0 8     | (111) | 0              | \(\times\)       | \(\times\)      | 3 (3)          | \(\times\)     |
| Weyl nodal line                              | WNL        | 1 2     | (11)  | \(\pi\)        | 1510 (395)        | 3525 (470)     | 1243 (262)     | 1082 (232)     |
| Weyl nodal line net                          | WNL net    | 1 2     | (11)  | \(\pi\)        | 1143 (274)        | 1222 (294)     | 685 (150)      | 148 (57)       |
| Quadratic nodal line                         | QNL        | 1 2     | (22)  | 0              | 740 (173)         | \(\times\)      | 61 (19)        | \(\times\)     |
| Cubic nodal line                             | CNL        | 1 2     | (33)  | \(\pi\)        | \(\times\)       | \(\times\)      | \(\times\)     | \(\times\)     |
| Dirac nodal line                             | DNL        | 1 4     | (11)  | 0              | 12 (4)            | \(\times\)      | 223 (52)       | 178 (51)       |
| Dirac nodal line net                         | DNL net    | 1 4     | (11)  | 0              | \(\times\)       | 6 (2)          | 8 (4)          | \(\times\)     |
| Nodal surface                                | NS         | 2 2     | (1)   | \(\times\)    | 1257 (147)        | \(\times\)      | 765 (94)       | \(\times\)     |
| Nodal surface net                            | NS net     | 2 2     | (1)   | \(\times\)    | 442 (62)          | \(\times\)      | 168 (30)       | \(\times\)     |

and C-3 WP only exists on the \(\Delta(00u)\) line in hexagonal systems. (ii) Accidental WP’s are much more common than essential WP’s, which is also true for TP (Triple point), DP (Dirac point), and C-2 DP. (iii) CDP (Cubic Dirac point), CCDP (Cubic crossing Dirac point), and OP (Octuple point) are very rare, especially CDP only exists at the double-valued small corep \((A)_{7}A_{7}A_{7}\) of MSG 192.251 \((P6/m1c’c’\) (see Appendix A for the corep label). (iv) WNL (Weyl nodal line) is more common than C-1 WP, and WNL net is also very common.

Compared with the emergent particles in type-II MSGs [38], 6 types of emergent particles, i.e. C-4 WP, C-4 DP, C-4 QDP (Charge-4 quadratic Dirac point), C-4 SP (Charge-4 sextuple point), QCSP (Quadratic contact sextuple point), and CNL (Cubic nodal line), do not exist in type-III MSGs. Detailed differences are emphasized in red in Tabs. I and II, in which red cross means the particle exists in type-II MSGs but not in type-III MSGs, red number means the particle does not exist in type-II MSGs but exists in type-III MSGs, and black number (cross) means the particle exists (do not exist) in both type-II and type-III MSGs. Consequently, one finds that all non-complex particles in type-III MSGs also exist in type-II MSGs, and the complex emergent particle QNL/NS is the only one which exists in type-III MSGs but not in type-II MSGs.
Table III. Part of the spinless emergent particles in MSG 56.370 excerpted from the tables in SM-SIIIA and SM-SIIIB. The line above the table indicates the information about the notation of MSG (its unitary subgroup in the parentheses), the Bravais lattice, the generators of the MSG, whether $I\Gamma$ exists, and whether SOC is considered. $k$ is a high-symmetry $k$-point or k-line defined in the Tab. 3.6 of [52], “generators” are the point parts for the generators of the MLG of $k$, “dim” is the dimension of the corep, and “matrices” are the corep matrices of the MLG generators. The unitary matrices $\lambda_m$, $\sigma_p$, and $\Gamma_q$ are defined in SM-SIV. All $k\cdot p$ Hamiltonians are defined in SM-SV. Node type is just the type of emergent particles.

56.370, \textit{Pc’cm’} (14, $P2_1/c$) \hspace{1cm} \Gamma_\nu, \{C_{2y}\{\frac{1}{2}\frac{1}{2}\frac{1}{2}\}\} \{I\{\frac{1}{2}\frac{1}{2}\frac{1}{2}\}\}, \{C_{2x} T\{\frac{1}{2}\frac{1}{2}\frac{1}{2}\}\}, Without \ IT, without \ SOC

| $k$ name | info | generators | corep | dim | matrices | $k\cdot p$ Hamiltonian type | $|C|$ |
|----------|------|------------|-------|-----|----------|----------------------------|------|
| $\Gamma$ 000 | $C_{2y}, I, C_{2x} T$ | (T)$\Gamma_{1}^+$ | 1 | | 1, 1, 1 | $H_{10.46}$ | 0 |
| $\Gamma$ 010 | $C_{2y}, I, C_{2x} T$ | (T)$\Gamma_{1}$ | 1 | | 1, 1, 1 | $H_{10.46}$ | 0 |
| $\Gamma$ 010 | $C_{2y}, I, C_{2x} T$ | (T)$\Gamma_{2}^+$ | 1 | | 1, 1, 1 | $H_{10.46}$ | 0 |
| $\Gamma$ 010 | $C_{2y}, I, C_{2x} T$ | (T)$\Gamma_{2}$ | 1 | | 1, 1, 1 | $H_{10.46}$ | 0 |
| $Y$ 100 | $C_{2y}, I, C_{2x} T$ | (Y)$Z_{1}$ | 2 | $\sigma_{4}, \sigma_{3}, \sigma_{3}$ | | $H_{50.282}$ | P-WNL |
| $U$ 012 | $C_{2y}, I, C_{2x} T$ | (U)$A_{1}A_{1}$ | 4 | $\Gamma_{49}, \Gamma_{70}, \Gamma_{4}$ | | $H_{56.370}$ | 0 |
| $S$ 012 | $C_{2y}, I, C_{2x} T$ | (S)$C_{1}$ | 2 | $\sigma_{4}, \sigma_{4}$ | | $H_{52.358}$ | P-Ns |
| $R$ 111 | $C_{2y}, I, C_{2x} T$ | (R)$E_{1}^{+}E_{2}^{+}$ | 2 | $\sigma_{3}, \sigma_{4}$ | | $H_{55.358}$ | P-WNL/NS |
| $D$ 012 | $C_{2y}, C_{2x} T$ | (D)$W_{1}W_{2}$ | 2 | $\lambda_{20}\sigma_{4}$ | | $H_{55.358}$ | L-NS |
| $E$ 012 | $C_{2y}, C_{2x} T$ | (E)$U_{1}U_{2}$ | 2 | $\lambda_{20}\sigma_{4}$ | | $H_{55.358}$ | L-NS |
| $\Delta$ $\Gamma Y$ | $C_{2y}, C_{2x} T$ | \{(\Delta)A_{1}, (\Delta)A_{2}\} | 2 | | | $H_{49.297}$ | C-1 WP |
| $\Sigma$ $\Gamma X$ | $C_{2y}, C_{2x} T$ | \{(\Sigma)U_{1}, (\Sigma)U_{2}\} | 2 | | | $H_{55.59}$ | P-WNL |

III. AN EXAMPLE: MSG 56.370

As discussed above, we explore all the possibilities of the emergent particles in type-III MSGs and tabulate the results one MSG by one. The resulting tables are listed in SM. We then use a spinless system with MSG No. 56.370 (\textit{Pc’cm’}) as an example to provide a glimpse of the encyclopedia. Tab. III is an example excerpted from the tables for MSG 56.370 in SM-SIIIA and SM-SIIIB. In Tab. III, the first line provides some basic information of MSG 56.370, including unitary subgroup, BZ type, generating elements, whether the MSG has $I\Gamma$ symmetry (combined spatial inversion symmetry $I$ and $\mathcal{T}$), and whether SOC effect is considered.

The main part of Tab. III can be divided into six parts: information of high-symmetry momentum $k$, the point parts of the generating elements of $M_k$, the corep information of $M_k$, and the effective Hamiltonian, the type and the topological charge of the degeneracies. Particularly, we find that many coreps share the same matrices and so do the $k\cdot p$ Hamiltonians. Thus, we also explicitly list all the possible corep matrices and Hamiltonians in SM-SIV and SM-SV respectively. For example, the corep matrices for the generators of $M_{k=Y}$ are $D\{C_{2y}\{\frac{1}{2}\frac{1}{2}\frac{1}{2}\}\} = \sigma_{4}$ and $D\{I\{\frac{1}{2}\frac{1}{2}\frac{1}{2}\}\} = D\{T\{C_{2x}\{\frac{1}{2}\frac{1}{2}\frac{1}{2}\}\}\} = \sigma_{3}$ [57] with

\[
\begin{pmatrix}
0 & 1 \\
-1 & 0
\end{pmatrix}, \quad \begin{pmatrix}
1 & 0 \\
0 & -1
\end{pmatrix},
\]

and the effective Hamiltonian is

\[
H_{50.282}^{(X)A_{2}} = c_{2}k_{x}\sigma_{1} - c_{3}k_{y}\sigma_{2} + c_{1}\sigma_{0}.
\]

The subscript and superscript in $H_{50.282}^{(X)A_{2}}$ means that this matrix form of effective Hamiltonian firstly appear for the degeneracy with corep $(X)A_{2}$ at MSG 50.282.

P-WNL (P-NS) indicates that the high-symmetry k-point (e.g. $Y$, $S$) or the accidental band-crossing point on
a high-symmetry k-line (e.g. Σ) is actually a point residing on a WNL (NS), and similarly L-NS indicates that the high-symmetry k-line (e.g. D) resides on a NS. Therefore, when counting the occurrence numbers in Tabs. I and II, P-WNL is regarded as WNL, P-WNL/NS is regarded as WNL/NS, and both P-NS and L-NS are regarded as NS.

IV. COMPLEX PARTICLE: QNL/NS

As mentioned above, QNL/NS is a novel complex emergent particle that does not exist in nonmagnetic systems. Here we take a spinful system hosting QNL/NS for example to demonstrate the existence of QNL/NS. There are three type-III MSGs hosting QNL/NS, i.e. 176.147 (P6̅3/m’), 193.259 (P6̅3/m’c’), and 194.268 (P6̅3/m’c’). Without loss of generality, we construct a tight-binding (TB) model under the symmetric constraints of MSG 176.147 by our homemade MagneticTB package [58]. The simplest s orbitals, i.e. |s↑⟩ and |s↓⟩, are adopted to construct the TB model, which is enough to capture QNL/NS. Fig. 1(a) is the unit cell with irrelevant atoms omitted, showing an A-type antiferromagnetic configuration. The TB Hamiltonian is given in Appendix B.

The energy bands of the model is shown in Fig. 1(c), from which we can see that line Γ-A, line A-H (in fact the whole plane AHL) and point K are doubly degenerate. The four bands are divided into upper and lower portions which are separated by a gap and possess the same degeneracy over the whole BZ. Accordingly, the lower two bands are enough to host all possible essential particles in MSG 176.147, including three non-complex types, i.e. a QNL along Γ-A, a NS on plane AHL, and two C-1 WP’s at ±K points, and a complex type QNL/NS at A point (cf. the 176.147 table in the SM-SHIC). The band splitting around any point on Γ-A, such as the Q point in Fig. 1(c), is quadratic along both (100) and (110) directions, as shown in Fig. 1(d), which indicates Γ-A is a QNL.

Figure 1. Unit cell (a), bulk BZ and its projection to (100) surface (b), bulk energy bands (c,d), and density of states of semi-infinite system with (100) surface (e) of the TB model of MSG 176.147. ΔE in (d) means the band splitting. The parameters used are $\varepsilon = -0.5$, $t_1 = 0.4$, $t_2 = -0.1$, $t_3 = 0$, $r = -0.8$, $s_1 = 0.2$, $s_2 = s_3 = s_4 = 0$.

It should be pointed out that the coexistence of both QNL along Γ-A and NS on plane AHL does not necessarily lead to QNL/NS at A point. The existence of QNL/NS requires that the coreps of QNL and NS satisfy the compatibility relation with the coreps of their intersection point. For example, the type-II MSG 176.144 (P6̅3/m1’) have both QNL along Γ-A and NS on plane AHL but does not have QNL/NS at A point [17, 33]. None of type-II MSGs satisfies such compatibility relation and this is why QNL/NS does not exist in type-II MSGs.

V. CONCLUSIONS

In conclusion, we have studied all the possible emergent particles that can be stabilized by type-III MSG symmetries and compiled the results to an encyclopedia. Band crossings at all high-symmetry k-points and k-lines and originated from both single-valued and double-valued small coreps are analyzed. In addition to the essential degeneracy protected by a single small corep, accidental degeneracy induced by a pair of small coreps is also considered. Compared with the results of type-II MSGs in [38], the non-complex emergent particles existing in type-III MSGs form a subset of those in type-II MSGs, missing C-4 WP, C-4 DP, C-4 QDP, C-4 SP, QCSP, and CLN in type-III MSGs. The complex particle QNL/NS is the only one which exists in type-III MSGs but not in type-II MSGs. One can easily check...
which type-III MSGs can host a certain emergent particle in SM-SI. Apart from the emergent particles, this encyclopedia provides a quick reference of all small coreps at/on every high-symmetry k-point/k-line defined in [52], and it also provides the \( k \cdot p \) Hamiltonians for these k-points/k-lines. This work will be a convenient reference for emergent particles, symmetries, and \( k \cdot p \) models in the studies of magnetic topological nodal materials and related fields, and it will also facilitate the search for required emergent particles in magnetic materials.

Note: Please find the supplementary material “MSGIII_emergent_SM.pdf” in the source file (gzipped tar file).

ACKNOWLEDGMENTS

YY acknowledges the support by the National Key R&D Program of China (Grant No. 2020YFA0308800), the NSF of China (Grants Nos. 11734003, 12061131002), and the Strategic Priority Research Program of Chinese Academy of Sciences (Grant No. XDB30000000). GBL acknowledges the support by the international cooperation project of NSF of China (Grant No. 52161135108), the National Key R&D Program of China (Grant No. 2017YFB0701600) and the Beijing Natural Science Foundation (Grant No. Z190006). ZZ acknowledges the support by the NSF of China (Grant No. 12004028), and the China Postdoctoral Science Foundation (Grant No. 2020M670106). ZMY acknowledges the support by the NSF of China (Grant No. 12004035).

Appendix A: label of small corep

The small corep of a type-III MSG \( M = S + T(G - S) \) is constructed from one or two of the small representations of its unitary subgroup \( S \). The BZ and k-point naming of \( M \) are the same with those of \( G \), but they may be different from those of \( S \). Taking MSG 118.309 (\( P4'\text{~}n2' \)) for example, its \( S \) subgroup is space group No. 21 (\( C2\text{~}22 \)). Hence \( M \) has a simple tetragonal BZ, while \( S \) has a base-centered orthogonal BZ. The symbol \( A \) in the parentheses explicitly indicates the k-point name for \( M \), which is different from the k-point name for \( S \) here. However, even if the k-point names for both \( M \) and \( S \) happen to be the same, we still keep the parentheses. For example, MSG 118.309 also has small coreps \((A)T_2, (V)H_1H_1, (A)\Lambda_1, (Z)Z_2Z_2, (R)R_1R_2\), and so on.

Appendix B: TB model of MSG 176.147

According to the symmetries in MSG 176.147, a TB model based on orbitals \( \{|s \uparrow\rangle, |s \downarrow\rangle\} \) at each of the two magnetic atoms in the hexagonal cell shown in Fig. 1(a) can be constructed by the MagneticTB package [58] to show the existence of QNL/NS emergent particle. The obtained Hamiltonian is

\[
H(k) = \begin{bmatrix}
\varepsilon \sigma_3 + h_1 & h_2 + h_3 \\
h_2^* + h_3^* & \varepsilon \sigma_3 + h_1^*
\end{bmatrix}
\]  

(B1)

\[
h_1 = \begin{bmatrix}
t_2 f_1(k_{||}) & t_1 f_3(k_{||}) \\
t_1^* f_2^*(k_{||}) & t_3 f_1(k_{||})
\end{bmatrix}
\]  

(B2)

\[
h_2 = r \cos \frac{k_z}{2} \sigma_1
\]  

(B3)

\[
h_3 = \begin{bmatrix}
s_3 f_2(k_{||}) \cos \frac{k_z}{2} & s_1 f_3(k_{||}) + s_2 f_4(k_{||}) \\
s_1 f_3(k_{||}) + s_2 f_4(k_{||}) & s_4 f_2^*(k_{||}) \cos \frac{k_z}{2}
\end{bmatrix}
\]  

(B4)

in which \( h_1, h_2, \) and \( h_3 \) are blocks from the 1st-, 2nd-, and 3rd-neighbour hoppings respectively, \( \varepsilon \) is a real parameter, and \( t_1, r, \) and \( s_j \) are complex hopping parameters (except \( t_2 \) and \( t_3 \) which are real). \( k_{||} = (k_x, k_y) \), and \( f_i \) is defined as follows

\[
f_1(k_{||}) = \cos k_x + \cos k_y + \cos (k_x + k_y)
\]  

(B5)

\[
f_2(k_{||}) = \cos k_x + e^{-i\frac{k_z}{2}} \cos k_y + e^{i\frac{k_z}{2}} \cos (k_x + k_y)
\]  

(B6)

\[
f_3(k) = \cos (k_x - \frac{k_z}{2}) + \cos (k_y - \frac{k_z}{2}) + \cos (k_x + k_y + \frac{k_z}{2})
\]  

(B7)

\[
f_4(k) = \cos (k_x + \frac{k_z}{2}) + \cos (k_y + \frac{k_z}{2}) + \cos (k_x + k_y - \frac{k_z}{2})
\]  

(B8)

Compared with the original output of MagneticTB, in order to make the result tidy, we have adjusted the bases by the transformation matrix \( \sigma_0 + \sigma_1 \) and substituted for the original parameters, i.e. \( \varepsilon = (e^2 - e^1)/2, t_1 = 2[t_1 + \sqrt[3]{(1 + 2t_3)}, t_2 = 2t_4, t_3 = 2t_2, r = (t_2 - i t_1), s_1 = 2(s_5 + i s_1), s_2 = 2(s_8 + i s_2), s_3 = 4[s_6 + \frac{i}{\sqrt{3}}(2s_3 + s_6)], \) and \( s_4 = 4[s_7 - \frac{1}{\sqrt{3}}(2s_4 + s_7)] \).
[1] X. Wan, A. M. Turner, A. Vishwanath, and S. Y. Savrasov, Topological semimetal and fermi-arc surface states in the electronic structure of pyrochlore iridates, Phys. Rev. B 83, 205101 (2011).

[2] S. M. Young, S. Zaheer, J. C. Y. Teo, C. L. Kane, E. J. Mele, and A. M. Rappe, Dirac Semimetal in Three Dimensions, Physical Review Letters 108, 140405 (2012).

[3] A. A. Burkov, M. D. Hook, and L. Balents, Topological nodal semimetals, Physical Review B 84, 235126 (2011).

[4] Z. Wang, Y. Sun, X.-Q. Chen, C. Franchini, G. Xu, H. Weng, X. Dai, and Z. Fang, Dirac semimetal and topological phase transitions in $A_2$Bi ($a=Na, k, rb$), Phys. Rev. B 85, 195320 (2012).

[5] C. Fang, M. J. Gilbert, X. Dai, and B. A. Bernevig, Multi-weyl topological semimetals stabilized by point group symmetry, Physical Review Letters 108, 266802 (2012).

[6] A. A. Burkov and L. Balents, Weyl semimetal in a topological insulator multilayer, Phys. Rev. Lett. 107, 127205 (2011).

[7] Z. K. Liu, B. Zhou, Y. Zhang, Z. J. Wang, H. M. Weng, D. Prabhakaran, S.-K. Mo, Z. X. Shen, Z. Fang, X. Dai, Z. Hussain, and Y. L. Chen, Discovery of a three-dimensional topological dirac semimetal, Na$_3$Bi, Science 343, 864 (2014).

[8] S. M. Young and C. L. Kane, Dirac Semimetals in Two Dimensions, Physical Review Letters 115, 126803 (2015).

[9] S.-Y. Xu, I. Belopolski, N. Alidoust, M. Neupane, G. Bian, C. Zhang, R. Sankar, G. Chang, Z. Yuan, C.-C. Lee, S.-M. Huang, H. Zheng, J. Ma, D. S. Sanchez, B. Wang, A. Bansil, F. Chou, P. P. Shibayev, H. Lin, S. Jia, and M. Z. Hasan, Discovery of a weyl fermion semimetal and topological fermi arcs, Science 349, 613 (2015).

[10] A. A. Soluyanov, D. Gresch, Z. Wang, Q. Wu, M. Troyer, X. Dai, and B. A. Bernevig, Type-II Weyl Semimetals, Nature 527, 495 (2015).

[11] Z. Zhu, G. W. Winkler, Q. Wu, J. Li, and A. A. Soluyanov, Triple point topological metals, Physical Review X 6, 031003 (2016).

[12] B. Bradlyn, J. Cano, Z. Wang, M. G. Vergniory, C. Felser, R. J. Cava, and B. A. Bernevig, Beyond dirac and weyl fermions: Unconventional quasiparticles in conventional crystals, Science 353, aaf5037 (2016).

[13] C.-K. Chiu, J. C. Teo, A. P. Schnyder, and S. Ryu, Classification of topological quantum matter with symmetries, Reviews of Modern Physics 88, 035005 (2016).

[14] N. P. Armitage, E. J. Mele, and A. Vishwanath, Weyl and dirac semimetals in three-dimensional solids, Reviews of Modern Physics 90, 015001 (2018).

[15] S. Li, Z.-M. Yu, Y. Liu, S. Guan, S.-S. Wang, X. Zhang, Y. Yao, and S. A. Yang, Type-II nodal loops: Theory and material realization, Phys. Rev. B 96, 081106 (2017).

[16] Z. Yan, R. Bi, H. Shen, L. Lu, S.-C. Zhang, and Z. Wang, Nodal-link semimetals, Physical Review B 96, 041103 (2017).

[17] W. Wu, Y. Liu, S. Li, C. Zhong, Z.-M. Yu, X.-L. Sheng, Y. X. Zhao, and S. A. Yang, Nodal surface semimetals: Theory and material realization, Physical Review B 97, 115125 (2018).

[18] R. Bi, Z. Yan, L. Lu, and Z. Wang, Nodal-knot semimetals, Physical Review B 96, 201305 (2017), publisher: American Physical Society.

[19] H. Weng, Y. Liang, Q. Xu, R. Yu, Z. Fang, X. Dai, and Y. Kawazoe, Topological node-line semimetal in three-dimensional graphene networks, Physical Review B 92, 045108 (2015).

[20] D.-S. Ma, J. Zhou, B. Fu, Z.-M. Yu, C.-C. Liu, and Y. Yao, Mirror protected multiple nodal line semimetals and material realization, Phys. Rev. B 98, 201104(R) (2018).

[21] B. Fu, X. Fan, D. Ma, C.-C. Liu, and Y. Yao, Hourglasslike nodal net semimetal in a2gbio3, Phys. Rev. B 98, 055146 (2018).

[22] M. Z. Hasan, G. Chang, I. Belopolski, G. Bian, S.-Y. Xu, and J.-X. Yin, Weyl, Dirac and high-fold chiral fermions in topological quantum matter, Nature Reviews Materials 6, 784 (2021).

[23] X.-P. Li, K. Deng, B. Fu, Y. Li, D.-S. Ma, J. Han, J. Zhou, S. Zhou, and Y. Yao, Type-III Weyl semimetals: (TaSe$_2$)$_3$I, Physical Review B 103, L081402 (2021).

[24] Z. Wang, H. Weng, Q. Wu, X. Dai, and Z. Fang, Three-dimensional dirac semimetal and quantum transport in c$_{2d}$as$_2$, Phys. Rev. B 88, 125427 (2013).

[25] H.-Z. Lu and S.-Q. Shen, Quantum transport in topological semimetals under magnetic fields, Frontiers of Physics 12, 127201 (2017).

[26] D. T. Son and B. Z. Spivak, Chiral anomaly and classical negative magnetoresistance of weyl metals, Physical Review B 88, 104412 (2013).

[27] E. V. Gorbar, V. A. Miransky, and I. A. Shovkovy, Chiral anomaly, dimensional reduction, and magnetoresistivity of weyl and dirac semimetals, Phys. Rev. B 89, 085126 (2014).

[28] T. Bzdušek, Q. Wu, A. Rüegg, M. Sigrist, and A. A. Soluyanov, Nodal-chain metals, Nature 538, 75 (2016).

[29] M. Ezawa, Loop-nodal and point-nodal semimetals in three-dimensional honeycomb lattices, Physical Review Letters 116, 127202 (2016).

[30] G. Bian, T.-R. Chang, H. Zheng, S. Velury, S.-Y. Xu, T. Neupert, C.-K. Chiu, S.-M. Huang, D. S. Sanchez, I. Belopolski, N. Alidoust, P.-J. Chen, G. Chang, A. Bansil, H.-T. Jeng, H. Lin, and M. Z. Hasan, Drumhead surface states and topological nodal-line fermions inTiTaSe2, Physical Review B 93, 121113 (2016).

[31] B. J. Wieder, Y. Kim, A. M. Rappe, and C. L. Kane, Double dirac semimetals in three dimensions, Physical Review Letters 116, 186402 (2016).

[32] Z.-M. Yu, Y. Yao, and S. A. Yang, Predicted Unusual Magnetoresponse in Type-II Weyl Semimetals, Physical Review Letters 117, 077202 (2016).

[33] Z.-M. Yu, W. Wu, X.-L. Sheng, Y. X. Zhao, and S. A. Yang, Quadratic and cubic nodal lines stabilized by crystalline symmetry, Phys. Rev. B 99, 121106(R) (2019).

[34] T. Bzdušek and M. Sigrist, Robust doubly charged nodal lines and nodal surfaces in centrosymmetric systems, Physical Review B 96, 155105 (2017).

[35] R. Yu, Z. Fang, X. Dai, and H. Weng, Topological nodal line semimetals predicted from first-principles calculations, Frontiers of Physics 12, 127202 (2017).
[36] W. Chen, H.-Z. Lu, and O. Zilberberg, Weak Localization and Antilocalization in Nodal-Line Semimetals: Dimensionality and Topological Effects, Physical Review Letters 122, 196603 (2019), publisher: American Physical Society.

[37] N. Nagaosa, T. Morimoto, and Y. Tokura, Transport, magnetic and optical properties of weak materials, Nature Materials 5, 621 (2020).

[38] Z.-M. Yu, Z. Zhang, G.-B. Liu, W. Wu, X.-P. Li, R.-W. Zhang, S. A. Yang, and Y. Yao, Encyclopedia of emergent particles in three-dimensional crystals, Science Bulletin 67, 375 (2021), arXiv:2102.01517 [cond-mat.mes-hall].

[39] P. Tang, Q. Zhou, G. Xu, and S.-C. Zhang, Dirac fermions in an antiferromagnetic semimetal, Nature Physics 12, 1100 (2016).

[40] Q. Wang, Y. Xu, R. Lou, Z. Liu, M. Li, Y. Huang, D. Shen, H. Weng, S. Wang, and H. Lei, Large intrinsic anomalous Hall effect in half-metallic ferromagnet Co3Sn2S2 with magnetic Weyl fermions, Nature Communications 9, 3681 (2018).

[41] S. Nie, Y. Sun, F. B. Prinz, Z. Wang, H. Weng, Z. Fang, and X. Dai, Magnetic Semimetals and Quantized Anomalous Hall Effect in EuB6, Physical Review Letters 124, 076403 (2020), publisher: American Physical Society.

[42] J. Wang, Antiferromagnetic topological nodal line semimetals, Physical Review B 96, 081107 (2017), publisher: American Physical Society.

[43] B. Wang, H. Gao, Q. Lu, W. Xie, Y. Ge, Y.-H. Zhao, K. Zhang, and Y. Liu, Type-I and type-II nodal lines coexistence in the antiferromagnetic monolayer CrAs2, Physical Review B 98, 115164 (2018), publisher: American Physical Society.

[44] Z. Zhang, Z.-M. Yu, and S. A. Yang, Magnetic higher-order nodal lines, Physical Review B 103, 115112 (2021).

[45] C. Cui, X.-P. Li, D.-S. Ma, Z.-M. Yu, and Y. Yao, Charge-four Weyl point: Minimum lattice model and chirality-dependent properties, Physical Review B 104, 075115 (2021).

[46] G.-B. Liu et al., MSGCorep: A package for corepresentations of magnetic space groups, to be published.

[47] Zeying Zhang et al., MagneticKP: A package for k · p model of magnetic and non-magnetic materials, to be published.

[48] The commands getMLGElem[[56,370],"Y"] and showMLGCorep[[56,370],"Y"] in the package MSGCorep [50] can easily give respectively the elements and coreps of this MLG.

[49] Z. Zhang, Z.-M. Yu, and Y. Yao, MagneticTB: A package for tight-binding model of magnetic and non-magnetic materials, Comput. Phys. Commun. 270, 108153 (2022).