Encyclopedia of emergent particles in type-IV magnetic space groups

Zeying Zhang,1,* Gui-Bin Liu,2,3,* Zhi-Ming Yu,2,3 Shengyuan A. Yang,4 and Yuguı Yao2,3,†

1College of Mathematics and Physics, Beijing University of Chemical Technology, Beijing 100029, China
2Centre for Quantum Physics, Key Laboratory of Advanced Optoelectronic Quantum Architecture and Measurement (MOE), School of Physics, Beijing Institute of Technology, Beijing, 100081, China
3Beijing Key Lab of Nanophotonics & Ultralıne Optoelectronic Systems, School of Physics, Beijing Institute of Technology, Beijing, 100081, China
4Research Laboratory for Quantum Materials, Singapore University of Technology and Design, Singapore 487372, Singapore

The research on emergent particles in condensed matters has been attracting tremendous interest, and recently it is extended to magnetic systems. Here, we study the emergent particles stabilized by the symmetries of type-IV magnetic space groups (MSGs) . Type-IV MSGs feature a special time reversal symmetry \( \{T|t_0\} \), namely, the time reversal operation followed by a half lattice translation, which significantly alters the symmetry conditions for stabilizing the band degeneracies. In this work, based on symmetry analysis and modeling, we present a complete classification of emergent particles in type-IV MSGs by studying all possible (spinless and spinful, essential and accidental) particles in each of the 517 type-IV MSGs. Particularly, the detailed correspondence between the emergent particles and the type-IV MSGs that can host them are given in easily accessed interactive tables, where the basic information of the emergent particles, including the symmetry conditions, the effective Hamiltonian, the band dispersion and the topological characters can be found. According to the established encyclopedia, we find that several emergent particles that are previously believed to exist only in spinless systems will occur in spinful systems here, and vice versa, due to the \( \{T|t_0\} \) symmetry. Our work not only deepens the understanding of the symmetry conditions for realizing emergent particles but also provides specific guidance for searching and designing materials with target particles.

**Introduction.** In crystals, the atoms are arranged in an orderly manner, forming crystal lattices extending in three directions in real space and leading to periodic band structure in momentum space [1]. The symmetries of the bare crystal lattice are described by the space groups, where all the operators can be made unitary. By further including the spin and orbital degrees of freedom in the crystal, anti-unitary operations such as time reversal and its combinations with certain spatial symmetries need to be considered, and the extension leads to the magnetic space groups. Correspondingly, the energy bands of crystals should be labeled by the corepresentation of the relevant MSG [2, 3].

With certain symmetry conditions, the energy bands may form degeneracies in the Brillouin zone (BZ), giving rise to topological semimetal states [4–16]. Because the degeneracies are singularities in momentum space, the excitations around the degeneracies show many novel and intriguing phenomena, such as chiral anomaly, quantum vortex, chiral Landau levels and divergent optical responses [16–26]. Hence the topological semimetals have been one of the most active research fields in the past ten years [27–31].

Rooted in the MSG symmetries and the corepresentations, the band degeneracies take diverse forms, and each kind of degeneracy can exhibit distinct properties [1, 32–37]. Thus, of fundamental importance to list and classify all possible band degeneracies, along with their symmetry conditions. A complete classification of emergent particles in type-II and type-III MSGs have recently been presented by us in Ref. [38] and Ref. [39], respectively. Here, we complete the last missing piece of the project, i.e., the classification for the type-IV MSGs.

There are 517 type-IV MSGs, of which share the following structure

\[
M = G + \{T|t_0\}G ,
\]

(1)

where \( G \) is a space group, \( T \) is the time reversal operation, and \( t_0 \) is a half lattice translation. The "shifted" time reversal operation \( \{T|t_0\} \) connects two lattice sites with opposite magnetic moments, indicating that type-IV MSGs describe systems with certain antiferromagnetic orders. The appearance of \( \{T|t_0\} \) is also reminiscent of nonsymmorphic symmetries, which are point group operations followed by a fractional lattice translation. Because of \( \{T|t_0\} \), although the crystals belonging to type-IV MSG are magnetic systems without the pure \( T \) symmetry, its energy band still exhibit the \( T \) symmetry, reflected as \( E_n(k) = E_n(Tk) \). However, the \( \{T|t_0\} \) here is quiet different from the pure \( T \) symmetry but similar to the nonsymmorphic spatial operators. The extra fractional translation may lead new possibilities of the emergent particles in type-IV MSGs. For example, consider the eight time-reversal invariant momenta (TRIMs) in spinless case, \( \{T|t_0\}^2 = e^{-2ik \cdot t_0} \) will generate double degeneracy at TRIMs which satisfy \( 2k \cdot t_0 = \pi \). This is distinct from other space groups, where the pure \( T \) symmetry can lead to the Kramers double degeneracy only for spinful systems.

In this work, we systematically study all the possible

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* These two authors contribute equally to this work.
† ygyao@bit.edu.cn
TABLE I. The main results of the difference between type-IV magnetic space group and type-II MSG. “√” ( “×”) means there (do not) exist corresponding emergent particles in magnetic space groups. “II” and “IV” represent the type-II MSG and type-IV magnetic space group, respectively. The “√” with red color means that the emergent particles exist in type-IV magnetic space group but not exist in type-II MSG, and the “√” with green color means that the emergent particles exist in type-II MSG but not exist in type-IV magnetic space group. “Single (Double)” is for emergent particles with (without) SOC.

| Notation                        | Abbr. | Single | Double |
|---------------------------------|-------|--------|--------|
| Charge-1 Weyl point             | C-1 WP| ✓ ✓ ✓ ✓ | ✓ ✓ ✓ ✓ |
| Charge-3 Weyl point             | C-3 WP| ✓ ✓ ✓ ✓ | ✓ ✓ ✓ ✓ |
| Triple point                    | TP    | ✓ × ✓ | ✓ ✓ ✓ |
| Quadratic triple point          | QTP   | ✓ ✓ ✓ | Quadratic contact triple point QCTP |
| Dirac point                     | DP    | ✓ ✓ ✓ ✓ | Charge-2 Dirac point C-2 DP |
| Charge-4 Dirac point            | C-4 DP| × ✓ ✓ ✓ | Quadratic Dirac point QDP |
| Charge-4 quadratic Dirac point  | C-4 QDP| × ✓ ✓ ✓ | Quadratic contact Dirac point QCDP |
| Cubic Dirac point               | CDP   | × ✓ ✓ ✓ | Cubic crossing Dirac point CCDP |
| Sextuple point                  | SP    | ✓ ✓ ✓ ✓ | Charge-4 sextuple point C-4 SP |
| Quadratic contact sextuple point| QCSP  | × × ✓ ✓ | |
| Octuple point                   | OP    | × × ✓ ✓ | |
| Weyl nodal line                 | WNL   | ✓ ✓ ✓ ✓ | Weyl nodal line (net) WNLs |
| Quadratic nodal line            | QNL   | ✓ ✓ ✓ ✓ | Cubic nodal line CNL |
| Dirac nodal line                | DNL   | ✓ ✓ ✓ ✓ | Dirac nodal line (net) DNLs |
| Nodal surface                   | NS    | ✓ ✓ ✓ ✓ | Multiple nodal surfaces NSs |

emergent particles protected by the symmetries of type-IV MSGs, and classify the emergent particles from four aspects, namely, the dimension of degeneracy manifold, the degree of degeneracy, the type of dispersion, and the topological charge. The main results are shown in Table 1, where one can find most of the emergent particles (except QCSP) can be realized in type-IV MSGs. The corepresentation information and the possible emergent particles, including spinless and spinful, essential and accidental particles for each of the 517 type-IV MSGs are given in easily accessible interactive tables in S5 of Supplemental Material (SM). We also compare the differences between results of type-IV MSGs and that of type-II MSGs (nonmagnetic systems with pure $T$ symmetry) in table I. For type-II MSGs, the C-4 WP only appears in spinless systems while the C-4 DP, the C-4 QDP and the C-4 SP only appear in spinful systems [38]. In contrast, for type-IV MSGs the C-4 SP only appear in spinless systems, and the C-4 WP, the C-4 DP, and the C-4 QDP can appear in both spinless and spinful systems, due to the $\{T|t_0\}$ symmetry. We construct concrete lattice models to demonstrate the existence of C-4 WP in spinful systems and the existence of C-4 DP in spinless systems. Together with Ref. [38] and [39], our work accomplishes the grand task of classifying all possible emergent particles in periodic lattices.

**Rationale.** To study the degeneracies stabilized by the symmetries of type-IV MSGs, we should obtain the corepresentation information of type-IV MSGs. The method to calculate the corepresentation information of type-IV MSGs are exactly same as that of type-II MSGs [1]. Specifically, the corepresentation of a type-IV MSG $M$ can be induced from the small corepresentations of $M_k$, where $M_k$ is the magnetic little group of $k$ in $M$. This step is done by our homemade package MSGCorep [40]. With the calculated small corepresentation information of $M_k$, we can easily identify the possible degeneracies protected by the symmetries of $M_k$ and establish the $k\cdot p$ Hamiltonians expanded around the corresponding degeneracy. Many crucial properties of the degeneracies can be inferred from the $k\cdot p$ Hamiltonians, such as the dimension of degeneracy manifold, the type of band splitting, and the topological charge. A complete list of all possible emergent particles and their detailed classification is presented in S4 of SM, arranged for each of the 517 type-IV MSGs.

**Compare with nonmagnetic systems.** We also compare the particles in type-IV MSGs with that in type-II MSGs
TABLE II. Complex emergent particles existing in type-IV MSGs. The format of this table is similar to Tab. I

| Notation                  | Abbr.       | Single II IV | Double II IV |
|---------------------------|-------------|--------------|--------------|
| Combined WNL and NS       | WNL/NS      | ✓ ✓ ✓ ✓      | ✓ ✓           |
| Combined QNL and NS       | QNL/NS      | × ✓ ✓ ✓      | ✓ ✓ ✓         |
| Combined QNLs and WNLs    | QNLs/WNLs   | ✓ ✓ ✓ ×      | ✓ ✓ ✓ ✓       |
| Combined CNL and WNLs     | CNL/WNLs    | × × ✓ ✓      | ✓ ✓ ✓ ✓       |

Kramers degeneracy \((IT)^2 \equiv -1\) and for spinless cases with \(IT\), one can always choose the proper basis to obtain a real Hamiltonian, then the degeneracy manifold for doubly degenerate point in those cases are always large than 0, i.e. the degenerate point is on a nodal line or NS [11]. (ii) The blue text in S5 of SM (marked as Greek letters and Latin capital letters) are clickable. One can directly click them to get the full form of corepresentation matrices and Hamiltonians. (iii) In order to avoid redundant data in S7 of SM, the Hamiltonian marked as \(H_{\alpha T}\), which means the expression of Hamiltonian is exactly the same as the Hamiltonian in \(R_t\) corepresentation of magnetic space group \(\alpha\), despite their corepresentation matrices may different. (iv) The symmetry operations for magnetic space groups are taken from Bradley and Cracknell’s (BC) book [1]. However, some magnetic space groups are mistaken in the BC book, which are not consistent with their BNS notations [2, 3]. These magnetic space groups are corrected in the package MSGCorep [40], and hence all magnetic space groups we used here are consistent with those used in Bilbao Crystallographic Server or ISOTROPY [41, 42].

For the spinful systems with MSG 198.11, one has \(\{T|t_0\}^2 = -1\) for \(\Gamma\), \(M\) and \(\{T|t_0\}^2 = 1\) for \(R, X\), as \(t_0 = (\frac{1}{2} \frac{1}{2} \frac{1}{2})\). Hence, the band in \(\Gamma\) and \(M\) must at least be doubly degenerate, while in \(R\) and \(X\) do not have such constraints. The generators of corepresentation matrices for \(R_5R_6\) of \(R\) point can be written as

\[
D(\{2z\frac{1}{2}\frac{1}{2}\}) = -D(\{2z\frac{1}{2}\frac{2}{2}\}) = 1
\]

\[
D(\{3z\{000\}) = \gamma \sigma_{19} = -\frac{1}{2}\sigma_0 - i\frac{\sqrt{3}}{2}\sigma_3
\]

\[
D(\{T\frac{1}{2}\frac{1}{2}\frac{2}{2}\}) = \sigma_1
\]

where the definition of \(\sigma_i\) and \(\gamma\) can be found in S6 of SM. Then the \(k \cdot p\) Hamiltonian at \(R\) point can be solved from the constraint equations

\[
H(k) = \begin{cases} 
D(Q)H(R^{-1}k)D^{-1}(Q) & \text{if } Q = \{R|t\} \\
D(Q)H^*(-R^{-1}k)D^{-1}(Q) & \text{if } Q = \{RT|t\}
\end{cases}
\]

where \(D(Q)\) is the corepresentation matrices for symmetry operation \(Q\) with rotation part \(R\) and translation part.
The $k \cdot p$ Hamiltonian for $R_5R_6$ is [43]

$$H = (c_1 + c_2 k^2) \sigma_0 + c_3 k_x k_y k_z \sigma_3$$
$$+ (c_3 k^2 + c_4 k_x^2 - c_5 k_y^2 - c_6 k_z^2) \sigma_1$$
$$+ \frac{\sqrt{3}}{3} (c_3 k^2 - 3c_5 k_y^2 - c_6 k^2 + 3c_6 k_z^2) \sigma_2$$

where $k^2 = k_x^2 + k_y^2 + k_z^2$. Such Hamiltonian host (223)

leading order of the band splitting and is a C-4 WP [38]. Moreover, for nonmagnetic spinful systems, the C-2 TP can not appear at $\mathcal{T}$-invariant point. But, as shown in Table II, the C-2 TP can appear at R point, which again demonstrate the fact that type-IV MSG can exhibit many intriguing phenomena that can not be realized in non-magnetic systems.

To further confirm our results, we construct both spinless and spinful lattice models for MSG 198.11. Notice the minimum Wyckoff position of 198.11 is 8a, consider the $|\phi_s\rangle$ (spinless) and $\{|\phi_s\uparrow\rangle, |\phi_s\downarrow\rangle\}$ (spinful) for each atom in 8a. Then we can construct two tight-binding models (see S2 of SM for Hamiltonian and parameters) [44]. The structure for active atom of the lattice model is shown in Fig. 1. Moreover, for spinful case there are another C-4 DP locate at $\Gamma$ as show in Fig. 1(b). The calculated band structure of this two models are plotted in Fig. 1(c-d). The topological charge for emergent particles can be obtained by calculating the Wilson loops on a sphere enclosing the WP (DP)

$$W(\theta) = \oint d\mathbf{k} \langle \psi(\mathbf{k}) | i \nabla | \psi(\mathbf{k}) \rangle$$

where $\theta$ is the polar angle of the sphere. The integration is over an enclosing loop of a constant polar angle of the sphere. The evolution of Wilson loop for $\Gamma$ and $R$ with considering SOC are shown in Fig. 1(e-f) which are consist with table III.

TABLE III: Part of the emergent particles in type-IV magnetic space group 198.11. The text above the double line of table are the basic information of magnetic space group, including the symbol of magnetic space group, the Bravais lattice, the generators of the magnetic space group, whether exist the combination of inversion symmetry ($I$) and $\mathcal{T}$, and whether SOC is considered. The column for $k$ show the name and coordinate of high-symmetry momenta [1]. The column for “corep” is the information of corepresentation of $k$’s magnetic little group, including the label, dimension and corepresentation matrices for generators. The last three column are the $k \cdot p$ Hamiltonian, type of emergent particles and topological charge respectively.

**198.11, P2_13**

| $\Gamma_c$ | $\{C_{2x}\|0\frac{1}{2}\frac{1}{2}\}, \{C_{2x}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\}, \{C_{31}\|000\}, \{\mathcal{T}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$, without $IT$ |
|---|---|

FIG. 1. (a) Structure of lattice model. (b) Schematic showing the C-4 WP C-4 DP and C-1 WPs in Brillouin zone, the red, purple and blue points represent C-4 WP, C-4 DP and C-1 WPs, receptively. (c-d) Band structure of lattice models without SOC(c) and with SOC(d). (e-f) Wilson loop of C-4 DP and C-4 WP located at $\Gamma$ and $R$ and the horizontal coordinates are polar angle $\theta$ of the sphere.
**Discussion and conclusion.** In this work, we have theoretically listed the emergent particles in type-IV magnetic space groups. However, it remains an important task to identify realistic materials that can host these emergent particles. To put it into practice, one can directly look up our tables in $S_5$ of SM to find the possible emergent particles by the MSG number in the material database [45–47]. Besides, $S_4$ of SM also shows in which emergent particles by the MSG number in the material group symmetries. However, it remains an important task to identify realistic materials that can host these emergent particles. To put it into practice, one can directly look up our tables in $S_5$ of SM to find the possible emergent particles by the MSG number in the material database [45–47]. Besides, $S_4$ of SM also shows in which emergent particles by the MSG number in the material group symmetries. However, it remains an important task to identify realistic materials that can host these emergent particles.

Spinless emergent particles

| $k$ name | $kinfo$ | generators | $T$ | $\Gamma_2 \Gamma_3$ | $\Gamma_4$ | $\Gamma_1, \sigma_1, \sigma_4, \sigma_4$ | $\Gamma_4^{195.3}$ | $\Gamma_4^{195.3}$ | $\Gamma_4^{195.3}$ |
|-----------|----------|-------------|-----|---------------------|----------|---------------------------------|----------------|----------------|----------------|
| Spinless emergent particles | | $C_{22}, C_{22}, C_{31}^+, T$ | | $\sigma_0, \sigma_0, -\gamma \sigma_19, \sigma_1$ | | | | | |
| $\Gamma$ | 000 | | | $\Gamma_2 \Gamma_3$ | $\Gamma_4$ | | | | |
| $X$ | 0$\frac{1}{2}$0 | $C_{22}, C_{22}, T$ | | | $\sigma_1, \sigma_4, \sigma_4$ | | | | |
| $R$ | 0$\frac{1}{2}$1 | $C_{22}, C_{22}, C_{31}^+, T$ | | | | | | | |
| | | | | | | | | | |

In conclusion, with the powerful tool—group representation theory, we establish the encyclopedia of emergent particles in type-IV magnetic space groups which can provides useful guidance to search and study magnetic topological materials. Two interesting directions for the future are: (i) investigate the emergent particles in spin-space groups which have decoupled spin and lattice symmetries, (ii) use compatibility relations to study the connectivity of energy bands and the coexistence of emergent particles for specific Wyckoff position.

**Acknowledgments.** This work is supported by the NSF of China (Grants Nos. 12004028, 12004035, 11734003, 1206131002), the China Postdoctoral Science Foundation (Grant No. 2020M670106), the Strategic Priority Research Program of Chinese Academy of Sciences (Grant No. XDB30000000), the National Key R&D Program of China (Grant No. 2020YFA0308800), the Beijing Natural Science Foundation (Grant No. Z190006) and the Singapore MOE AcRF Tier 2 (Grant No. MOE2019-T2-1-001).

**Note added.** During completion of our paper, two independent and complementary works with a list of $k \cdot p$ Hamiltonians for 1651 magnetic space groups appeared in Ref. [51, 52]. The SM of this manuscript can be found in gzipped tar source file (TYPE-IV-EP-SM.pdf).
A. Burkov, Chiral Anomaly and Diffusive Magneto-

A. A. Zyuzin and A. A. Burkov, Topological response in

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

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

A. A. Zyuzin and A. A. Burkov, Topological response in Weyl semimetals and the chiral anomaly, Physical Review B 88, 115133 (2012).

A. Burkov, Chiral Anomaly and Diffusive Magnetotransport in Weyl Metals, Physical Review Letters 112, 247203 (2014).

X. Huang, L. Zhao, Y. Long, P. Wang, D. Chen, Z. Yang, H. Liang, M. Xue, H. Weng, Z. Fang, X. Dai, and G. Chen, Observation of the Chiral-Anomaly-Induced Negative Magnetoresistance in 3D Weyl Semimetal TaAs, Physical Review X 5, 031023 (2015).

T. Morimoto, S. Zhong, J. Orenstein, and J. E. Moore, Semiclassical theory of nonlinear magneto-optical responses with applications to topological Dirac/Weyl semimetals, Physical Review B 94, 245121 (2016).

M. Hirschberger, S. Kushwaha, Z. Wang, Q. Gibson, S. Liang, C. Belvin, B. Bernevig, R. Cava, and N. Ong, The chiral anomaly and thermopower of Weyl fermions in the half-Heusler GdPtBi, Nature Materials 15, 1161 (2016).

T. Liu, M. Franz, and S. Fujimoto, Quantum oscillations and Dirac-Landau levels in Weyl superconductors, Physical Review B 96, 224518 (2017).

J. E. Moore, Optical properties of Weyl semimetals, National Science Review 6, 206 (2019).

Y. Okamura, S. Minami, Y. Kato, Y. Fujishiro, Y. Kaneko, J. Ikeda, J. Muramoto, R. Kaneko, K. Ueda, Y. Kocsis, N. Kanazawa, Y. Taguchi, T. Kuretsume, K. Fujisawa, A. Tsukazaki, R. Arita, Y. Tokura, and Y. Takahashi, Giant magneto-optical responses in magnetic Weyl semimetal Co3Sn2S2, Nature Communications 11, 4619 (2020).

X. Yuan, C. Zhang, Y. Zhang, Z. Yan, T. Lyu, M. Zhang, Z. Li, C. Song, M. Zhao, P. Leng, M. Ozzerov, X. Chen, N. Wang, Y. Shi, H. Yan, and F. Xiu, The discovery of dynamic chiral anomaly in a Weyl semimetal NbAs, Nature Communications 11, 1259 (2020).

Z. Song, J. Zhao, Z. Fang, and X. Dai, Detecting the chiral magnetic effect by lattice dynamics in Weyl semimetals, Physical Review B 94, 214306 (2016).

Z. Zhang, Z.-M. Yu, G.-B. Liu, and Y. Yao, MagneticTB: A package for tight-binding model of magnetic and non-magnetic materials, Computer Physics Communications 270, 108153 (2022).

S. Curtarolo, W. Setyawan, S. Wang, J. Xue, K. Yang, R. H. Taylor, L. J. Nelson, G. L. Hart, S. Sanvito, M. Buongiorno-Nardelli, N. Mingo, and O. Levy, AFLLOWLIB.ORG: A distributed materials properties repository from high-throughput ab initio calculations, Computational Materials Science 58, 227 (2012).

S. V. Gallego, J. M. Perez-Mato, L. Elcoro, E. S. Tasci, R. M. Hanson, K. Momma, M. I. Aroyo, and G. Madariaga, MAGNEDITA: towards a database of magnetic structures. I. The commensurate case, Journal of Applied Crystallography 49, 1750 (2016).
[47] A. Jain, S. P. Ong, G. Hautier, W. Chen, W. D. Richards, S. Dacek, S. Cholia, D. Gunter, D. Skinner, G. Ceder, and K. A. Persson, Commentary: The Materials Project: A materials genome approach to accelerating materials innovation, APL Materials 1, 011002 (2013).

[48] B. Lv, T. Qian, and H. Ding, Angle-resolved photoemission spectroscopy and its application to topological materials, Nature Reviews Physics 1, 609 (2019).

[49] Z. Wang, Y. Chong, J. D. Joannopoulos, and M. Soljačić, Observation of unidirectional backscattering-immune topological electromagnetic states, Nature 461, 772 (2009).

[50] L. Lu, C. Fang, L. Fu, S. G. Johnson, J. D. Joannopoulos, and M. Soljačić, Symmetry-protected topological photonic crystal in three dimensions, Nature Physics 12, 337 (2016).

[51] F. Tang and X. Wan, Exhaustive construction of effective models in 1651 magnetic space groups, Physical Review B 104, 085137 (2021).

[52] Y. Jiang, Z. Fang, and C. Fang, A kp Effective Hamiltonian Generator, Chin. Phys. Lett. 38, 077104 (2021).