Topological correspondence between magnetic space group representations and subdimensions

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(Dated: June 18, 2021)

The past years have seen rapid progress in the classification of topological materials. These diagnostic methods are increasingly getting explored in the pertinent context of magnetic structures. We report on a general class of electronic configurations within a set of anti-ferromagnetic-compatible space groups that are necessarily topological. Interestingly, we find a systematic correspondence between these anti-ferromagnetic phases to necessarily nontrivial topological ferro/ferrimagnetic counterparts that are readily obtained through physically motivated perturbations. Addressing the exhaustive list of magnetic space groups in which this mechanism occurs, we also verify its presence on planes in 3D systems that were deemed trivial in existing classification schemes. This leads to the formulation of the concept of subdimensional topologies, featuring non-triviality within part of the system that coexists with stable Weyl points away from these planes, thereby uncovering novel topological materials in the full 3D sense that have readily observable features in their bulk and surface spectrum.

I. INTRODUCTION

With the advent of topological insulators (TIs) – gapped quantum matter having a topological entity by virtue of symmetry – the past years have seen a reinvigorated interest in band theory. Time reversal symmetry (TRS) has played a major role in these developments, standing at the basis of the developments of the first models of the general notion of symmetry protected states [1, 2]. More recently, the interplay with crystalline symmetries has provided a plethora of topological characterizations [3–22]. In particular, it was found that a substantial fraction of topological materials can be diagnosed by refined symmetry eigenvalue methods. Heuristically this pertains to considering combinatorial constraints between high symmetry momenta in the Brillouin zone (BZ), which can be shown to reveal classes of band structures that actually match the full machinery of K-theory analysis in certain cases [23], and then comparing them to real space atomic limits in order to define non-triviality with respect to this reference [24, 25].

Despite the crucial role of TRS, arguably the most paradigmatic TI model actually involves the formulation of TRS-breaking Chern bands [26], manifesting the original inspiration of these pursuits by Quantum Hall effects. Hence, it is of natural interest to consider the role of magnetism in combination with the above recent developments. While the interplay of topology and magnetism entails a vast and established literature, ranging from spin liquids to axion insulators [27–33], there have been rather fruitful results on both essential symmetry eigenvalues indicated schemes [34], that is symmetry indicators [35] and, very recently, topological quantum chemistry [36].

Already in the non-magnetic case the refined evaluations resulted in new insights. In particular, the discrepancies between different approaches culminated in the formulation of the concept of fragile topology [37]. These are topological invariants that, unlike stable counterparts, characterize band-subspaces separated by energy gaps from the other bands that can be trivialized upon the closing of the gaps [38–41]. Of particular interest are systems with PT or C2T symmetry that were early characterized through a stable Z2 invariant [42–45], and more recently through a fragile Z invariant [38, 46] given by the Euler class [47–49] for which new physical effects have been predicted [50]. In fact, taking into account multiple gap conditions [49], these phases go beyond any symmetry eigenvalue indicated notion and relate to the momentum space braid trajectories of non-Abelian framecharge characterized spectral nodes [48, 51, 52]. The role of C2T symmetry has also been pointed out in the non-trivial topology of the low energy bands of twisted bilayer graphene [53, 54].

Here we revert to the question what physical implications the extension to magnetic space groups (MSG) symmetries can bring within the above context. To this end we start by a case study in space group family (SG) 75 and find that within a magnetic background some Wyckhoff positions necessarily imply non-triviality. Turning to anti-ferromagnetic case we, for the first time, defining anti-ferromagnetic (AFM) order is however broken upon adding a generic Zeeman term, giving rise to a ferro/ferrimagnetic-compatible (FM) phase within the

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same family. The correspondence subsequently manifests itself by conveying that the fragile topological nature has to translate into bands of finite Chern number in the FM counterpart. Going beyond fragile topology, we find that the other remaining possibility of this configuration entails a symmetry protected Weyl semi-metallic phase, characterized by a quantizedπ-Berry phase. The stable nodal phase corresponds to finite $\mathbb{Z}_2$ symmetry indicator [35] that is protected by the combination of the $C_4$ and $C_2T$ symmetries. We moreover show that this phase possesses a systematic correspondence to a non-trivial Chern insulating FM counterpart at half-filling, characterized by an even Chern number $C = 2 \mod 4$. We then generalize our findings by formulating an exhaustive list of tetragonal MSGs featuring this necessarily present topological configurations and their systematic correspondences relating AFM and FM counterparts. We moreover address the effect of adding and removing unitary symmetries leading to the identification of magnetic Dirac points [55], and the generalization of the $C_2T$ protected Weyl semi-metallic phases to numerous MSGs. Most importantly, we find that this mechanism can occur on planes in 3D systems that were previously diagnosed as trivial. At the crux of the argument lies that the in-plane topology must coexist with symmetry indicated nodes away from the subdimensional regions, such that the 3D conditions appear trivial. Nonetheless, these subdimensionally enriched topological nodal topologies exhibit robust topological features, such as corner modes plus Fermi arcs in the subdimensional gapped fragile AFM case [56], or Fermi arcs plus Fermi arcs in the subdimensional Weyl nodal AFM case, and thus pinpoint to a new class of gapped-nodal topological materials to explore.

II. MAGNETIC SPACE GROUP AND MAGNETIC STRUCTURE: A FIRST CASE STUDY IN SG P4 (NO. 75)

To concretize matters we depart from a simple model for the tetragonal magnetic space group P4 \(_1\) (MSG No. 75.5 using the BNS convention) [57, 58]. The MSG can be decomposed into left cosets as $G_{75.5}/G_{75.1} = (E)0G_{75.1} + (E)\tau G_{75.1}$, where the space group $G_{75.1} = C_4 \times T$ (P4, No. 75.1 in the BNS convention) has no anti-unitary symmetry [57] ($E$ is the identity, the prime (') stands for time reversal, and $\tau = a_1/2 + a_2/2$). MSG75.1 (P4) has point group $C_4$ with the normal subgroup of translations $T$ corresponding to the primitive tetragonal Bravais lattice $\{n_1a_1 + n_2a_2 + n_3a_3\}_{n_1, n_2, n_3 \in \mathbb{Z}}$ where the primitive vectors are $a_1 = a(1, 0, 0)$, $a_2 = a(0, 1, 0)$, and $a_3 = c(0, 0, 1)$. In the foregoing we first focus on the two-dimensional projection $z = 0$, namely we study the corresponding magnetic layer group $p_4$ (denoted MLG[4.4.35] in [58]). In addition, we use the fact that MSG75.5 ($Pc\_4$) is generated by $(C_{4z}0)T$ ($C_{4z}$ is the rotation by $\pi/2$ around the z-axis in the positive trigonometric orientation) and $(E)\tau' T$ (we call $(E)\tau'$ a non-symmorphic time reversal symmetry (TRS) as it contains a fractional translation).

Generally, magnetic space groups with non-symmorphic TRS, called Shubnikov space groups of type IV [57], correspond to AFM structure. Writing $(r, m)$ for a magnetic moment $m$ located at $r$, the action of $(E)\tau'$ gives $(E)\tau'(r, m) = (r + \tau, -m)$, and the square $[(E)\tau']^2(r, m) = (r + a_1 + a_2, m)$, i.e. the moment is conserved under translation by a Bravais lattice vector while it is flipped under a fractional translation. Hence MSG75.5 ($Pc\_4$) is compatible with the AFM structure drawn over one unit cell in Fig. 1a), where all the moments of equal sign (pointing in the direction of the vertical $\hat{z}$-axis) are obtained under the action of elements generated by $(C_{4z}0)T$. In the following, we assume the existence of a magnetic background and describe its effect on the band structure’s topology of itinerant electrons. We note that such magnetism can be obtained directly as localized atomic magnetism within density functional theory frameworks [59], or as the solution of an effective spin Hamiltonian mapped from the Green’s functions of interacting electrons [60, 61]. Alternatively, effective electronic tight-binding Hamiltonians were derived from the double exchange model, i.e. non self-interacting electrons coupled through Hund’s coupling to local classical magnetic moments that interact via super-exchange coupling [62], where the electron spins anti-align with the local moments, and for which line-nodal semimetallic phases were recently discussed [63].
A. Necessary crystalline fragile antiferromagnetic topology

Adopting maximal Wyckoff position 2b [58], spanned by the sub-lattice sites \( r_A = a_1/2 \) and \( r_B = \tau - r_A = a_2/2 \), and setting one \( s \)-electronic orbital and both spin-
-1/2 components per site, we define the corresponding Bloch orbital basis functions

\[
|\varphi_{\alpha,\sigma}, k\rangle = \sum_{R \in T} e^{ik \cdot (R + r_\alpha)} |w_{\alpha,\sigma}, R + r_\alpha\rangle, \tag{1}
\]

with \( \alpha = A, B \) and \( \sigma = \uparrow, \downarrow \) (taking \( \hat{z} \) as the quantization axis of the spins). Ordering the degrees of freedom as \( \varphi = \{ \varphi_A, \varphi_B \} \), the generators of MSG75.5 (Pc\{4\}, i.e. \( C_{4z} \) rotation and non-symorphic time reversal, are then represented through

\[
\begin{align*}
\langle \varphi, D_{\pi/2}k | (C_{4z} | 0) | \varphi, k\rangle &= (\sigma_x \otimes M_4), \\
\langle \varphi, -k | (E | \tau) | \varphi, k\rangle &= e^{i\kappa \cdot \tau}(\sigma_x \otimes -i\sigma_y)\mathcal{K},
\end{align*}
\]

where \( M_4 = \text{diag}[-e^{-i\pi/4}, e^{i\pi/4}] \), and \( D_{\pi/2} \) is the 3D rotation matrix by an angle \( \pi/2 \) along the \( k_z \)-axis, \( \{ \sigma_i \}_{i=x,y,z} \) are the Pauli matrices, and \( \mathcal{K} \) is complex conjugation. Combining the two generators, we also obtain

\[
\langle \varphi, -D_{\pi/2}k | (C_{4z} | \tau) | \varphi, k\rangle = e^{iD_{\pi/2}k \cdot \tau}(1 \otimes -i\sigma_y M_4^* \mathcal{K}). \tag{3}
\]

It follows that the orbit of the action of the symmetries \( \{ (E | 0), (C_{4z} | 0), (E | \tau), (C_{4z} | \tau) \} \) on \( \varphi_A, \varphi_A, \varphi_B, \varphi_B \) is \( \{ \varphi_A, \varphi_A, \varphi_B, \varphi_B \} \), i.e. all four degrees of freedom are intertwined by the symmetries of MSG75.5 (Pc\{4\}). It can be easily checked that this remains true for any change of basis (i.e. under any general rotation among the sub-lattice and spinor components). Furthermore, it can be verified that the atomic orbitals cannot be moved to any other Wyckoff position without breaking the symmetries. We therefore conclude that \( \{ |\varphi, k\rangle \}_{k \in \mathbb{BZ}} \) defines a four-dimensional elementary band representation (EBR) [25, 64–66] as it is formed by the minimal set of localized (atomic like) orbitals at the sites 2b that is compatible with the magnetic space group symmetries, and we denote it EBR\( _{75.5}^{2b} \). This agrees with Ref. [36] which lists 2b as a maximal Wyckoff position and excludes this EBR from the exceptional composite EBRs.

A minimal tight-binding model for EBR\( _{75.5}^{2b} \) is given by

\[
H(k) = t_1 f_1(k) \sigma_z \otimes \sigma_z + t_2 f_2(k) \sigma_y \otimes \mathbb{1} + t_3 f_3(k) \sigma_x \otimes \mathbb{1} + \lambda_1 g_1(k) \mathbb{1} \otimes \sigma_+ + \lambda_2 g_2(k) \mathbb{1} \otimes \sigma_- + \lambda_3 g_3(k) \sigma_x \otimes \sigma_+ + \lambda_4 g_4(k) \sigma_x \otimes \sigma_-,
\]

with \( \sigma_{\pm} = (\sigma_x \pm i\sigma_y)/2 \) and the lattice form factors

\[
\begin{align*}
f_1 &= \cos a_1 k - \cos a_2 k, \\
f_2 &= \cos \delta_1 k - \cos \delta_2 k, \\
f_3 &= \sin \delta_1 k - \sin \delta_2 k, \\
g_1 &= \sin a_1 k - i \sin a_2 k, \\
g_2 &= \sin \delta_1 k - i \sin \delta_2 k, \\
g_3 &= \cos \delta_1 k + \cos \delta_2 k,
\end{align*}
\]

defined in terms of the bond vectors \( \delta_{\{j\}} = (a_1 \uparrow a_2)/2 \). It is assumed that \( \{ t_1, t_2, t_3 \} \) are real, while \( \{ \lambda_1, \lambda_2 \} \) can be complex. In the following, we first set \( t_1, t_2, t_3 = 1 \), and \( \lambda_1, \lambda_2 = (1/2)e^{i\pi/5} \).

Of importance for the analysis of the band structure and its topology are the squares of the twofold unitary symmetries [67, 68]. The non-symmorphic time reversal squares as

\[
\langle \varphi, k \rangle |(E | \tau)^2 | \varphi, k\rangle = -e^{-ik \cdot 2\tau} \mathbb{1}_{4 \times 4}, \tag{6}
\]

from which we get

\[
\langle \varphi, \Gamma |(E | \tau)^2 | \varphi, \Gamma\rangle = \langle \varphi, M |(E | \tau)^2 | \varphi, M\rangle = -\mathbb{1}_{4 \times 4}. \tag{7}
\]

We thus conclude that there must be a twofold Kramers degeneracy at \( \Gamma \) and \( M \), and we call them TRIM (time reversal invariant momentum) in the following. Combining the non-symmorphic time reversal with \( C_{2z} \), we get \( (C_{2z} | \tau)^{\prime} \) that is represented through

\[
\langle \varphi, -C_{2z}/k |(C_{2z} | \tau)^{\prime} | \varphi, k\rangle = e^{iD_{\pi}k \cdot \tau}(\sigma_x \otimes i\sigma_x)\mathcal{K}, \tag{8}
\]

and squares as

\[
\langle \varphi, k \rangle |(C_{2z} | \tau)^{\prime2} | \varphi, k\rangle = \mathbb{1}_{4 \times 4}. \tag{9}
\]

The existence of such an antiunitary symmetry that leaves the momentum invariant and squares to +1 implies that there exists a change of orbital basis in which the Hamiltonian is real symmetric [52]. This is here achieved through \( H(k) = V \cdot H(k) \cdot V^{\dagger} \) where \( V = \sqrt{\sigma_x \otimes \sigma_x} \). We symbolically refer to this symmetry as the “\( C_{2z}^T \)” symmetry.

The bands are then effectively analyzed using the (co-)reducible representations at the \( \Gamma \), \( M \) and \( X \) points. These are summarized in Table I (and discussed further in Appendix D1). Whenever a band structure of an EBR may be split by an energy gap, at least one band subspace must be topological, namely either both band subspaces are stable or fragile topological, or one is trivial and the other must be fragile topological [25, 37, 38]. Heuristically this is the case because there must be an obstruction forbidding the mapping of Bloch eigenstates of EBR subspaces to localized Wannier functions (i.e. atomic limits) as a result of the space group symmetries, since the dimensionality of any band subspace’s Wannier basis (here two) is necessarily smaller than the dimensionality of the by definition minimal EBR (here four). As a consequence, the Wannier functions representing an EBR’s subspace are either delocalized if we impose all symmetry constraints, or are incompatible with the space group symmetries. From the induced irreducible co-representations (coIRREPs) and the compatibility relations among these [23, 69, 70], we conclude that EBR\( _{75.5}^{2b} \) can be split over all high symmetry regions of the Brillouin zone. We actually obtain a gapped band structure over the whole Brillouin zone in our minimal model, see Fig. 2a) and b) that gives the
TABLE I. Character table for the magnetic space group IRREPs of MSG75.1 (P4), and coIRREPs of the unitary symmetries of MSG75.5 (Pc4), at Γ, M, and X, with ω = e^iπ/4.

The coIRREPs of MSG75.5 (Pc4) are given by the pairing of the two IRREPs of MSG75.1 (P4) within the same column (e.g. \( ΓT\) to \( ΓT\)). Retrieved from the Bilbao Crystallographic Server [69]. The second column gives the spin components located at the Wyckoff position 2c of MSG75.1 (P4) from which the IRREPs are induced.

| 2c | \( ΓT\) | \( ΓT\) | \( ΓT\) | \( M4\) | \( M5\) | \( M6\) | \( X3\) | \( X4\) |
|----|--------|--------|--------|--------|--------|--------|--------|--------|
| \( C_{4z} \) | \( ↑_z \) | \(-ω^*\) | \( ω^*\) | \( ω\) | \( -ω\) |
| \( C_{2z} \) | \( ↑_z \) | \(-i\) | \( -i\) | \( i\) | \( -1\) | \( -i\) | \( -i\) |

\footnote{We note that for any maximal Wyckoff position (WP) of MSG75.1 (P4) \{1a, 1b, 2c\} [36, 69] the spin-z components are good quantum numbers at Γ and M, which originates from the fact that the vertical \( C_{4z}\)-axes (for WPs 1a and 1b) and \( C_{2z}\)-axes (for WPs 2c) give natural quantization axes for the spins. At the Wyckoff position 2c (compatible with the Wyckoff position 2b of MSG75.5), the spin-z +1/2 (+3/2) induces \( \{\Gamma_t, \Gamma_l, \Gamma_7, \Gamma_8\} \), and the spin-z −1/2 (−3/2) induces \( \{\Gamma_7, \Gamma_8, \Gamma_7, \Gamma_8\} \).}

ordering in energy of the induced coIRREPs[71] (defined in Table I). The rational behind the splitting of the EBR will be explained when we address the symmetry indicator, which turns out to be trivial for the IRREPs ordering of Fig. 2b). In the following we refer to the lower (higher) two-band subspace as the valence (conduction) subspace at half-filling. The question is then to determine the topology of each gapped subspace as in that case there is no stable symmetry indicated topology.

As pointed out above, the \( C_{2z}T \) symmetry implies that the Bloch eigenvectors can be made real through the appropriate change of basis. It follows that (oriented) two-band subspace are the valence (conduction) subspace of Bloch eigenvectors [49]. The Wilson loop (\( W[l] \), see Appendix A) of each two-band subspace winds along both directions (i.e. integrating along the base path \( k_x = \{(k_x, k_y) | k_x \in [0, 2π]\} \) and scanning through \( k_y \in [0, 2π] \), and similarly if we exchange \( k_x \leftrightarrow k_y \), see Fig. 2d). We moreover find that the Berry phase \( e^{iμ\pi[l]} = \text{Det} W[l] \) of both two-band subspaces is \( π \) along both directions, see Fig. 2d (red dashed line), pointing to the non-orientability of the subspace frames of Bloch eigenvectors [49]. While the Euler class is not defined strictly speaking for an unorientable band subspace [72], we still obtain the winding of Wilson loop as an element of \( π_1(O(2)) = Z \) since \( W[l] \in O(2) \) when computed in the real gauge (i.e. using the Bloch eigenvectors of the real symmetric form) [73]. We thus conclude that each two-band subspace has a non-orientable non-trivial fragile topology [49]. Moreover, we also point out that the non-trivial \( π \) Berry-phases are actually appealing from a bulk-boundary perspective [74]. Indeed, they culminate in-gap edge states, reflecting a physical signature, see [56] for a detailed analysis.

We further derive in Appendix A the necessary non-triviality of the split EBR2_75.5. Following Ref. [38] we show that the crystal symmetries impose a finite fractional winding of Wilson loop over one quarter of the Brillouin zone, i.e. the patch bounded by the paths ΓXΓ and ΓMΓ (blue dashed lines) in Fig. 2c). This results from the difference in the symmetry protected quantizations of the Wilson loops over the two base paths, i.e. \( \text{Arg}[\text{det}(W[l_{ΓXΓ}]) = 0, π] \) and \( \text{Arg}[\text{det}(W[l_{ΓMΓ}]) = π/2, π/2] \), which depends on both the IRREPs and the spinor structure of the bands (i.e. spin-parallel vs. spin-flip parallel transports, see Appendix A), as is also verified through direct numerical evaluation of the Wilson loop over the patch in Fig. 2c).

Then, by \( C_4 \) symmetry, the Wilson loop must have a finite integer winding over the whole Brillouin zone, as confirmed by Fig. 2d). We later refer to it as the crystalline Euler fragile topology (written CEF in Table III) when we address the generalization to other MSGs.

We furthermore compute the \( C_4 \)-symmetric Wilson loop flow [38, 75, 76] from the point \( l_0 = Γ \) to the contour of the Brillouin zone \( l \in \partial BS \), shown in green in Fig. 2c), and between which we extrapolate by taking the scaled contour \( ν \partial BS \) for \( ν \in [0, 1] \). This also exhibits a full winding shown in Fig. 2f). The \( C_4 \)-symmetric Wilson loop winding alludes to the persistence of nontrivial fragile topology after breaking \( C_{2z}(0)^2 \) symmetry, i.e. without Euler class. We refer to it as the crystalline fragile topology (written CF in Table III).

These results thus constitute three complementary ways to reveal the necessary non-triviality of the crystalline fragile topology of the split EBR2_75.5.

**B. Stable nodal topological phases**

We can characterize the symmetry indicators of a given band structure by using the matrix containing all allowed magnetic EBRs. This results in a \( Z_2 \) indicator for MSG75.5 (Pc4). As detailed in Appendix D, the explicit expression for this indicator is

\[ z_2 = n_{X_3} \mod 2, \]

where \( n_{X_3} \) is the number of occupied bands at the X-point with the IRREP \( X_3 \). In agreement with the discussion in the previous section, the indicator is trivial for the fragile phase of EBR2_75.5 at half-filling, as can be verified from the coIRREPs of Fig. 2b). We emphasize that this symmetry indicator readily generalizes for an arbitrary even number of occupied bands, i.e. at a filling \( ν \in 2Z + 2 \).

We thus conclude that a stable topological phase can be reached through a band inversion at X. This is achieved for the model Eq. (4) by taking \( |λ_2| > √2|t_1| \). Setting \( λ_2 = (6/5)√2 \), we obtain the band structure of
Fig. 2. Non-triviality in MSG75.5. a) Full band structure of model defined in Eq. (4) and b) along the high symmetry directions with coIRREPs indicated. c) Symmetry-based paths within the Brillouin zone used as base loops for the patch Wilson loop (dashed blue), the $C_4$-symmetric Wilson loop (green), and the symmetry indicated Berry phase (red). The small arrows show the direction of flow (deformation of base loops). d) Two-band Wilson loop (blue lines), integrated along $k_x \in [0, 2\pi]$, and total Berry phase (red dashed line) for the valence (equivalently, conduction) bands of EBR$_{25\gamma \tau}^{2\gamma \tau}$. Integrating along $k_y \in [0, 2\pi]$ gives equivalent results. e) Wilson loop flow over a patch from the base loop $\Gamma X \Gamma'$ to $\Gamma M \Gamma'$. f) $C_4$-symmetric Wilson loop flow from the point $l_0 = \Gamma$ to the boundary of the Brillouin zone, $l_1 = \partial BZ$. Notation follows conventions of the main text.

Fig. 3. Stable topological semimetallic phase of MSG75.5 ($P\gamma\tau$) indicated by $z_2 = 1 \bmod 2$, here represented by EBR$_{25\gamma \tau}^{2\gamma \tau}$ at half-filling. Full band structure over a) BZ and b) along high symmetry lines where two coIRREPs at X have been inverted when compared to figure 2b).

Fig. 3 that exhibits a semimetallic phase with four nodal points around $\Gamma$ at half-filling. We find that the stable symmetry indicator $z_2$ corresponds to a $\pi$-Berry phase for the valence (conduction) bands along the path $l_0$ (see Fig. 2(c)], i.e. (see derivation in Appendix B)

$$\gamma_B^{(1:2)}[l_0] = -\log \left| \text{Det} \left( \mathbf{W}^{(1:2)}[l_0] \right) \right|$$

$$= -\log \left\{ \xi_2^X(1)\xi_2^X(2)\xi_2^M(1)\xi_2^M(2) \right\}$$

$$= -\log \left\{ \left( -1 \right)^{\left( +1 \right)} \xi_2^X(1)\xi_2^X(2) \right\}$$

$$= 0 \mod 2\pi$$

$$\text{if } z_2 = 0,$$

$$\pi \mod 2\pi$$

$$\text{if } z_2 = 1.$$  \(11\)

Let us first note that, similarly to Eq. (10), Eq. (11) can also be generalized for an arbitrary even number of occupied bands (i.e. a filling $\nu \in 2\mathbb{Z} + 2$). Importantly, $C_2\gamma T$ symmetry (with $[C_2\gamma T]^2 = +1$) imposes the vanishing of the $U(1)$ Berry curvature over the two-band occupied eigen-subspaces, since within the real basis we have $\mathcal{F} = \text{Pr}[\mathcal{F}]_{\sigma_y} [52]$ and thus $\text{tr}\mathcal{F} = 0$. As a consequence, the Chern number of the gapped AFM phase at half-filling is identically zero. From there results that the nontriviality of the Berry phase indicates a nodal phase (i.e. it indicates the obstruction to define a smooth projector on the occupied bands over the whole Brillouin zone due to the presence of topologically stable band crossings with the unoccupied bands), i.e. the necessary existence of an odd number of nodal points inside the domain bounded by $l_0$. Upon the breaking of the non-symmorphic TRS, $C_2\gamma T$ is also broken, and the $\pi$ Berry phase indicates a $C_4$-symmetry protected Chern number at half-filling, or more generally at a filling $\nu \in 2\mathbb{Z} + 2$.

$$\mathcal{C} = 2z_2 \bmod 4.$$ \(12\)

The nontrivial Chern phases are discussed in detail in the next section.

We emphasize that the nodal points at general momenta are not indicated by the compatibility relations. Indeed, these are stabilized by the $(C_{2\gamma \tau})^4$-symmetry ($C_{2\gamma T}$) for which there is not an eigenvalue structure. Instead, the $C_{2\gamma T}$ symmetry quantizes the Berry phase to the values $\{0, \pi\}$, with $\pi$ indicating an odd number of nodes encircled by $l_0$. Embedded in 3D the nodal points correspond to single Weyl points that are pinned on the $C_{2\gamma T}$ invariant plane (i.e. at $k_z = 0$ where $-C_{2\gamma T}k = IC_{2\gamma T}k = m_z k = k$) by virtue of the chirality-preserving property of $C_{2\gamma T}$. Indeed, any Weyl point leaving the $k_z = 0$ plane must have a mirror symmetric image with equal chirality by $C_{2\gamma T}$ symmetry. It is therefore forbidden for a single node to leave the plane by conservation of Chern number. We refer to these phases in the 3D context as the crystalline Weyl topology (written CW in Table III).

### III. AFM-FM CORRESPONDENCE

We now turn to ferro/ferrimagnetic (FM) phases associated with SG75 obtained from the fragile and stable
nodal AFM phases discussed above through the breaking of the antinumity symmetry \((E|\tau)'\), thereby effectively realizing MSG75.1 \((P4,\text{ Shubnikov type I})\). This is done in Eq. (4) by adding a Zeeman coupling term \(\epsilon_Z(1 \otimes \sigma_z)\). We find that the topology of the FM-compatible phases are necessarily nontrivial, exhibiting Chern numbers constrained by crystalline symmetries that intricately relate to the topology of the AFM counterparts.

We note that the correspondence discussed here must be contrasted from the Chern phases obtained under an external magnetic field \([77]\) which are in general not symmetry indicated.

\[ \lambda \]

\[ \epsilon \]

\[ \sigma \]

\[ \tau \]

\[ \Delta \]

\[ \Delta \]

\[ \lambda_{\text{soc}} \]

\[ \epsilon_Z > 0 \]

\[ C \]

\[ \epsilon_Z > \Delta, \lambda_{\text{soc}} \]

A. General mechanism

Let us first generally address the AFM-FM correspondence and its physical mechanisms. For this purpose it is worth starting from MSG83.49 \((P4_4/m)\) which is obtained from MSG75.5 by simply adding inversion symmetry, i.e. SG83 has point group \(C_{4h}\). The presence of \((I|\tau)'\) symmetry which squares to \(-1\) leads to the twofold Kramers degeneracy of the bands over the whole Brillouin zone. The parent EBR, which we write EBR\(_{83}^{49}\), also splits with a topology characterized by symmetry indicated mirror Chern numbers \([36]\). We readily obtain the corresponding Hamiltonian by taking \(\lambda_1, \lambda_2 = 0\) in Eq. (4). The full splitting of EBR\(_{83}^{49}\) requires \(\epsilon_{k_1}, \epsilon_{k_2}, \epsilon_{k_3} > 0\) (which we symbolize by a single variable \(\Delta\) in Fig. 4), where \(t_1\) is a spin-z-preserving spin-orbit coupling that acts as a delocalized Zeeman coupling on each sub-lattice orbital but changes sign between sub-lattice sites, and \(t_2\) and \(t_3\) are spin-preserving inter-sub-lattice site couplings. Due to the basal mirror symmetry \(\langle \varphi, m, k | \varphi, k \rangle = \hat{1} \otimes -i \sigma_z\), each band-doublet can be separated into the \(-i\) and \(i\) mirror-eigenvalue sectors, matching with the spin-up and spin-down components (i.e. the spin-\(z\)-components are good quantum numbers over the whole Brillouin zone).

The terms in \(\{\lambda_1, \lambda_3\}\) in Eq. (4) break inversion symmetry and correspond to combined Dresselhaus and Rashba spin-orbit couplings. The effect of the latter (symbolized by \(\lambda_{\text{soc}}\)) is to split the Kramers degeneracy away from \(\Gamma\) and \(M\), as represented schematically in Fig. 4a) for \(z_2 = 0\) in Eq. (10). The conservation of Kramers doublets at \(\Gamma\) and \(M\) is due to the non-symmorphic time reversal which still squares to \(-1\) at these points, as derived above. While the bands now have pseudo-spin components at generic momenta, the pure spin-up and spin-down components are still good quantum number at \(\Gamma\) and \(M\) since the terms in \(\lambda_{1,2}\) vanish there.

The AFM-FM transition can then be modeled through a Zeeman term \((\epsilon_Z)\) that breaks the non-symmorphicTRS leading to the splitting of the \((\Gamma, M)\) Kramers doublets. This leads to the pure spin polarization of the bands at \(\Gamma\) and \(M\) since, for any maximal Wyckoff position of MMSG75.1 \((P4)\) \([36, 69]\), spin-up and spin-down induce distinct sets of IRREPs at \(\Gamma\) and at \(M\) (see the footnote of Table I). In the following we thus refer to the pseudo-spin-polarizations \(\uparrow\) and \(\downarrow\) of the bands in the sense that the band \(\uparrow\) \((\downarrow)\) at \(k\) has the pure spin component \(\uparrow\) \((\downarrow)\) at \(\Gamma\) and \(M\). This does not exclude the case, for dominant spin-flip terms as compared to Zeeman splitting, of a band subspace with an opposite pure spin configuration at \(\Gamma\) (say spin-up) and \(M\) (spin-down), see the discussion around Eq. (A6) in Appendix A. Such a configuration typically requires long-range spin-flip terms \([36]\). This results in energy ordered pseudo-spin-polarized Chern bands (column \(\epsilon_Z > 0\) in Fig. 4, Fig. 5, and Fig. 12 in Appendix C) with the relative chirality of the minimal model set by \(\text{sign}[t_2]\). Further increasing Zeeman coupling (while keeping \(\lambda_{\text{soc}}\) fixed, see below) leads to fully pseudo-spin-polarized valence and conduction subspaces illustrated in the right column in Fig. 4a).

As a next step, by switching off the spin-flip \(\lambda_{1,2}\)-terms, while maintaining a dominant Zeeman splitting, we adiabatically map the fully pseudo-spin-polarized bands into pure spin-polarized split EBRs of MSG75.1 \((P4)\). Indeed, the sub-lattice sites \(A\) and \(B\) still span a single maximal Wyckoff position, now labeled 2e for MSG75.1 \((P4)\) \([69, 78]\), and from the absence of spin-mixing sym-
crystalline Chern topology refer to these symmetry indicated Chern phases as the EBR (i.e. for Band 1 and 2. Below we also use the pseudo-spin polarization into spin-polarized split EBRs as EBR\textsuperscript{2c\uparrow} \sim EBR\textsuperscript{2c\uparrow} \sim EBR\textsuperscript{2c\uparrow} + EBR\textsuperscript{2c\uparrow}. The symmetry breaking term (Zeeman) thus induces the following phase transition from one four-dimensional split EBR (of MSG75.5) to two-dimensional split EBRs (of MSG75.1),

$$\text{EBR}^{2b}_{75.5} \rightarrow \text{EBR}^{2c\uparrow}_{75.1} + \text{EBR}^{2c\downarrow}_{75.1} \sim \text{EBR}^{2c\uparrow}_{75.1} + \text{EBR}^{2c\downarrow}_{75.1}. \quad (13)$$

We emphasize that this mapping is model independent, in the sense that it continues to exist when we add any extra term in Eq. (4) that satisfies the symmetries of MSG75.5 (Pc-4) and MSG75.1 (P4). The symmetry broken band structure is now split into four separated bands and the question is to characterize the topology of each single band.

The symmetry indicated Berry phase for Band n (using the bottom-up labeling of the energy values, i.e. $E_n \leq E_{n+1}$) along the path $l_q = \Gamma M \Xi M \Gamma$ (M = M- $b_2$), see (in red) Fig. 2a), is [6, 13, 79] (one-band reduction of Eq. (11), see derivation in Appendix B)

$$\gamma_B^{(n)}[l_q] = -i \log[\xi_B^J(n)\xi_B^M(n)^{-1}\xi_B^J(n)\xi_B^M(n)^{-1}], \quad (14)$$

where $\xi_B^J(n)$ and $\xi_B^M(n)$ are the C\textsubscript{4} and C\textsubscript{5}-eigenvalues, respectively, at the high-symmetry point k listed in Table I. The Chern number of Band n, given through $e^{-i2\pi\mathcal{C}(n)} = (e^{i\gamma_B^{(n)}[l_4]}), \text{ mod 4,}$ is thus

$$\mathcal{C}(n) = -(2/\pi)\gamma_B^{(n)}[l_4] \text{ mod 4}, \quad (15)$$

see also [36]. We show below that whenever the FM phase is obtained from one of the (necessarily) nontrivial AFM phases of EBR\textsuperscript{2b}_{75.5}, it must be made of nontrivial Chern bands. Remarkably, the Zeeman splitting of the stable nodal phase of MSG75.5 (Pc-4), i.e. with $z_2 = 1$ in Eq. (10), necessarily generates a nontrivial Chern FM phase at half-filling, with $C = 2 \text{ mod 4}$ according to Eq. (12), see Fig. 4b). This is discussed in detail below where we show that Eq. (12) matches with Eq. (14,15) for Band 1 and 2. Below we also use the pseudo-spin polarization to predict single bands of higher Chern number (i.e. C = ±3 mod 4) in some regime. In the following we refer to these symmetry indicated Chern phases as the crystalline Chern topology (we call it CC topology in the following).

Before we study the AFM to FM phases correspondence for the model Eq. (4) in more detail, we importantly note that the same nontrivial AFM phases, as well as the AFM to FM correspondence, can be obtained from the following EBRs (for MSG75.5 (Pc-4) \rightarrow MSG75.1 (P4)):

$$\text{EBR}^{2a}_{1a} \oplus \text{EBR}^{2a}_{1b} \rightarrow \text{EBR}^{1m}_{1a} \oplus \text{EBR}^{1m}_{1b} \oplus \text{EBR}^{1m}_{1a} \oplus \text{EBR}^{1m}_{1b}, \qquad \text{EBR}^{2i}_{4c} \rightarrow \text{EBR}^{2i}_{4d}. \quad (16)$$

FIG. 5. Non-triviality in MSG75.1. a) Band structure for MSG75.1 obtained from the model in Eq. (4) together with Zeeman coupling, and b) along high-symmetry lines with the IRREPs indicated. We have taken $\epsilon_{\pm} = 1/2$. Applying Eq. (14) we find that each band hosts a nonzero Chern number.

where EBR\textsuperscript{2c} is an EBR formed with non-colinear in-plane spinors \{(-), C_{\pm\pm}(-), C_{\pm\mp}(-), C_{\mp\mp}(-)\}, i.e. with a quantization axis that is perpendicular to the vertical $C_{\pm}$-axis [80] (we chose $\hat{y}$ in Table III with $\gamma_{\pm} = \mp y$).

B. Small Zeeman splitting

Here we derive the topology of the FM phases obtained from each of the nontrivial AFM phases of EBR\textsuperscript{2b}_{75.5}, when the Zeeman splitting is small compared to the other energy scales (i.e. $\epsilon_{\pm} < \Delta, \lambda_{SOC}$ in Fig. 4), underpinning the general mechanism outlined previously.

1. Crystalline Chern ferro/ferrimagnetic topology from fragile AFM phase

Starting from the gapped fragile phase of EBR\textsuperscript{2b}_{75.5} ($z_2 = 0$) and given the sign of the Zeeman coupling ($\epsilon_{\pm} > 0$, i.e. $E_{1\pm} > E_{2\pm}$) we predict the ordering in energy of the IRREPs of each split Kramers degeneracy to be $E(\Gamma_7) < E(\Gamma_5) < E(\Gamma_8) < E(\Gamma_6)$, and $E(\tilde{M}_3) < E(\tilde{M}_1) < E(\tilde{M}_2) < E(\tilde{M}_5)$. We show the band structure for MSG75.1 in Fig. 5a) and b) together with the IRREPs along high-symmetry lines thus confirming the IRREPs ordering.

Substituting the symmetry eigenvalues in Eq. (14) we then readily find $\mathcal{C}(1) = \mathcal{C}(4) = +1$ mod 4, and $\mathcal{C}(2) = \mathcal{C}(3) = -1$ mod 4. We conclude that each split EBR\textsuperscript{2c}_{75.1} has a stable Chern class topology. This is confirmed by direct evaluation of the flow of Berry phase for each band, see Fig. 12 in Appendix C.

2. Crystalline Chern FM from stable nodal AFM phase

We now start from the stable nodal phase of EBR\textsuperscript{2b}_{75.5} ($z_2 = 1$). The breaking of non-symmorphic TRS unlocks the nodal (Weyl) points which then become free to leave the basal momentum plane (when embedded in 3D). As for the fragile topological phase this results in a fully gapped band structure at $k_z = 0$ where each band
acquires a symmetry indicated Chern number given by Eq. (14). Given the band inversion at X between Band 2 and 3 required in the fragile to stable topological transition (see the IRREPs ordering in Fig. 3b)), we now find band Chern numbers

$$C(1) = C(2) = C(3) = C(4) = +1 \text{ mod } 4. \quad (17)$$

Then, together with the cancellation sum rule $$\sum_{i=1}^{4} C(i) = 0$$, we predict $$C(2) = -3$$ and $$C(3) = +1$$ (or, equivalently, $$C(2) = +1$$ and $$C(3) = -3$$). This is confirmed numerically in Fig. 13 of Appendix C. We thus reach the conclusion that for small Zeeman coupling the bands in the vicinity of the half-filling energy must exhibit a higher Chern number. Also, contrary to the gapped FM phase obtained from the fragile topological phase where the valence (conduction) subspace has a trivial summed topology (i.e. $$C(1) + C(2) = 0$$), we here necessarily obtain a nontrivial Chern phase at half-filling with $$C(1) + C(2) = \pm 2$$, thus recovering the general prediction of Eq. (12).

C. Fully pseudo-spin-polarized FM phases

Given the spin-$$z$$ components associated with the induced IRREPs of the EBR at $$\Gamma$$ and M (Table I), we anticipate that by increasing $$\epsilon_2$$ there must be a second transition into a phase with fully pseudo-spin-polarized valence (conduction) bands (right column of Fig. 4), i.e. the $$\uparrow(-\downarrow)$$-band has a $$\uparrow(-\downarrow)$$-spin component at $$\Gamma$$ and M. This phase transition must happen through two band inversions, i.e. at $$\Gamma$$ and at M. Assuming $$\epsilon_2 > 0$$, we infer that beyond the transition the IRREPs ordering at $$\Gamma$$ and M are $$E(\mathbf{T}_7) < E(\mathbf{T}_8) < E(\mathbf{T}_5) < E(\mathbf{T}_6)$$, and $$E(\mathbf{M}_5) < E(\mathbf{M}_6) < E(\mathbf{M}_8) < E(\mathbf{M}_7)$$, respectively (importantly, note the difference with the ordering of the previous section and Fig. 5b)). The question of the Chern numbers, as determined by Eq. (14), is then reduced to the IRREPs ordering at X.

First, without loss of generality we can assume that the lowest (highest) energy level has IRREP $$\overline{X}_4$$ ($$\overline{X}_3$$), as in Fig. 2b) and Fig. 3b), from which we get $$C(1) = C(4) = +1 \text{ mod } 4$$. Then, for dominant values of $$\epsilon_2$$ and $$\lambda_{SOC}$$, we get $$C(2) = C(3) = -1 \text{ mod } 4$$. If we assume intermediary values of $$\epsilon_2$$ and $$\lambda_{SOC}$$ (see below), we instead obtain $$C(2) = C(3) = +1 \text{ mod } 4$$. In the later case, (similarly to the discussion below Eq. (17)) one of the two middle bands must exhibit a high Chern number of $$-3$$, giving a total Chern number of $$\pm 2$$ at half-filling for the valence/conduction space.

We now detail the phase transition to the fully polarized phase in the context of the model Eq. (4) to underpin the general scheme outlined above. The fully pseudo-spin-polarized phase must happen through two band inversions, at $$\Gamma$$ and M, which are analytically defined for Eq. (4) by the conditions $$\epsilon_2 > 2t_3$$ and $$\epsilon_2 > 2t_2$$, respectively (assuming $$t_{2,3} > 0$$), and with the IRREPs ordering at $$\Gamma$$ and M given above for $$\epsilon_2 > 0$$. The general form of

the energy eigenvalues at X for Eq. (4) including the Zeeman term is $$\epsilon_{s_1,s_2} = s_12t_1 + s_2\sqrt{2|\lambda_2|^2 + \epsilon_2^2}$$ with $$s_{1,2} = \pm 1$$, and we find $$E_{\pm}(\overline{X}_4) = \epsilon_{-\pm}$$ and $$E_{\pm}(\overline{X}_3) = \epsilon_{\pm\pm}$$. Fixing $$t_1 > 0$$, we note that $$E_{-}(\overline{X}_4) \leq E_{-}(\overline{X}_3) \leq E_{+}(\overline{X}_3)$$ and $$E_{-}(\overline{X}_4) \leq E_{-}(\overline{X}_3) \leq E_{+}(\overline{X}_3)$$. Hence, the lowest and highest energy levels are $$E_1 = E_{-}(\overline{X}_4)$$ and $$E_3 = E_{+}(\overline{X}_3)$$, respectively, from which we get $$C(1) = C(4) = 1 \text{ mod } 4$$.

The topology of the two remaining bands is then determined by the sign of

$$E_{-}(\overline{X}_3) - E_{+}(\overline{X}_4) = 2t_1 - \sqrt{2|\lambda_2|^2 + \epsilon_2^2}. \quad (18)$$

Let us first we assume $$|\lambda_2| > \sqrt{2t_1}$$, for which we find $$E_2 = E_{-}(\overline{X}_4) < E_{+}(\overline{X}_3) = E_3$$ for all $$\epsilon_2 > 2t_2, 2t_3$$, and $$C(2) = C(3) = -1 \text{ mod } 4$$. This case thus has zero Chern number at half-filling.

If we take instead $$t_1 > |\lambda_2|/\sqrt{2}$$, then either $$\epsilon_2 > \sqrt{4t_1^2 - 2|\lambda_2|^2}/2t_2, 2t_3$$, and we reach the same conclusion as before, or $$\sqrt{4t_1^2 - 2|\lambda_2|^2} > \epsilon_2 > 2t_2, 2t_3$$, in which case $$E_2 = E_{+}(\overline{X}_4) < E_{-}(\overline{X}_3) = E_3$$, and we find $$C(2) = C(3) = +1 \text{ mod } 4$$ which, we have shown, leads to a higher Chern number for Band 2 or 3, thus leading to a finite Chern number at half-filling ($$C = 2 \text{ mod } 4$$).

We conclude this section by noting that the bands of a single split EBR $$2C,7^{(4)}$$ must always carry non-zero Chern numbers irrespectively of the ordering of IRREPs.

IV. 3D TOPOLOGY AND GENERAL MSG

Having determined the topology of the 2D projection of MSG75.5 ($$PC_4$$) (i.e. for the corresponding magnetic layer group), we now address the 3D topology introducing the third momentum component $$k_z$$. First of all, we note that each Kramers doublet at $$\Gamma$$, M, Z, and A, are Weyl points carrying a chirality (Chern number). This results from the chirality of any crystal structure with MSG75.5 ($$PC_4$$, see Section VI. This nodal topology will be manifested in terms of Fermi arcs on surface spectra only at quarter-filling, and more generally at a filling $$\nu \in 2Z + 1$$. In the following we instead focus on the topology at half-filling, and more generally at a filling $$\nu \in 2Z + 2$$.

The above results are directly transferable to the $$k_z = 0$$ and $$k_z = \pi$$ planes of the 3D Brillouin zone, which leads to a $$\mathbb{Z}_2^{8}$$ classification. If the two symmetry indicators are distinct, e.g. $$(z_{0}, z_{2}) = (1, 0)$$, they indicate the presence of $$C_{4z}$$ protected Weyl points (at half-filling) on the $$\mathbb{R}\mathbb{R}$$ high-symmetry axis, on top of the four Weyl points on the $$k_z = 0$$-plane, while the plane at $$k_z = \pi$$ has CEF topology. These thus form a $$\mathbb{Z}_2$$ octuplet of Weyl points (i.e. the CW topology). It is interesting to note that by $$C_4$$ symmetry the Weyl points in plane must all have the same chirality, while the Weyl points on the $$\mathbb{R}\mathbb{R}$$ axis must all be of the opposite chirality by $$C_2T$$ symmetry, which leads to the configuration of Fig. 6a)
Fragile topology is colored in green. Weyl points all have equal chirality.

When both symmetry indicators are nonzero (obtained from above through a band inversion at R) both planes are stable nodal and we either obtain two quadruplets of Weyl points of opposite chirality in each horizontal plane as illustrated in Fig. 6b) (after the annihilation on the vertical axes of the nodes with opposite chirality visible in Fig. 6c)), or we have two octuplets of Weyl points with all Weyl points on the horizontal planes with the same chirality and all Weyl points on the vertical axes with the opposite chirality as shown in Fig. 6d).

Only when both symmetry indicators are zero do we retrieve a gapped 3D phase where both planes $k_z = 0$ and $k_z = \pi$ are fragile topological. Our classification thus characterizes and refines the earlier prediction of a $\mathbb{Z}_2$ symmetry indicator for the 3D MSG75.5 ($P_4$) phases [35]. As a side remark, we note that planes hosting the four TRIM ($\Gamma,M,Z,A$) characterized by (non-symmorphic) TRS, i.e. an anti-unitary symmetry squaring to $-1$ and inverting the momentum, give rise to a non-symmetry indicated $\mathbb{Z}_2$ index of a strong two-dimensional TI [32]. We note that the non-symmorphic TRS squares to $-1$ over the whole plane that contains the four TRIMPs. Therefore, restricting any 3D model on that plane, it can be seen effectively as a 2D system with TRS and the index can be computed in the same way as the Kane-Mele $\mathbb{Z}_2$ invariant [81].

For completeness, let us also mention the axion insulating phases protected by $C_2T$, i.e. the three-dimensional gapped topological phases indicated by the difference in the second Stiefel Whitney class between the two $C_2T$ symmetric planes $k_z = 0, \pi$ [29, 30, 42, 82]. This phase requires that $C_2T$ squares to $+1$ on both planes and, contrary to its parent phases with inversion symmetry [36], it is not symmetry indicated.

The mechanism discussed so far is directly transferable to the other tetragonal AFM candidate MSG81.37 ($P_4$) and its FM counterpart MSG81.33 ($P_4$), where the fourfold rotoinversion point symmetry $S_4$ takes the place of $C_4$. The only differences with MSG75.5 ($P_4$) are the reversal of chirality of the Weyl points under the action of $S_4 = IC_{4z}$ symmetry and, for the 3D gapped phase, the existence of an additional $z'_2 \in \mathbb{Z}_2$ symmetry indicator [35] of a strong 3D TI protected by $S_4$-symmetry and (non-symmorphic) TRS [83] (see also Appendix D 3 where this symmetry indicator is derived for MSG81.36 ($P_4$) for which it is the unique symmetry indicator of the 3D gapped phase, similarly to MSG81.38 ($P_4$)). The nontrivial value of the symmetry indicator $z'_2$ in Eq. (D4), corresponding to the indicator $z_2$ identified for MSG81.33 ($P_4$) in Ref. [36], indicates a 3D axion topological insulating phase with a non-trivial axion angle $\pi$ [36] and a quantized magnetoelectric response [28, 84].

We conclude this section by noting the candidate MSSG77.17 ($P_4$) that has a $\mathbb{Z}_2$ symmetry indicator [35] which indicates $C_2T$ protected Weyl semi-metallic phases, as in MSG75.5 ($P_4$), but now with a minimal connectivity of bands of 4, i.e. the filling must be $\nu \in 4\mathbb{Z} + 4$. The 2D gapped phases at $k_z = 0, \pi$ are thus either trivial, or host the second Stiefel Whitney topology that is not symmetry indicated, since the non-trivial Euler class topology only exists within two-band subspaces.

V. COEXISTENCE OF NODAL AND SUBDIMENSIONAL TOPOLOGIES

In the previous MSG candidates we were guided by the possibility of having a non-trivial symmetry indicator of the 3D gapped phase, signaling the possibility of splitting groups of bands (possibly EBRs) into (fragile) topological bands, see also Appendix D. We now address a class of MSGs that host a similar mechanism that nonetheless appear trivial from a standard symmetry indicator or topological quantum chemistry perspective. At the crux of the argument lies the observation that these MSGs host groups of bands (possibly EBRs) that
can be split at planes in the Brillouin zone, hosting the same (stable) topological features, while their total three-dimensional band structure must be connected. Consequently, within these “trivial” groups of bands, i.e. in the sense that they lack 3D symmetry indicators, the in-plane non-trivial signatures must coexist with symmetry indicated nodal structures located away from the (possibly) gapped planes. We discuss below one example where the connectivity of the three-dimensional EBR by itself indicates the presence of protected Weyl points in the direction perpendicular to the 2D topological planes. It thus has stable 3D signatures, such as Fermi arcs [85], which topological origin is independent of the 2D topologies and their signatures. Since the 3D symmetry indicators are blind to this kind of coexistence, these topological phases can thus only be perceived in this refined context of sub-dimensional topology.

We emphasize that our use of subdimensional topology is distinct from the usual correspondence between the topological charges of a d-dimensional node, with codimension δ within a d + δ = D-dimensional Brillouin zone, and the p-dimensional gapped topologies for δ − 1 ≤ p ≤ D − 1 [46, 86]. The archetypical example of this usual decent approach is the stability of a Weyl point being captured by the Chern number of a gapped sphere surrounding it [87]. We discuss below such as a situation for the case of Weyl nodes protected by the screw axis 4_2 with a chirality χ = ±2 captured by gapped Chern planes with C = 2 mod 4. Many correspondences of this kind have been formulated recently for new types of crystal-symmetry protected gapped topologies, e.g. [86, 88–90].

In contrast, the new sub-dimensional topology we are referring to is independent of the charges of the Weyl nodes protected by the screw symmetry, since we show that the Chern number must be zero on the 2D planes that host the sub-dimensional topology. This leads to the prediction of new phases with coexisting topological features, i.e. the manifestations of the nodal topology in 3D together with the manifestations of the nontrivial sub-dimensional topology.

### A. Case study of MSG77.18 (P_42)

As an example, we take MSG77.18 (P_42) that hosts the mechanism discussed for MSG77.5 (P_24) as a 2D sub-dimensional topology. The coset decomposition of the AFM compatible MSG77.18 (P_42) in terms of its FM partner MSG77.13 (P_42) is \( \Gamma_{77,18}/\Gamma_{77,13} = (E(0)\Gamma_{77,13} + \Gamma_{77,13}) \) with \( \Gamma_{77,13} = A_1 + a_2 + a_3, \) where \( T \) is the primitive Bravais lattice and \( \Gamma_{77,13} \) is generated by \( (C_{4z}|\tau_3)T \) with \( \tau_3 = a_3/2. \) We consider the Wyckoff position (WP) 2c [69] that is spanned by the sub-lattice sites \( r_A = a_1/2 \) and \( r_B = a_2/2 + a_3/2. \) The same sites correspond to WP 2c of MSG77.13. Populating the sites with s-electronic orbitals and both spin-2/3-1/2 components we get the Bloch orbital basis \( \{\varphi, \overline{\varphi}\} \) forming an elementary band representation which we write EBR\(^{27}_{77,18}\). EBR\(^{27}_{77,18}\) resembles EBR\(^{25}_{75,5}\) except that it is indecomposable over the 3D Brillouin zone.

An other important difference with MSG77.5 (P_24) is the algebra of symmetries at \( k_z = \pi. \) Taking a point on the \( k_z = \pi \) plane \( \tilde{k} = (k_x, k_y, \pi), \) the \( C_2T \) symmetry in MSG77.18 (P_42) is represented for EBR\(^{27}_{77,18}\) by

\[
\langle \varphi, \tilde{k} | (C_{2z}|\tau_3)^T \rangle \langle \varphi, \tilde{k} \rangle = e^{ikC_{2z}|\tau_3}e^{iC_2T}e^{i\delta}e^{i\sigma_x \delta}e^{i\sigma_y \delta}e^{i\sigma_z \delta}K = e^{iC_2T}e^{i\delta}e^{i\sigma_x \delta}e^{i\sigma_y \delta}e^{i\sigma_z \delta}K = e^{iC_2T}T(-b_3)(\sigma_x \otimes i\sigma_y)K,
\]

(19)

with \( T(-b_3) = \text{diag}(e^{i\pi/4}, e^{i\pi/4}, e^{-i\pi/4}, e^{-i\pi/4}) \). The \( \langle \varphi, \tilde{k} | (C_{2z}|\tau_3)^T \rangle \langle \varphi, \tilde{k} \rangle = -1 \times 4 \times 4, \) i.e. the \( C_2T \) symmetry squares to \(-1. \) The bands hence exhibit a twofold Kramers degeneracy over the whole \( k_z = \pi \)-plane.

| WP | \( Z_5 \) | \( Z_6 \) | \( \bar{X}_5 \) | \( \bar{X}_6 \) | \( \bar{A}_7 \) | \( \bar{R}_4 \) | \( K_4 \) |
|----|-----|-----|-----|-----|-----|-----|-----|
| \( (C_{4z}|\tau_3) \) | ↑_z = -ω | ω | -ω | ω | -ω | ω | -ω |
| ↓_z = -ω | ω | -ω | ω | -ω | ω | -ω | ω |
| \( (C_{2z}|0) \) | ↑_z = i | -i | i | i | i | -i | -i |
| ↓_z = i | -i | i | i | i | -i | -i | -i |

#### 1. Model and band structure

We illustrate this with the following minimal 3D extension of Eq. (4) which we rewrite as \( H[f_1, f_2, f_3, g_1, g_2](\kappa), \)

\[
H'(\kappa) = H[f_1, f_2, f_3, g_1, g_2](\kappa) + \rho_1 h_1(\kappa) + \rho_2 h_2(\kappa) + \rho_3 h_3(\kappa),
\]

(20)

where the new lattice form factors are now extended to 3D momentum space,

\[
f_1(\kappa) = (\cos \delta_1 \kappa - \cos \delta_2 \kappa + \cos \delta_3 \kappa) / 2,
f_2(\kappa) = (\cos \delta_1 \kappa + \cos \delta_2 \kappa + \cos \delta_3 \kappa) / 2,
g_1(\kappa) = (\sin \delta_1 \kappa - \sin \delta_2 \kappa - \sin \delta_3 \kappa - \sin \delta_4 \kappa) / 2,
g_2(\kappa) = (\sin \delta_1 \kappa - \sin \delta_2 \kappa - \sin \delta_3 \kappa - \sin \delta_4 \kappa) / 2,
\]

(21)

with \( \delta_1 = \delta_2 + \delta_3/2, \) \( \delta_4 = -\delta_1 + \delta_3/2, \) and with the new real parameters \( \rho_1, \rho_2, \rho_3, \) we (take \( \rho_1 = -1 \) and \( \rho_2 = -2/5 \).
We show the band structure of model Eq. (20) in Fig. 7a) where the \( k_z \)-axis covers \([0, 2\pi]\), and the other axis corresponds to the successive paths \( \Gamma X \) and \( XM \) within the plane \( k_z = 0 \). The band structure along the high-symmetry lines is shown in Fig. 8a), and c) after a band inversion at X. We note the twofold degeneracy at \( k_z = \pi \) which explains the degeneracies along \( ZR \) and \( RA \) in Fig. 7a), and in Fig. 8a) and c).

Importantly, the compatibility relations along the \( C_4 \)-symmetric axes \( \Gamma Z \) and \( MA \) imply that the EBR cannot be split [69], see Appendix D 2. Indeed, the fourfold screw symmetry \( 4_2 \equiv (C_4z|\tau_3) \) imposes an exchange of branches between the Kramers doublets of \( \Gamma \) and \( Z \) (and \( M \) and \( A \)), see the coIRREPs given in Table II retrieved from [69]. This leads to two \( 4_2 \)-protected nodal points on the \( \Gamma Z \)-line (resp. the \( MA \)-line) at half-filling (marked by circles in Fig. 7a)), and more generally at a filling \( \nu \in \frac{4}{2} \mathbb{Z} + 2 \). We note that this exchange of IRREPs along the \( 4_2 \)-axes originates from the monodromy of the irreducible representations of the screw symmetry \( 4_2 \) [6, 69, 86, 91, 92].

### 2. Chirality of Weyl nodes protected by a screw axis \( 4_2 \)

Following the algebraic argument of Ref. [6], see also Ref. [86], we now derive the symmetry enforced chirality of \( \chi = 2 \text{mod} 4 \) for each Weyl point protected by \( 4_2 \). Let us start with a sphere \( S \) surrounding one of the Weyl points, say the one on the upper half of the \( \Gamma Z \) line. We fix the south pole at \( \Gamma \) and the north pole at \( Z \), see Fig. 9a). Then, we divide the sphere in four quarters, one of which, let us call it \( S \), is bounded by an oriented loop \( \partial S \equiv l = l_b \circ l_a \) (which we read as first \( l_a \) followed by \( l_b \)) with \( l_a = C_4zl_b^{-1} \) (where \( l_b^{-1} \) is the reversed oriented path), see Fig. 9a).

Since we can recompose the total sphere through \( C_4z \) actions, i.e. \( S = S \cup C_4zS \cup C_4z^2S \cup C_4z^3S \), the Chern number of the two occupied bands over the gapped sphere thus reads

\[
e^{-2i\pi c[S]} = \left(e^{-i\gamma_B[l]}\right)^4 = e^{-4i\gamma_B[l]},
\]

by the invariance of the Berry curvature under rotation symmetry [6], and where \( \gamma_B[l] \) is the Berry phase of the two occupied bands over the loop \( l = l_b \circ l_a \), i.e. (see the definition of symmetry transformation of the Wilson
FIG. 9. Chirality of $\chi = 2 \text{mod} 4$ for each Weyl point protected by the 4$_2$ screw axis on the $\Gamma Z$ and MA lines, at half-filling ($\nu \in 4Z + 2$), derived from the symmetry reduction of the Wilson loop (see text).

loop in Appendix A)

$$e^{-i \gamma_B[l]} = \det \mathcal{W}[l] = \det (\mathcal{W}[l_a] \cdot \mathcal{W}[l_b])$$

$$= \det (R_{4_a}^\Gamma \cdot \mathcal{W}[l]^{-1} \cdot (R_{4_b}^\Gamma)^{-1} \cdot \mathcal{W}[l])$$

$$= \det (R_{4_a}^\Gamma \cdot (R_{4_b}^\Gamma)^{-1})^{-1} = \chi_{4_a}(\Gamma_5) \chi_{4_a}(\Gamma_7) \chi_{4_b}(\Gamma_7)$$

$$= (-i)^2 = -1,$$

where $R_{4_a}^\Gamma = e^{iC_{4_a} k \cdot \tau_3 S_{4_a}^\Gamma (\Gamma_5, \Gamma_7)} = S_{4_a}^\Gamma (\Gamma_5, \Gamma_7)$ and $R_{4_b}^\Gamma = e^{iC_{4_b} k \cdot \tau_3 S_{4_b}^\Gamma (\Gamma_7, \Gamma_7)} = S_{4_b}^\Gamma (\Gamma_7, \Gamma_7).$

We finally conclude that $\chi_{4_a}(\Gamma_7) = \chi_{4_b}(\Gamma_7)$ is the character of the IRREP $\tilde{\mathcal{K}}_j$ at a momentum $\mathbf{k}$, and $\chi_{4_a}(\mathbf{k}_{\ast})$ is the representation of symmetry $(g |\tau g)$ in the valence band basis $S_{4_a}^\Gamma (\mathcal{K}_j, \mathcal{K}_j)$ for a coIRREP $\mathcal{K}_j$, $\mathcal{K}_j$ in the plane the $\mathcal{K}_j$ indicates a crystalline (non-Euler) fragile (CF) topology.

FIG. 10. $C_4$-symmetry Wilson loop for the conduction a) and valence b) bands of EBR$_{77.18}^{2\tilde{a}}$ at $k_z = \pi$.

We now determine how the subdimensional topologies (at $k_z = 0, \pi$) interact with the topology of the 4$_2$-symmetry protected Weyl points. We first note that the Chern number at half-filling vanishes on the $k_z = 0, \pi$-planes as a consequence of $C_2T$ symmetry (see the discussion below Eq. (11) for $k_z = 0$, and at $k_z = \pi$, we have $\mathcal{F} \equiv 0$ by $[C_2T]^2 = -1$). As a consequence, we can deform the sphere $S$ of Fig. 11a) into the pyramid $P$ of Fig. 11b) while conserving the Chern number, i.e. $\mathcal{C}[S] = \mathcal{C}[P] = 2$ mod 4. This equality can be readily verified through the symmetry reduction of the Wilson loop $W[l \circ l_a \circ l_b \circ l_a]$ (Fig. 11a) into the pyramid $P$ (Fig. 11b) while conserving the Chern number, i.e. $\mathcal{C}[S] = \mathcal{C}[P] = 2$ mod 4. This equality can be readily verified through the symmetry reduction of the Wilson loop $W[l \circ l_a \circ l_b \circ l_a]$ similarly to the above derivation for $S$ but now using both $C_{4a}$ and $C_{2a}$ transformations.

We note that even if there are nodal points on the $k_z = 0$ plane (for $z_2 = 1$), by $C_4$ symmetry they must contribute to an increase of the Chern number by $\pm 4$, which leaves the quantity mod 4 unchanged. An other consequence of $C_2T$ symmetry is that any Weyl point above the $k_z = 0$ plane must have its mirror symmetric image underneath (k$_z \rightarrow IC_{2z}k_z = -k_z$) with the same chiral charge. Combining the top of the pyramid in Fig. 9b) with its mirror image in the $k_z$-direction, we obtain an octahedron $\mathcal{O} = \tilde{\mathcal{O}} \cup m_3\tilde{\mathcal{O}}$ that wraps the pair of Weyl points on the $\Gamma Z$ line, and over which there is a total Chern number (chirality) of $\mathcal{C}[\mathcal{O}] = (2 + 2) \times 8 = 4 \times 4$ mod 8.

We now discuss the global topology of the AFM topological phases for MSG77.18 ($P^*_1, 42$). We first note that EBR$_{77.18}^{2\tilde{a}}$ can be gapped over the planes $k_z = 0, \pi$. The 2D topology at $k_z = 0$ for EBR$_{77.18}^{2\tilde{a}}$ is the same as the topology discussed for EBR$_{75.5}^{2\tilde{a}}$, that is, CEF topology versus stable nodal (CW topology) indicated by $z_2$ in Eq. (10). We therefore can define a sub-dimensional $z_2^0 \in \mathbb{Z}_2$ symmetry indicator. We have seen that on the $k_z = \pi$ plane the $C_2T$ symmetry squares to $-1$, such that there is no (real) Euler class topology. Nevertheless, we show in Fig. 10 the $C_4$-symmetric Wilson loop on the plane $k_z = \pi$ for the model for MSG77.18 ($P^*_1, 42$) Eq. (20), over a) the conduction and b) valence bands. The winding of Wilson loop for the conduction bands indicates a crystalline (non-Euler) fragile (CF) topology.

3. AFM topological phases

We now discuss the global topology of the AFM topological phases for MSG77.18 ($P^*_1, 42$). We first note that EBR$_{77.18}^{2\tilde{a}}$ can be gapped over the planes $k_z = 0, \pi$. The 2D topology at $k_z = 0$ for EBR$_{77.18}^{2\tilde{a}}$ is the same as the topology discussed for EBR$_{75.5}^{2\tilde{a}}$, that is, CEF topology versus stable nodal (CW topology) indicated by $z_2$ in
We now consider the effect of breaking the non-symmorphic TRS, i.e. inducing a transition from the AFM phase of MSG77.18 \( (P4_2) \) to the FM phase of MSG77.13 \( (P4_2) \). This can be done by including a Zeeman splitting as we did for MSG75. We show the band structure in Fig. 7b), and along the high-symmetry lines in Fig. 8b), and d) after a band inversion at X. We find that all the Kramers degeneracies are split leaving gapped bands on the \( k_z = 0 \) and \( \pi \) planes. Similarly to the case of MSG75.1 \( (P4) \), the topology of the gapped bands at fixed \( k_z \) are characterized through symmetry indicated Chern numbers (i.e. with CC topology). Interestingly, for moderate Zeeman coupling, the four bands remain fully connected along the \( C_4 \)-symmetric axes through the persistence of the \( C_4 \)-symmetry protected Weyl nodes, as indicated by the IRREP order at \( \Gamma, Z, M, \) and \( A \), as it is clearly shown in Fig. 8b) and d).

We note however that, by relaxing the pairing conditions (i.e. from 2D colIRREPs to 1D IRREPs), there are more combinatorial ways of connecting the bands allowed by the compatibility relations for MSG77.13 \( (P4_2) \). In particular, the bands can be ordered at \( \{ \Gamma, Z, M, A \} \) as to avoid Weyl points at half-filling (more generally at a filling \( \nu \in 4\mathbb{Z} + 2 \)).

## 5. Stable 3D signatures

We emphasize that the rational of sub-dimensional topologies thus works in two manners. Firstly, because the total 3D EBR is connected, and thus trivial, these phases are missed by previous schemes. Reciprocally, the presence of in plane topology together with the nodes to make the EBR globally connected implies the coexistence of topological signatures of qualitatively distinct origins. On one hand, the connectivity condition directly induces symmetry indicated Weyl points, and in turn, Fermi arcs in the surface spectra. On the other hand, the subdimensional topology is either gapless, in which case it induces additional Weyl points and thus additional Fermi arcs, or it is gapped fragile topological, in which case it induces corner modes [56]. In this sense this mechanism can thus be used to find new topological signatures that are directly detectable via the usual routes of e.g. angle resolved photoemission spectroscopy, quantum oscillation techniques or scanning tunneling microscopy.

### B. Generalization

We end by generalizing our sub-dimensional topology scheme and search systematically for candidate MSGs hosting the planar topologies discussed so far— that is, CEF, CF, and CW phases for the AFM cases and CC phases for their FM counterpart—and the outlined mechanisms relating them. Remarkably, our results are directly transferable to all tetragonal MSGs with the point groups \( C_4 \) and \( S_1 \), i.e. comprising space group families SG75-SG82. For each family we then consider all the Shubnikov type IV AFM MSGs and the one type I FM MSG. This amounts to a total of 26 MSGs which we list in Table III, where we give the type of planar topologies for \( k_z = 0 \) and \( k_z = \pi \), and the list of EBRs hosting these. On top of the single EBRs that split on both planes, \( k_z = 0 \) and \( k_z = \pi \), and which must necessarily host a nontrivial planar topology of type indicated, we have also listed the sums of EBRs that can lead to a listed topology upon the permutation of their IRREPs. Whenever there is the choice CEF/CW, the topology is determined by the ordering of IRREPs. We note that \( [C_2T]^2 = \pm 1 \) indicates CEF or CEF/CW \( (+1) \) versus CF \( (-1) \) topology [98][99] as the only alternative since the Chern number must vanish. Finally, all FM candidates acquire CC topology when obtained from their AFM parents through Zeeman splitting. In particular, every nodal AFM phase at half-filling must give rise to a nontrivial Chern FM phase at half-filling, thus constituting a systematic correspondence between necessarily
TABLE III. Candidate MSGs for the (Euler) fragile/stable-nodal AFM to Chern FM mechanism, including those profiting from the subdimensional topological analysis. The table lists the AFM and corresponding FM counterparts as well as their time reversal invariant momenta (TRIM) which host Kramers doublets (i.e. Weyl nodes). Moreover, it details the topology by enumerating the value of $C_2T = \pm 1$ and the two-band subspace (2-BS) characterization on the $k_z = 0, \pi$ momentum planes. $C_2T = \pm 1$ indicates Euler class (real) topology, while $C_2T = -1$ implies the twofold Kramers degeneracy of the bands. The labels CEF, CW, and CC indicate crystalline Euler fragile (with symmetry-indicated Wilson loop quantization), crystalline fragile (with the winding of $C_4$-symmetric Wilson loop), and crystalline Weyl semimetallic (with a symmetry-indicated $\pi$-Berry phase), respectively. When the 2-BS Topology is CW, we mean that there must be Weyl nodes connecting adjacent two-band subspaces. When we write CEF/CW, we mean that either of the topologies is realized depending on the ordering of IRREPs.

| AFMSG | TRIM | $k_z$ | $|C_2T|^2$ | 2-BS Topology | EBRs | FMSG |
|-------|------|------|----------|--------------|------|------|
| 75.4 (P$_4$) | $\Gamma,M,X,X'$ | $\pi$ | $-1$ | CEF | $\{2a, \uparrow_x\} \oplus \{2b, \downarrow_z\}$, $(4c, \uparrow_z)$, $(4c, \downarrow_z)$ | 75.1 (P4) |
| 75.5 (P$_C$4) | $\Gamma,M,Z,A$ | $\pi$ | $-1$ | CEF/CW | $\{2a, \uparrow_x\} \oplus \{2b, \downarrow_z\}$, $(4c, \uparrow_z)$, $(4c, \downarrow_z)$ | 75.1 (P4) |
| 75.6 (P$_4$) | $\Gamma,M,R,R'$ | $\pi$ | $-1$ | CEF/CW | $(2a, \uparrow^1/2_x) \oplus (2a, \downarrow^1/2_z) \oplus (2a, \downarrow^1/2_z)$, $(4b, \uparrow_z)$, $(4b, \downarrow_z)$ | 75.1 (P4) |
| 76.10 (P$_C$4) | $\Gamma,M,X,X'$ | $\pi$ | $-1$ | CEF/CW | $(4a, \rightarrow_y)$, $(4b, \rightarrow_y)$, $(4c, \rightarrow_y)$ | 76.7 (P41) |
| 75.7 (P$_C$4) | $\Gamma,M,A$ | $\pi$ | $-1$ | CEF/CW | $(2a, \uparrow_x \oplus \downarrow_x)$, $(2b, \uparrow_x \oplus \downarrow_x)$, $(4c, \uparrow_z)$, $(4c, \downarrow_z)$ | 77.13 (P42) |
| 77.17 (P$_C$4) | $\Gamma,M,A$ | $\pi$ | $-1$ | CEF/CW | $(4a, \uparrow_x) \oplus (4a, \downarrow_x)$, $(4b, \uparrow_x) \oplus (4b, \downarrow_x)$, $(4c, \rightarrow_y)$ | 77.13 (P42) |
| 77.18 (P$_C$4) | $\Gamma,M,R,R'$ | $\pi$ | $-1$ | CEF/CW | $(2a, \uparrow_x \oplus \downarrow_x)$, $(4b, \uparrow_x)$, $(4b, \down_x)$, $(4c, \rightarrow_y)$ | 77.13 (P42) |
| 78.22 (P$_C$4) | $\Gamma,M,X'$ | $\pi$ | $-1$ | CEF/CW | $(4a, \rightarrow_y)$, $(4b, \rightarrow_y)$, $(4c, \rightarrow_y)$ | 78.19 (P43) |
| 78.23 (P$_C$4) | $\Gamma,M,A$ | $\pi$ | $-1$ | CEF/CW | $(4a, \rightarrow_y)$, $(4b, \rightarrow_y)$, $(4c, \rightarrow_y)$ | 78.19 (P43) |
| 78.24 (P$_C$4) | $\Gamma,M,R,R'$ | $\pi$ | $-1$ | CEF/CW | $(4a, \rightarrow_y)$, $(4b, \rightarrow_y)$, $(4c, \rightarrow_y)$ | 78.19 (P43) |
| 79.28 (I$_4$) | $\Gamma,M,X'$ | $\pi$ | $-1$ | CEF | $(4a, \uparrow_x) \oplus (4a, \down_x)$, $(4b, \up_x)$, $(4c, \rightarrow_y)$ | 79.25 (I4) |
| 80.32 (I$_4$) | $\Gamma,M,X'$ | $\pi$ | $-1$ | CEF | $(8a, \rightarrow_y)$, $(8b, \rightarrow_y)$, $(8c, \rightarrow_y)$ | 80.29 (I41) |
| 81.36 (P$_4$) | $\Gamma,M,X'$ | $\pi$ | $-1$ | CEF | $(2a, \uparrow_x \oplus \down_x)$, $(2b, \up_x)$, $(2c, \down_x)$, $(4g, \up_z)$, $(4g, \down_z)$ | 81.33 (P4) |
| 81.37 (P$_C$4) | $\Gamma,M,Z,A$ | $\pi$ | $-1$ | CEF/CW | $(2a, \uparrow_x \oplus \down_x)$, $(2b, \up_x)$, $(2c, \down_x)$, $(4g, \up_z)$, $(4g, \down_z)$ | 81.33 (P4) |
| 81.38 (P$_4$) | $\Gamma,M,R,R'$ | $\pi$ | $-1$ | CEF/CW | $(2a, \uparrow_x \oplus \down_x)$, $(2b, \up_x)$, $(2c, \down_x)$, $(4g, \up_z)$, $(4g, \down_z)$ | 81.33 (P4) |
| 82.42 (I$_4$) | $\Gamma,M,X'$ | $\pi$ | $-1$ | CEF | $(4a, \up_x)$, $(4b, \down_x)$, $(4c, \up_z)$, $(4d, \down_z)$, $(8y, \rightarrow_y)$ | 82.39 (I4) |

- The EBRs are defined for a given Wyckoff position and a fixed spin basis. We either take the vertical $\tilde{z}$-axis ($C_4$-axis) as the quantization axis for the spin-1/2 (3/2) with the spin basis (\uparrow_x, \down_x), or we take a quantization axis that is perpendicular to \tilde{z}, e.g. \tilde{y} for which the spin basis is \(\rightarrow_y\) = \(\uparrow_x \oplus \down_x\), \(\up_x \oplus \down_x\) / \(\sqrt{2}\).
- In the case of a single EBR, splitable at $k_z = 0$ and $k_z = \pi$, we mean that it must host one of the listed nontrivial topologies. In the case of a (direct) sum of EBRs, we mean that the topology can be achieved through the permutation of IRREPs between the EBRs.

nontrivial topological phases associated to MSG representations.

VI. CHIRAL FERMIONS AT HIGH-SYMMETRY MOMENTA AND LARGE FERMI ARCS

All the MSGs of the table with point group $C_4$ (i.e. the type IV AFM MSG75.4-MSG81.36, and the type I FM
MSG75.1-MSG80.29) have only proper symmetries, a consequence of which is that any crystal structure that explicitly breaks all symmetries not included in their MSG must be chiral, i.e. enantiomorphous (the SGs 75-76-77-78-79-80 are all among the 65 Schocke space groups with no inversion, no mirror, nor roto-inversion symmetries [100]). Then, the absence of improper symmetry allows the existence of Weyl nodes at high-symmetry momenta, i.e. with non-vanishing Chern numbers. This is the rationale for the chiral Fermions found in many (non-magnetic) material candidates with a Schocke space group [6, 101–105].

We have noted that MSG75.5 (PC4) and MSG77.18 (P42) exhibit Weyl nodes at every TRIMP at a filling $2Z + 1$. MSG77.18 must also exhibit Weyl nodes on the $\Gamma Z$- and $M A$-lines at a filling $4Z + 2$ due to the monodromy of the irreducible representation of the screw axis 42. The same results apply to the FM parents MSG75.1 (P4) and MSG77.13 (P42). The Weyl points at high-symmetry momenta for all the other MSGs of the table can be found similarly.

In Ref. [6] we have given a detailed analysis of the symmetry indicated higher Chern number generated by the Weyl points locked on a screw axis at half-filling, and derived the necessary existence of large Fermi arcs due to the compensation of chirality across the Brillouin zone. This analysis can be readily transferred to the present situation (e.g. here $C = \pm 2$ on the 42-axes). Large Fermi arcs has also been reported in other non-magnetic chiral materials [102, 103].

In the next section, we discuss the fate of the Weyl points when extra improper point symmetries are included.

We now turn to the MSGs with roto-inversion symmetry $IC_{4z}$. Since the chirality of Weyl points is reversed under $IC_{4z}$, the Kramer’s degeneracies at the TRIMPs (which are also $IC_{4z}$ invariant momenta) cannot form Weyl nodes at the filling $2Z + 1$. Instead, each double degeneracy at a TRIMP on the $k_z = 0$ plane is continued as a nodal line for all values of $k_z$ [69].

Remarkably the four bands become all connected through a fourfold magnetic Dirac node at M, similarly to the examples discussed in Ref. [55]. The same happens for MSG89.93 (P42), obtained by including one horizontal $\pi$-rotation symmetry (say $C_{2y}$) leading to the point group $D_4$ (422), as well as for MSG83.49 (P4/m), obtained by including the basal mirror symmetry $m_z$ leading to the point group $C_{4h}$ (4/m).

The structural chirality is lost for MSG99.169 (P4mm) and MSG83.49 (P4/m), thus preventing the existence of Weyl nodes at the TRIMPs, i.e. the Weyl points are absorbed within vertical nodal lines on the $C_{4z}$-axes, and, respectively, within a global twofold Kramer’s degeneracy. For MSG89.93 (P42) instead, the structural chirality, and thus the Weyl nodes, are preserved.

We note that the introduction $m_z$ allows the definition of $C_4$-symmetry indicated mirror Chern numbers [13, 83, 106]. The systematic study of the magnetic topological phases for the next magnetic super-space groups, however, lies beyond the scope of the present work.

B. Weyl phases protected by $|C_2T|^2 = +1$

The symmetry indicator Eq. (10) and its interpretation in terms of a $Z_2$ quantized Berry phase Eq. (11), derived here for MSG75.5 (PC4), can be readily applied to many other MSGs with gapped 2D planes in the Brillouin zone where $|C_2T|^2 = +1$. The simplest example MSG3.4 (P42), obtained by forgetting the $C_4$ symmetry, has a $Z_2$ symmetry indicator that readily corresponds to $z_2$ Eq. (10) [35].

For many MSGs though, there are symmetry indicated nodal points between the gapped planes, i.e. similarly to MSG77.18 (P42), such that they cannot be identified by a (3D) symmetry indicator and they have been listed as trivial [35].

C. Chern and Weyl phases of type I MSGs

We have discussed in detail the transition from the AFM Weyl phase of MSG75.5 (PC4), and MSG77.18 (P42), to the sub-dimensional Chern insulating FM phases of MSG75.1 (P4), and MSG77.13 (P42), respectively, obtained upon the breaking of the non-symmorphic TRS. The effect of breaking TRS is to unlock the Weyl nodes that were pinned on the $C_{2}T$ planes, so that they move within the Brillouin zone. We conclude that the symmetry indicator $Z_4$ of the type I MSG75.1 (P4) [35] indicates a Weyl semi-metallic phase, while there is no symmetry indicator for MSG77.13 (P42) [35] with a Weyl semi-metallic phase that must be assessed in terms of sub-dimensional topology.

In the same way as we predict many AFM phases with $C_{2}T$ protected Weyl nodal phases, we predict many FM
VIII. CONCLUSIONS

In conclusion, starting from the specific case study, MSG 75.5 (Pc4), we find that specific Wyckoff positions (2b) in this magnetic ground group necessarily results in (fragile) topological bands. In this regard we formulated a first generic model exhibiting fragile topology in the context of magnetic space group symmetries. Breaking the essential symmetry by a Zeeman term then relates the underlying AFM-compatible MSG with a FM counterpart in the same space group family and ensures that the fragile topology gaps into bands with finite Chern number. After translating the $Z_2$ symmetry indicator of the AFM MSG into a quantized Berry phase of a stable topological semimetallic phase, which originates from the combination of $C_4$ symmetry and $C_2T$-protected Euler class topology, we also discuss a similar correspondence to FM Chern phases. We thus unveil a systematic correspondence between necessarily nontrivial topological phases associated with MSG representations. Moreover, we then promote this mechanism to three spatial dimensions, where we also find novel phases characterized by the concept of subdimensional topologies. The latter feature the same in-plane mechanism but have 3D elementary band representations that are fully connected. As a result, the non-trivial 2D topology must coexists with nodes away from the high symmetry planes, e.g. Weyl points, giving rise to additional topological nodal features, such as Fermi arcs, that can be diagnosed with established experimental methods. As a result, our work culminates in an exhaustive list of tetragonal MSGs (with the point groups $C_4$ and $S_4$) and their EBR content hosting the above correspondence. We have then addressed the effect of adding and removing unitary symmetries that lead to the identification of magnetic Dirac (four-fold) points, and have outlined how the symmetry indicated Weyl semi-metallic phases protected by $C_2T$ can be found in numerous MSGs as a result of our refined subdimensional topological analysis. Given the generality of these insights and relevance of parameters to access this physics, we hope our results pave the way for new pursuits in topological band structures. In fact, we anticipate that this coexistence effect, i.e. of gapped subdimensional topology together with independent topological nodes, can also occur in the non-magnetic context culminating in novel gapped-nodal topological phases.

ACKNOWLEDGMENTS

R.-J. S. acknowledges funding from the Marie Skłodowska-Curie programme under EC Grant No. 842901 and the Winton programme as well as Trinity College at the University of Cambridge. G.F.L acknowledges funding from the Aker Scholarship.

Note added.– We finally note that our results agree with expressions for magnetic EBRs, compatibility relations and symmetry indicators tabulated in [36], which was posted during the finalizing stages of this manuscript.

Note added.– We comment here on Ref. [106] that appeared several months after the first version of this paper and has some overlap with our work. Among many results not covered by our work, they give a complete list of MSGs that have $z_2$ (called $z_4$ in their work) as one of the 3D symmetry indicators, including some of the MSGs discussed here. While the scope of our work was more restricted, our approach based on sub-dimensional topologies, i.e. allowing symmetry indicated nodes between gapped planes, leads us to predict many more MSGs with $C_2T$ protected Weyl semi-metallic phases. Ref. [106] also considers other Weyl semi-metallic phases in type I MSGs protected by $JC_{12}$ symmetry, among which are MSG81.33 ($P\bar{4}$) and MSG82.39 ($P\bar{4}$). Alternatively, these FM phases can be readily obtained, upon the breaking of the non-symmorphic TRS, from the (sub-dimensional) AFM Weyl phases of the following type IV MSG81.36 ($Pc\bar{4}$), MSG81.37 ($PC\bar{4}$), MSG81.38 ($P\bar{I}4$), and MSG82.42 ($Ic\bar{4}$), all listed in our table.
Appendix A: Wilson loop winding for the fragile topological phase

We algebraically derive the symmetry obstruction on the winding of Wilson loop over one quarter of the Brillouin zone, and following over the whole Brillouin zone, for the valence (conduction) subspace of the split EBR_{75.5}. For this we choose the patch of the Brillouin zone bounded by $l_{1\Gamma X\Gamma}$ and $l_{1\Gamma M\Gamma}$, see Fig. 2c (blue dashed). We design a flow starting with the base path $l_{1\Gamma X\Gamma}$ and ending with $l_{1\Gamma M\Gamma}$. Defining the Wilson loop phases

$$\{\varphi_1, \varphi_2\} = \text{Arg} \{\text{eig}\{W[l_{1\Gamma X\Gamma}]\}\}$$
$$\{\varphi'_1, \varphi'_2\} = \text{Arg} \{\text{eig}\{W[l_{1\Gamma M\Gamma}]\}\}$$  \hspace{1em} (A1)

they must extrapolate smoothly between $\{\varphi_1, \varphi_2\}$ and $\{\varphi'_1, \varphi'_2\}$ as we smoothly deform the base path from $l_{1\Gamma X\Gamma}$ to $l_{1\Gamma M\Gamma}$. The Wilson loop over an oriented base path $l : k_1 \rightarrow k_2$ is defined through $W_{k_2k_1} = \langle u, k_2 | W | u, k_1 \rangle$ where $|u, k_1\rangle$ is the matrix of Bloch eigenvectors of the band subspace under consideration, and $W = \prod_{k \in \text{Brillouin}} P(k)$ with the projector $P(k) = |u, k\rangle \langle u, k|$. We now show that the crystal symmetries act as an obstruction imposing the quantization of Wilson loop phases. First, we find

$$W[l_{1\Gamma X\Gamma}] = W[l_{1\Gamma X\Gamma}^{-1}] \cdot W_{X\Gamma}^{-1}$$
$$= R_a^X \cdot W_{X\Gamma}^{-1} \cdot (R_a^X)^{-1} \cdot W_{X\Gamma}^{-1},$$  \hspace{1em} (A2)

where $R_a^X = \langle u, D_{a\Gamma} | \tilde{U}(C_{2z}) | u, \bar{k} \rangle$ is the sewing matrix of the valence Bloch eigenvectors basis (with $\tilde{U}(C_{2z}) = \mathbb{1} \otimes e^{-i\pi z}$) of $C_{2z}$ at the high symmetry point $\bar{k}$ in the valence Bloch eigenvectors basis (with $\tilde{U}(C_{2z}) = \mathbb{1} \otimes e^{-i\pi z}$) of $C_{2z}$ in the orbital basis $\{\varphi, k\}$, and $D_a$ is the permutation operator, we retrieve irreducible representations $R_4^\xi$ and $R_3^\xi$ which depend on the coIRREPs realized at $\Gamma$ and $M$ (see Table I).

Considering now the base path $l_{1\Gamma M\Gamma}$, we have

$$W[l_{1\Gamma M\Gamma}] = W[l_{1\Gamma M\Gamma}^{-1}] \cdot W_{M\Gamma}^{-1}$$
$$= R_b^M \cdot W_{M\Gamma}^{-1} \cdot (R_b^M)^{-1} \cdot W_{M\Gamma},$$  \hspace{1em} (A4)

where $R_b^\rho = \langle u, D_{b\Gamma} | \tilde{U}(C_{4\Gamma}) | u, \bar{k} \rangle$ is the representation in the basis of Bloch eigenvectors of $C_{4\Gamma}$ at $\bar{k}$, with, in the orbital basis $\{\varphi, k\}$, $\tilde{U}(C_{4\Gamma}) = \sigma_x \otimes M_4$ where $M_4 = \text{diag}(e^{-i\pi/4}, e^{i\pi/4})$, and we have used $|u, D_{b\Gamma} | \bar{k} \rangle = \tilde{U}(C_{4\Gamma}) | u, \bar{k} \rangle R_b^\rho$. Using parallel transported Bloch eigenvectors the Wilson loop becomes diagonal, and we write $W_{M\Gamma}^{-1} = \text{diag}(e^{i\pi/2}, e^{i\pi/2})$. The above expression thus reduces to

$$\tilde{W}[l_{1\Gamma M\Gamma}] = R_b^M \cdot \left( \begin{array}{cc} e^{-i\pi/2} & 0 \\ 0 & e^{i\pi/2} \end{array} \right) \cdot (R_b^M)^{-1} \cdot \left( \begin{array}{cc} e^{i\pi/4} & 0 \\ 0 & e^{i\pi/4} \end{array} \right).$$  \hspace{1em} (A5)

Since at $C_{4\Gamma}$-symmetric momenta the parallel transported Bloch eigenvectors are also eigenvectors of the $C_{4\Gamma}$ operator, we retrieve irreducible representations $R_4^\xi = (\pm)\text{diag}(\omega, \omega^*)$ and $R_3^\xi = (\pm)\text{diag}(\omega, -\omega^*)$, where the signs depend on the coIRREPs realized at $\Gamma$ and $M$ (see Table I).

The quantization of the Wilson loop $\tilde{W}[l_{1\Gamma M\Gamma}]$ depends on the relative spin-$z$ components of the parallel transported Bloch eigenstates at $\Gamma$ and $M$, see the discussion in Ref. [38]. Writing $R_4^\xi = \text{diag}(e^{i\Gamma(a)}, e^{i\Gamma(b)})$, we find

$$\tilde{W}[l_{1\Gamma M\Gamma}] = \left( \begin{array}{cc} \xi_4^\Gamma(\Gamma_a)/\xi_4^\Gamma(\Gamma_b) & 0 \\ 0 & \xi_4^\Gamma(\Gamma_b)/\xi_4^\Gamma(\Gamma_a) \end{array} \right).$$  \hspace{1em} (A6)

Assuming the same spin-$z$ component at $\Gamma$ and $M$, e.g. with $\{\Gamma_a, \bar{\Gamma}_a, \bar{\Gamma}_b, \bar{\Gamma}_b\} = \{\Gamma_5, \bar{\Gamma}_5, \Gamma_7, \bar{\Gamma}_7\}$ (see Table I), we find

$$\{\varphi', \varphi''\} = \{\pi/4, \pi/4\} \mod 2\pi.$$  \hspace{1em} (A7)

This matches exactly with the direct numerical evaluation of the Wilson loop shown in Fig. 2c in the main text. If instead we assume opposite spin-$z$ components at $\Gamma$ and $M$, e.g. with $\{\Gamma_5, \bar{\Gamma}_5, \Gamma_7, \bar{\Gamma}_7\}$ (see Table I), we find

$$\{\varphi', \varphi''\} = \{0, \pi\} \mod 2\pi.$$  \hspace{1em} (A8)

This later quantization thus corresponds to a system where there is a twisting spin texture from $\Gamma$ to $M$, which would require strong Rashba-type spin-orbit coupling.

It thus follows that, in the absence of a twisted spin texture, the Wilson loop phases must wind from $\{\varphi_1, \varphi_2\} = \{0, \pi\}$ to $\{\varphi'_1, \varphi'_2\} = \{\pi/4, \pi/4\}$ mod $2\pi$, as we scan over one quarter of the Brillouin zone through the deformation of the base path from $l_{1\Gamma X\Gamma}$ to $l_{1\Gamma M\Gamma}$. There is thus a minimal winding of $(\Delta \varphi_1, \Delta \varphi_2) = (\varphi'_1, \varphi'_2) - (\varphi_1, \varphi_2) = (+\pi/2, -\pi/2)$. By the action of $C_4$ symmetry we can recover the whole Brillouin zone for which we predict a minimal winding of the Wilson loop phases of

We emphasize that the quantization of the Wilson loop over $\Gamma X \Gamma$ comes from the repetition of the IRREPs at X (equivalently at $\Gamma$). An alternative source of Wilson loop quantization is when both $\Gamma$ and $X$ are TRIMs in which case the Wilson loop phases are Kramers degenerated at $\{0, 0\}$ or $\{\pi, \pi\}$. 

This later quantization thus corresponds to a system where there is a twisting spin texture from $\Gamma$ to $M$, which would require strong Rashba-type spin-orbit coupling.

It thus follows that, in the absence of a twisted spin texture, the Wilson loop phases must wind from $\{\varphi_1, \varphi_2\} = \{0, \pi\}$ to $\{\varphi'_1, \varphi'_2\} = \{\pi/4, \pi/4\}$ mod $2\pi$, as we scan over one quarter of the Brillouin zone through the deformation of the base path from $l_{1\Gamma X\Gamma}$ to $l_{1\Gamma M\Gamma}$. There is thus a minimal winding of $(\Delta \varphi_1, \Delta \varphi_2) = (\varphi'_1, \varphi'_2) - (\varphi_1, \varphi_2) = (+\pi/2, -\pi/2)$. By the action of $C_4$ symmetry we can recover the whole Brillouin zone for which we predict a minimal winding of the Wilson loop phases of
4(Δφ₁, Δφ₂) = (±2π, −2π). This precisely predicts algebraically the numerical evaluation of the Wilson loop over the whole Brillouin zone shown in Fig. 2d).

We finally conclude that the valence (conduction) subspace of the split EBR₂₅蹉 is topologically non-trivial as indicated by the finite winding of Wilson loop phases.

Appendix B: Derivation of formula Eq. (14) and Eq. (11)

We give here the algebraic derivation of the Wilson loop over \( l_\xi = \Gamma M X M \) (red loop in Fig. 2c) as given in Eq. (11), from which Eq. (14) readily follows by reducing to a single band-subspace. We use the algebraic Wilson loop techniques developed in [13, 79] and [6, 38, 86].

It is convenient to decompose the Wilson loop into the contributions of each segment that connects two successive high-symmetry points, i.e. \( W[l_\xi] = W_0 W_1 W_2 W_3 \), with

\[
W_a = \langle u, \Gamma | \tilde{W} | u, M \rangle, \quad W_c = \langle u, X | \tilde{W} | u, M' \rangle, \quad W_b = \langle u, M' | \tilde{W} | u, \Gamma \rangle, \quad W_d = \langle u, M | \tilde{W} | u, X \rangle,
\]

where \( M' = M - b_2 \).

We now use symmetries to rewrite \( W_a \) and \( W_d \), as

\[
W_a = \langle u, \Gamma | \tilde{W} | u, M \rangle = \langle u, C_{4z} \Gamma | \tilde{W} | u, C_{4z} M \rangle = R^T \cdot \langle u, \Gamma | \tilde{U} | \tilde{W} \tilde{U} | (C_{4z}) | u, M' \rangle \cdot (R^M)^\dagger
\]

\[
= R^T \cdot W^{-1}_d \cdot (R^M)^\dagger,
\]

\[
W_d = \langle u, M | \tilde{W} | u, M' \rangle = \langle u, C_{2z} M' | \tilde{W} | u, C_{2z} M' \rangle = R^T \cdot \langle u, M' | \tilde{T}(-b_1) \tilde{U} \tilde{T}(C_{2z}) \tilde{W} \rangle
\]

\[
= R^T \cdot \langle u, M' | \tilde{T}(-b_1) \tilde{U} \tilde{T}(C_{2z}) \tilde{W} \rangle
\]

\[
\quad = R^T \cdot W^\prime_3 \cdot (R^M)^\dagger,
\]

where \( M' = M' - b_1 \) and \( X' = X - b_1 \). We thus have,

\[
\text{Det} W[l_\xi] = \text{Det} \left[ R^M_2 \cdot (R^X_2)^\dagger \cdot R^T \cdot (R^M_3)^\dagger \right].
\]

Defining the irreducible representation of the symmetry \( (g|\tau_\eta) \) in the basis of Bloch eigenstates as

\[
S^k_g = e^{-ik \cdot x} \tau_\eta R^k_b,
\]

and substituting in the above expression, we get

\[
\text{Det} W[l_\xi] = e^{i N_{\text{occ}} \left[ (M-X) \cdot \tau_{C_{2z}} + (\Gamma-M) \cdot \tau_{C_{4z}} \right]}
\]

\[
\text{Det} \left[ S^M_2 \cdot (S^X_2)^\dagger \cdot S^T \cdot (S^M_3)^\dagger \right]
\]

\[
= e^{i N_{\text{occ}} \left[ (M-X) \cdot \tau_{C_{2z}} + (\Gamma-M) \cdot \tau_{C_{4z}} \right] \prod_{i=1}^{N_{\text{occ}}} \xi^{i}_{\tau}\left(\xi^{M}_{\tau}\xi^{X}_{\tau}\right)}
\]

where \( N_{\text{occ}} \) is the number of occupied bands, and \( \xi^{k}_{\tau}(i) \) is the eigenvalue of the symmetry \( (g|\tau_\eta) \) of the \( i \)-th band at the high-symmetry momentum \( \bar{k} \). For magnetic space groups with symmorphic \( C_{4z} \) and \( C_{2z} \) symmetries (i.e. \( \tau_{C_{4z}} = \tau_{C_{2z}} = 0 \)) as MSG75.5 (and MSG75.1), it simplifies to

\[
\text{Det} W[l_\xi] = \prod_{i=1}^{N_{\text{occ}}} \xi^{\tau}_{\tau}\left(\xi^{M}_{\tau}\xi^{X}_{\tau}\right)
\]

Appendix C: Numerical computation of Berry phase flows for MSG75.1 (P4)

We present here the numerical evaluation of the non-triviality of the case MSG75.1 (P4), i.e. for the model Eq. (4) with an additional Zeeman coupling. In Fig. 12, we show the numerically obtained Berry phase for the individual bands of the band structure in Fig. 5 obtained for the model of MSG75.1 (P4). These evaluations corroborate the analytical results. That is, each band shows a finite Chern number \( C \). While bands 2 and 3 exhibit a value of \( C = 1 \), the other two bands have opposite Chern number. Finally, we also show in Fig. 13 the Berry phase of the bands as obtained from gapping the stable nodal topological MSG75.5 (P4) band structure of Fig. 3. As described in the main text, the resulting spectrum features a single band (band number two in this case) with Chern number \( C = -3 \), whereas the others exhibit a Chern number \( C = 1 \).

Appendix D: Details on symmetry indicator analysis

We here give further detail on the symmetry indicator analysis for some of the MSGs considered.
Bilbao Crystallographic Server operator (to form coIRREPs of MSG75.5 (P\textsubscript{c4}). Pairing the IRREPs of SG75, and pair them appropriately for the possible band structures for our model by considering the constraints imposed by the antiunitary symmetries. These can be determined from the Herring rule \cite{herring57} applied at each high-symmetry point. We only consider spinful IRREPs. At \Gamma and M (and A and Z), this gives pairing of inequivalent IRREPs. At X (and R), no additional pairing is required. To determine which IRREPs are paired to form the coIRREPs at \Gamma and M, we pair representations of \(g\) with representations of \(AgA^{-1}\), where \(g\) is an element of the unitary little group at \Gamma or M and \(A = (E|\tau)^r\). The allowed pairings at \Gamma are \(\Gamma_5\Gamma_7, \Gamma_6\Gamma_8\) and the pairings at M are \(\overline{M}_6M_7, \overline{M}_5M_8\). The magnetic EBRs for the MSG75.5 (\(PC_4\)) can be found from the EBRs for SG75 \cite{barkbout19}. We note that the vector \(\tau\) relates WP 1a \((0,0,0)\) and 1b \((1/2,1/2)\) in SG75, so the EBRs from these WPs are paired. Similarly, \(\tau\) maps WP 2c \((0,1/2),(1/2,0)\) in SG75 to itself, so we pair EBRs at WP 2c directly. We can uniquely determine which EBRs are paired, by realizing that the magnetic EBRs must satisfy the magnetic compatibility relations detailed above. This gives the following magnetic EBRs for MSG75.5 (\(PC_4\)) (using the WP labels from SG75):

\[
\begin{align*}
\Gamma_5 &\rightarrow \overline{Z}_5 \\
\Gamma_6 &\rightarrow \overline{Z}_6 \\
\Gamma_7 &\rightarrow \overline{Z}_7 \\
\Gamma_7 &\rightarrow \overline{Z}_8
\end{align*}
\]  
(D1)

The compatibility relations between M and A display a similar structure. Finally, the compatibility relations between X and R are:

\[
\begin{align*}
\mathbf{X}_3 &\rightarrow \overline{\mathbf{X}}_3 \\
\mathbf{X}_4 &\rightarrow \overline{\mathbf{X}}_4
\end{align*}
\]  
(D2)

From the above relations it is evident that it suffices to consider the points \(\Gamma, \mathbf{X}\) and \(\mathbf{M}\) as the compatibility relations uniquely link IRREPs at these points to all IRREPs at all other high-symmetry points in the 3D BZ \cite{barkbout19}. To form the coIRREPs, we consider the additional constraints imposed by the antiunitary symmetries. These full compatibility relations for the \(\Gamma\) point are given by:

\[
\begin{align*}
\Gamma_5 &\rightarrow \overline{Z}_5 \\
\Gamma_6 &\rightarrow \overline{Z}_6 \\
\Gamma_7 &\rightarrow \overline{Z}_7 \\
\Gamma_7 &\rightarrow \overline{Z}_8
\end{align*}
\]  
(D1)

To compute the compatibility relations for the \(\Gamma\) point are given by:

\[
\begin{align*}
\Gamma_5 &\rightarrow \overline{Z}_5 \\
\Gamma_6 &\rightarrow \overline{Z}_6 \\
\Gamma_7 &\rightarrow \overline{Z}_7 \\
\Gamma_7 &\rightarrow \overline{Z}_8
\end{align*}
\]  
(D1)

From our magnetic EBRs, we see that it is not possible to construct a band structure with an odd number of

\[
\begin{align*}
\Gamma_5 &\rightarrow \overline{Z}_5 \\
\Gamma_6 &\rightarrow \overline{Z}_6 \\
\Gamma_7 &\rightarrow \overline{Z}_7 \\
\Gamma_7 &\rightarrow \overline{Z}_8
\end{align*}
\]  
(D1)

From the above relations it is evident that it suffices to consider the points \(\Gamma, \mathbf{X}\) and \(\mathbf{M}\) as the compatibility relations uniquely link IRREPs at these points to all IRREPs at all other high-symmetry points in the 3D BZ \cite{barkbout19}. To form the coIRREPs, we consider the additional constraints imposed by the antiunitary symmetries. These full compatibility relations for the \(\Gamma\) point are given by:

\[
\begin{align*}
\Gamma_5 &\rightarrow \overline{Z}_5 \\
\Gamma_6 &\rightarrow \overline{Z}_6 \\
\Gamma_7 &\rightarrow \overline{Z}_7 \\
\Gamma_7 &\rightarrow \overline{Z}_8
\end{align*}
\]  
(D1)

From our magnetic EBRs, we see that it is not possible to construct a band structure with an odd number of
bands in the $\overline{X}_3$ (or equivalently the $\overline{X}_4$) IRREP from an integer combination of magnetic EBRs. Every other combination consistent with the compatibility relations can be constructed from the magnetic EBRs. Thus, the $Z_2$ indicator can be conveniently computed as:

$$n_{\overline{X}_3} \mod 2$$

in agreement with the expression in the main text.

2. Symmetry indicators for MSG77.18 ($P_{1}4_2$)

MSG77.18 ($P_{1}4_2$) is formed from SG77, by including the operator $(E|\tau)'$ with $\tau = \frac{1}{2}(a_1 + a_3)$. For the $C_4$ symmetric points (Γ,Z,M,A), the Herring test gives the same result as for 75.5. At X, the Herring test gives that the antiunitary symmetries impose no further degeneracies, whereas at R, the Herring test gives that each IRREP must be doubly degenerate. Additional degeneracies are imposed by the non-symmorphic symmetry elements of SG77. For the $C_4$ symmetric points, the non-symmorphic symmetries constrain that the IRREPs must switch partners when moving through the BZ. This enforces gap closings along the $k_z$ direction, which acts as an obstruction to defining two-band subspaces across the entire BZ, see figure 7a) and c). Thus the minimal connectivity of bands in the BZ is 4.

The symmetry indicator group can be computed as before. WP 1a (0, 1/2, z), (0, 1/2, z + 1/2) of SG77 goes into WP 2a of MSG77.18 ($P_{1}4_2$), and the two spinful site-symmetry IRREPs glue together. Similarly, WP 2a (0, 0, z), (0, 0, z + 1/2) and 2b (1/2, 1/2, z), (1/2, 1/2, z + 1/2) of SG77 go into WP 4b of MSG77.18 ($P_{1}4_2$), and by checking the compatibility relations, we realize that IRREPs $1E$ pairs with $1E$ at the different sites. Thus, we get three spinful magnetic EBRs, which are given by (using the WP labels from SG77):

$$\begin{align*}
2c : & \quad E_1 + 2c : E_2 \uparrow G = (\Gamma_5 \Gamma_6 \Gamma_8, Z_5 Z_6 Z_8, M_5 M_6 M_8, A_5 A_6 A_8, 2\overline{X}_3 2\overline{X}_4, 2R_3 2R_4) \\
2a : & \quad E_1 + 2b : E_2 \uparrow G = (\Gamma_5 \Gamma_6 \Gamma_8, Z_5 Z_6 Z_8, M_5 M_6 M_8, A_5 A_6 A_8, 4\overline{X}_3, 4R_4) \\
2a : & \quad E_2 + 2b : E_1 \uparrow G = (\Gamma_5 \Gamma_6 \Gamma_8, Z_5 Z_6 Z_8, M_5 M_6 M_8, A_5 A_6 A_8, 4\overline{X}_3, 4R_4)
\end{align*}$$

Using the Smith normal form decomposition as before, we see that there’s no nontrivial indicator in this MSG, in agreement with [35].

3. Symmetry indicator for MSG81.36 ($P_4$

As a final example, we here compute the symmetry indicators for MSG81.36 ($P_4$), as an example of an MSG with $S_4$ rotoinversion symmetry. This MSG is generated from SG81 by including the operator $(E|\tau)'$ with $\tau = \frac{1}{2}a_3$. SG81 is similar to SG75, but the $C_4$ rotations are combined with inversion. The Herring test gives that the $C_2$ IRREPs must glue together at the $C_2$ symmetric points X and R. At the $C_4$ symmetric points, the Herring test gives together $\Gamma_5 \Gamma_7$ and $\Gamma_6 \Gamma_8$ respectively, and similarly at M. At Z, $Z_5 Z_8$ and $Z_6 \overline{Z}_7$ glue together respectively, and similarly at A. This assignment satisfies the compatibility relations, so the minimal connectivity of bands in the BZ is 2, and two-band subspaces can be defined throughout the BZ.

To compute the symmetry indicator group, we note that $\tau$ connects WP 1a (0, 0, 0) and 1b (0, 0, 1/2) of SG81 to form magnetic WP 2a. Similarly, WP 1c (1/2, 1/2, 0) and 1d (1/2, 1/2, 1/2) of SG81 connect to form magnetic WP 2c. Some of the non-maximal WPc of SG81 become maximal WPc for MSG81.36 ($P_4$), e.g. WP 2c (0, 0, z), (0, 0, z) of SG81 goes into maximal magnetic WP 2b (0, 0, 1/4), (0, 0, 3/4), and similarly for non-magnetic WP 2f going into magnetic WP 2d. As the EBRs at these WPc have to satisfy compatibility relations, however, it is straightforward to investigate which site-symmetry IRREPs to pair. This gives the following magnetic EBRs (labelled using the WPc of SG81):
Computing the Smith normal form gives a single $\mathbb{Z}_2$ factor. Inspecting the solution space, we see that the corresponding indicator is given by whether the IRREPs at the $C_4$ invariant points contain an odd or an even number of representations with subscript 5 (or any other subscript). Thus, an explicit expression for the symmetry indicator is:

$$z'_2 = n_{\Gamma_5} + n_{\overline{Z}_5} + n_{\overline{M}_5} + n_{\overline{K}_5} \text{ mod } 2 \quad (D4)$$

It has been shown in [36] for MSG81.33 ($P\overline{4}$) that this

symmetry indicator relates to a 3D axion topological insulating phase.

We finally note that our results in this Appendix agree with general expressions for magnetic EBRs, compatibility relations and symmetry indicators in [36], which we became aware of during the finalizing stages of this manuscript.

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