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Nonsymmorphic symmetries like screws and glides produce electron band touchings, obstructing the formation of a band insulator and leading instead to metals or nodal semimetals even when the number of electrons in the unit cell is an even integer. Here we calculate the electron fillings compatible with being a band insulator for all 230 space groups, for non-interacting electrons with time-reversal symmetry. Our bounds are tight – that is we can rigorously eliminate band insulators at any forbidden filling, and produce explicit models for all allowed fillings – and stronger than those recently established for interacting systems. These results provide simple criteria that should help guide the search for topological semimetals and also have implications for both the nature and stability of the resulting nodal Fermi surfaces.

Introduction. — Recent advances in the understanding of topological phases of matter have rekindled the interest in the interplay between electron filling and electronic phases of matter. When is a system of electrons insulating? For non-interacting electrons in the presence of time-reversal (TR) symmetry, basic band theory dictates that a band insulator (BI) is possible only if the electron filling ν, defined as the average number of electrons per primitive unit cell, is an even integer.

Since all crystals possess space group (SG) symmetries, it is of fundamental importance to ask whether the filling constraints are tightened due to the crystal structure, i.e. do the extra spatial symmetries forbid BIs even when $\nu \in 2\mathbb{N}$? When spin-orbit coupling (SOC) is negligible, it has long been established that nonsymmorphic symmetries can enforce certain patterns of band degeneracies and lead to tighter filling constraints [1, 2]. Numerous recent works also pointed out that these nonsymmorphic filling constraints survive even when spin-rotation invariance is broken by SOC [3–13]. Weakly-correlated materials forbidden to be insulating by such tightened filling constraints tend to favor nodal semimetals — electronic systems with Fermi surfaces of reduced dimensionality and consequentially feature low-energy excitations with unconventional dispersion.

Similar filling constraints have also been derived for interacting systems using various non-perturbative methods [14–19]. However, none of the previous works provide tight constraints for all 230 SGs — in our recent work on interacting systems [18], we could only prove the tightness of the filling constraints for 218 SGs. That is, for the remaining 12 SGs at certain fillings, there was neither a general argument forbidding an insulator, nor an explicit construction of an insulating ground state.

Here we report the results from a comprehensive study of filling obstructions to realizing non-interacting TR-invariant BIs for all 230 SGs, with or without SOC. Our key result is summarized in Table I, which tabulates the set of electron fillings $\mathcal{S}_{\mathcal{G}}^{\mathrm{BI}}$ compatible with a TR-symmetric BI in any given SG $\mathcal{G}$. [See Tables S1, S2 of Supplementary Materials (SM) [20] for an expanded version]. Compared to the interacting results presented in [18], the current work serves as an independent verification of the tight filling constraints for 218 SGs using band-theory analysis, and provides the tight bounds for the remaining 12 SGs in the non-interacting limit. In addition, the band-theory arguments presented here form the basis for further $\boldsymbol{k} \cdot \boldsymbol{p}$ effective Hamiltonian analysis, which constrains the generic dispersion about the degeneracy point [13, 21–23]. In contrast, our previous interacting argument does not constrain the spectrum of low-energy excitation.

Before we move on to presenting the results we comment on how such tight filling constraints for all possible crystal structures should be useful for materials design and screening. Materials with $\nu \notin \mathcal{S}_{\mathcal{G}}^{\mathrm{BI}}$ are necessarily (semi-)metallic or strongly interacting. At the same time, since the Luttinger volume of a system with any even filling $\nu = 2n$ is zero, no Fermi surfaces are required [19, 24, 25]. The simplest Fermiology that has vanishing Luttinger volume, but at the same time is not an insulator, is a nodal point. Such systems are attractive candidates for realizing nodal semimetals, although we should note that other outcomes involving compensated Fermi surfaces are also admissible. Therefore the tight filling constraints we presented should be viewed as a general guide to help narrow down the search space to materials with a combination of SG symmetries and fillings that naturally favor nodal semimetals.

Actually, it may be worth noting that in spin-orbit-coupled systems lacking inversion symmetry, a similar argument on the Fermiology applies even when $\nu = 2n + 1$. Conventionally this filling is associated with a large Fermi surface, encompassing half the Brillouin zone; in the presence of SOC, however, the individual spin components cannot be distinguished and the Luttinger volume constraint only applies to the total number of electrons. Hence one could in principle realize a nodal semimetal at such fillings. However, if SOC is negligible or when the crystal is centrosymmetric, each band is doubly degenerate and the Luttinger's count is effectively halved. Consequently, unless both spatial inversion and spin-rotation symmetries are strongly broken, such systems typically possess two big Fermi surfaces each enclosing approximately half of the first Brillouin zone.

Let us mention some examples of existing materials that

TABLE I. The list of fillings $\mathcal{S}^{\mathrm{BI}}_{\mathcal{G}}$ corresponding to TR symmetric BIs in the presence / absence of SOC. $m\mathbb{N}$ represents the set $\{m, 2m, 3m, \cdots\}$ and $A \setminus B$ means deleting elements of B from A. $\mathcal{S}^{\mathrm{AI}}_{\mathcal{G}}$'s are the corresponding fillings for AIs. $\cap_{\Gamma \leq \mathcal{G}}(\mathcal{S}^{\mathrm{BI}}_{\Gamma}/v_{\mathcal{G},\Gamma})$ is the tightest constraints obtainable from Bieberbach subgroups Γ.

$\mathcal{G}$ (ITC No.)	$\mathcal{S}^{\mathrm{BI}}_{\mathcal{G}\times\mathrm{SU}(2)} = \mathcal{S}^{\mathrm{AI}}_{\mathcal{G}}$	$\mathcal{S}^{\mathrm{BI}}_{\mathcal{G}}$	$\cap_{\Gamma \leq \mathcal{G}}(\mathcal{S}^{\mathrm{BI}}_{\Gamma}/v_{\mathcal{G},\Gamma})$
1	$2\mathbb{N}$	$2\mathbb{N}$	$2\mathbb{N}$
4, 7, 9	$4\mathbb{N}$	$4\mathbb{N}$	$4\mathbb{N}$
144≃*145*	$6\mathbb{N}$	$6\mathbb{N}$	$6\mathbb{N}$
19, 29, 33, 76≃*78*	$8\mathbb{N}$	$8\mathbb{N}$	$8\mathbb{N}$
169≃*170*	$12\mathbb{N}$	$12\mathbb{N}$	$12\mathbb{N}$
73, 106, 110, 133, *135, 142, 206, 228*	$8\mathbb{N}$	$8\mathbb{N}$	$4\mathbb{N}$
199, 214	$4\mathbb{N} \setminus \{4\}$	$4\mathbb{N}$	$4\mathbb{N}$
220	$4\mathbb{N} \setminus \{4, 8, 20\}$	$4\mathbb{N} \setminus \{4\}$	$4\mathbb{N}$
230	$8\mathbb{N} \setminus \{8\}$	$8\mathbb{N}$	$4\mathbb{N}$
all other SGs	$2|\mathcal{W}^{\mathcal{G}}_{\mathrm{a}}|\mathbb{N}$	$2|\mathcal{W}^{\mathcal{G}}_{\mathrm{a}}|\mathbb{N}$	$2|\mathcal{W}^{\mathcal{G}}_{\mathrm{a}}|\mathbb{N}$

illustrate how our results apply. The proposed nodal-ring semimetal SrIrO$_3$ [26], which has a topologically protected nodal Fermi surface [5], has $\nu = 4$. For this SG (*62*), however, the allowed BI fillings are $\mathcal{S}^{\mathrm{BI}}_{62} = 8\mathbb{N}$, hence the necessity of at least nodal points at the lower filling. Now consider the stability of this nodal structure to a symmetry-lowering distortion $\mathcal{G} \to \mathcal{G}'$. If $\mathcal{S}^{\mathrm{BI}}_{\mathcal{G}} = \mathcal{S}^{\mathrm{BI}}_{\mathcal{G}'}$, the nodal Fermi surface is guaranteed to be protected from a full gapping out, although it can change from, say, a collection of nodal lines to nodal points. Conversely, if $\nu \in \mathcal{S}^{\mathrm{BI}}_{\mathcal{G}'}$, a possibly nontrivial BI, such as a topological (crystalline) insulator, is in principle achievable via such distortion.

Identification of special SGs. — We start by identifying some simple rules that reduce the analysis to a small number of special SGs. Consider a class of system X satisfying certain defining properties, like SG symmetries. We will be interested in $\mathcal{S}_X$, the set of electron fillings (defined with *primitive* unit cell) for which a BI in class X is possible. Imagine a 'less constrained' class X' for which we lift some of the constraints imposed on X. By definition, a BI lying in class X also lies in class X', but the converse is not necessarily true. So the sets of fillings satisfy $\mathcal{S}_X \subseteq \mathcal{S}_{X'}$ provided the filling is defined with respect to the same unit cell on the two sides.

Such relations will greatly reduce the work required to establish the BI filling bounds for all 230 SGs. For instance, if SG $\mathcal{G}'$ is a subgroup of $\mathcal{G}$, systems symmetric under $\mathcal{G}'$ belong to a 'less-constrained' class compared to those symmetric under $\mathcal{G}$. Therefore, we get an 'upper'-bound, $\mathcal{S}^{\mathrm{BI}}_{\mathcal{G}} \subseteq \mathcal{S}^{\mathrm{BI}}_{\mathcal{G}'}/v_{\mathcal{G},\mathcal{G}'}$ for $\mathcal{G}' < \mathcal{G}$. The factor $v_{\mathcal{G},\mathcal{G}'} \geq 1$ is needed because $\mathcal{G}'$ and $\mathcal{G}$ may have different unit cell volumes. For instance, if $\mathcal{G}$ differs from $\mathcal{G}'$ only by a body-centered translation, we have $v_{\mathcal{G},\mathcal{G}'} = 2$. More generally, $v_{\mathcal{G},\mathcal{G}'} = |T_{\mathcal{G}}/T_{\mathcal{G}'}|$, where $T_{\mathcal{G}}$ is the translation subgroup of $\mathcal{G}$ [27].

Atomic insulators (AIs) are special instances of BIs in which each electron is tightly localized to a single atomic orbital, or which can be smoothly deformed to such a configuration while preserving the symmetries. This is a restriction on the phase, and thus $\mathcal{S}^{\mathrm{AI}}_{\mathcal{G}} \subseteq \mathcal{S}^{\mathrm{BI}}_{\mathcal{G}}$ for the same $\mathcal{G}$, establishing a useful 'lower' bound. Whenever the upper and lower bounds agree with each other, i.e. $\mathcal{S}^{\mathrm{AI}}_{\mathcal{G}} = \mathcal{S}^{\mathrm{BI}}_{\mathcal{G}'}/v_{\mathcal{G},\mathcal{G}'}$ for some $\mathcal{G}' \leq \mathcal{G}$, one obtains the tight constraint $\mathcal{S}^{\mathrm{BI}}_{\mathcal{G}} = \mathcal{S}^{\mathrm{AI}}_{\mathcal{G}}$.

At first sight, it may appear nontrivial to deduce $\mathcal{S}^{\mathrm{BI}}_{\mathcal{G}}$ from this approach, since (i) one would still need to determine $\mathcal{S}^{\mathrm{AI}}_{\mathcal{G}}$, and (ii) there are numerous subgroup $\mathcal{G}'$ for any $\mathcal{G}$, and it is unclear which $\mathcal{G}'$ will provide maximal information about $\mathcal{S}^{\mathrm{BI}}_{\mathcal{G}}$. Fortunately (i) can be accomplished with little effort: by definition a TR-symmetric AI can be smoothly deformed into a phase with Kramers pairs of electrons localized to well-defined points in space, and these points must form a SG symmetric lattice. Such lattices are classified under the 'Wyckoff positions', which are exhaustively tabulated in [28]. Each Wyckoff position $\mathcal{W}^{\mathcal{G}}_w$ ($w = \mathrm{a}, \mathrm{b}, \dots$) corresponds to a lattice with some number of points within each *primitive* unit cell, which we denote by $|\mathcal{W}^{\mathcal{G}}_w|$. Thus $\mathcal{S}^{\mathrm{AI}}_{\mathcal{G}}$ is spanned by adding together arbitrary multiples of $2|\mathcal{W}^{\mathcal{G}}_w|$ (see Sec. II of SM).

For (ii), we take advantage of nonsymmorphic symmetries, which generally require extra band crossings and lead to tighter bounds on $\mathcal{S}^{\mathrm{BI}}_{\mathcal{G}}$ [2]. To systematically study the effects of nonsymmorphic elements of $\mathcal{G}$, we first consider a special class of SGs that contains only screws, glides, and translations. When acting on $\mathbb{R}^3$ such groups are fixed-point free, i.e. $\boldsymbol{r} \neq g(\boldsymbol{r})$ for any pair of $\boldsymbol{r} \in \mathbb{R}^d$ and $g \in \mathcal{G}$ unless g is the identity, and are known as 'Bieberbach' groups. Up to chirality there are only 10 such SGs in 3D [28]: *1*, *4*, *7*, *9*, *19*, *29*, *33*, *76*($P4_1$)≃*78*($P4_3$), *144*($P3_1$)≃*145*($P3_2$), *169*($P6_1$)≃*170*($P6_5$). (To avoid possible confusions, we denote a specific SG by its SG number used in [28] in ***bold italic*** face.)

In Sec. IV of SM, we establish that $\mathcal{S}^{\mathrm{AI}}_{\Gamma} = \mathcal{S}^{\mathrm{BI}}_{\Gamma}$ for each of the 10 Bieberbach groups Γ (the first row of Table I). The 10 Bieberbach groups then serve as an anchor for most of the analysis. In particular, for many SGs $\mathcal{G}$ there exists a Bieberbach subgroup $\Gamma \leq \mathcal{G}$ satisfying $\mathcal{S}^{\mathrm{AI}}_{\mathcal{G}} = \mathcal{S}^{\mathrm{BI}}_{\Gamma}/v_{\mathcal{G},\Gamma}$, which therefore establishes a tight bound on $\mathcal{S}^{\mathrm{BI}}_{\mathcal{G}}$. In fact, determining $\mathcal{S}^{\mathrm{AI}}_{\mathcal{G}}$ and $\mathcal{S}^{\mathrm{BI}}_{\Gamma}$ allows us to derive $\mathcal{S}^{\mathrm{BI}}_{\mathcal{G}}$ for 218 out of the 230 SGs [entries in Table I with $\mathcal{S}^{\mathrm{AI}}_{\mathcal{G}} = \mathcal{S}^{\mathrm{BI}}_{\mathcal{G}} = \cap_{\Gamma \leq \mathcal{G}}(\mathcal{S}^{\mathrm{BI}}_{\Gamma}/v_{\mathcal{G},\Gamma})$]. The 12 remaining SGs require a case-by-case study, though there are still group-subgroup relations among them that we can use to our advantage. With that, our main result can be tersely summarized as: *For spinful electrons symmetric under both TR and SG $\mathcal{G}$, $\mathcal{S}^{BI}_{\mathcal{G}} = \mathcal{S}^{AI}_{\mathcal{G}}$ unless $\mathcal{G}$ belongs to one of the following four exceptions: 199, 214, 220 and 230.* These four exceptions allow for BIs even when no AI is possible at the same filling, and their topological properties are the focus of another study [29].

Lastly, we address the case of systems with $\mathrm{SU}(2)$ spin-rotation invariance, relevant when SOC is negligible. The filling constraints satisfy $\mathcal{S}^{\mathrm{AI}}_{\mathcal{G}\times\mathrm{SU}(2)} \subseteq \mathcal{S}^{\mathrm{BI}}_{\mathcal{G}\times\mathrm{SU}(2)} \subseteq \mathcal{S}^{\mathrm{BI}}_{\mathcal{G}}$. Since each entry in $\mathcal{S}^{\mathrm{AI}}_{\mathcal{G}}$ corresponds to localizing an even number of electrons on each site, one can as well imagine putting them into a spin-singlet wavefunction, i.e. $\mathcal{S}^{\mathrm{AI}}_{\mathcal{G}\times\mathrm{SU}(2)} = \mathcal{S}^{\mathrm{AI}}_{\mathcal{G}}$.

Again by composing these relations, we have $\mathcal{S}_{\mathcal{G}\times\mathrm{SU}(2)}^{\mathrm{BI}} = \mathcal{S}_{\mathcal{G}}^{\mathrm{BI}}$ whenever $\mathcal{S}_{\mathcal{G}}^{\mathrm{BI}} = \mathcal{S}_{\mathcal{G}}^{\mathrm{AI}}$. Hence, to establish the complete list of $\mathcal{S}_{\mathcal{G}\times\mathrm{SU}(2)}^{\mathrm{BI}}$ one simply studies the four SGs with $\mathcal{S}_{\mathcal{G}}^{\mathrm{BI}} \neq \mathcal{S}_{\mathcal{G}}^{\mathrm{AI}}$. The result is: *For spinful electrons symmetric under TR, SG $\mathcal{G}$, and spin rotation, $\mathcal{S}_{\mathcal{G}\times\mathrm{SU}(2)}^{\mathrm{BI}} = \mathcal{S}_{\mathcal{G}}^{\mathrm{AI}}$ for all 230 SGs.*

Band theoretical analysis for 73. — We have reduced the analysis to that of the 10 Bieberbach SGs Γ, and the 12 SGs for which knowledge on $\mathcal{S}_{\mathcal{G}}^{\mathrm{AI}}$ and $\mathcal{S}_{\Gamma}^{\mathrm{BI}}$ alone does not guarantee tightness of the bounds on $\mathcal{S}_{\mathcal{G}}^{\mathrm{BI}}$. The filling constraints for some of these SGs, like those with a single screw or glide, have been derived in the literature [2–13]. As briefly reviewed in Sec. III of SM, the main strategy is to derive the little group irreducible representations (irreps) at the high symmetry momenta, and then study the compatibility between irreps connected by high symmetry lines. Such analysis, however, can become quite technical when the SG possesses a larger number of symmetries. Instead of presenting all the arguments for the $10 + 12$ SGs mentioned above, here we focus only on *73* in the presence of SOC, which illustrates the key ingredients needed to derive filling constraints for a SG with multiple nonsymmorphic symmetries and extra point group symmetries. We refer the interested readers to Sec. IV and V of SM for a detailed discussion on all the other SGs and the cases with spin-rotation invariance.

73 (*Ibca*) is centrosymmetric (i.e., contains the spatial inversion P) and belongs to the body-centered orthorhombic system. It is generated by P and (two of the) three orthogonal screws $S_{\alpha} \equiv T_{\boldsymbol{\tau}_{\alpha}} R_{\alpha,\pi}$ with $\alpha = x, y, z$. $R_{\alpha,\theta}$ represents the anti-clockwise rotation by angle θ around the positive α-axis; $T_{\boldsymbol{t}}$ represents the translation by $\boldsymbol{t}$, where for the screws we have $\boldsymbol{\tau}_x = (1/2, 1/2, 0)$, $\boldsymbol{\tau}_y = (0, 1/2, 1/2)$ and $\boldsymbol{\tau}_z = (1/2, 0, 1/2)$.

We first study the constraints arising from the screws. S_z is a symmetry of the Bloch states along the line $\boldsymbol{k} = (\pi, \pi, k_z)$, which connects two high-symmetry points $\boldsymbol{k} = (\pi, \pi, 0)$ (a time-reversal invariant momentum) and (π, π, π) (*not* time-reversal invariant due to the body-centered structure). Since $S_z^2 = T_{(0,0,1)} R_{z,2\pi}$ and 2π-rotation is -1 for a spin-1/2 electron, the allowed eigenvalues of S_z along this line are $\xi_{z,k_z}^{(l)} = \xi_{z,0}^{(l)} e^{-ik_z/2} = \pm i e^{-ik_z/2}$ (l is the band index). At $(\pi, \pi, 0)$, bands with $\xi_{z,0}^{(l)} = \pm i$ are paired into Kramers doublets. Assuming a BI, the two bands forming a doublet at $(\pi, \pi, 0)$ are either both filled or both empty. Therefore, along the line (π, π, k_z) the number of filled bands having $\xi_{z,k_z}^{(l)} = i e^{-ik_z/2}$ will always equal to that with $\xi_{z,k_z}^{(l)} = -i e^{-ik_z/2}$. The same argument, using the lines (k_x, π, π) and (π, k_y, π) applies equally well to ξ_{x,k_x} and ξ_{y,k_y}.

Now suppose there exists a BI at $\nu = 2$, and we focus on the symmetry representation at (π, π, π) where all three screws are symmetries. On the one hand, the preceding discussion implies the two bands have opposite $\xi_{\alpha,\pi}$, i.e. $\xi_{\alpha,\pi}^{(1)} \xi_{\alpha,\pi}^{(2)} = -1$ for each $\alpha = x, y, z$. On the other hand, the screw eigenvalues of a single band are constrained by the group relations. Since the product of three screws satisfies $S_x S_y S_z = 1$, we have
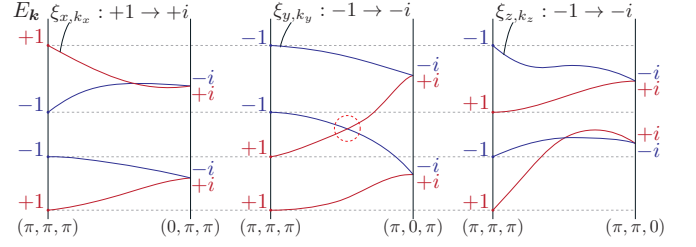

FIG. 1. Typical band structure of a TR-symmetric free electron system with SG *73*. Each branch is doubly degenerate due to presence of TR and inversion. Note that the product $\xi_{x,\pi}^{(l)} \xi_{y,\pi}^{(l)} \xi_{z,\pi}^{(l)}$ is identical for all bands (chosen to be $+1$ here). The red dashed circle indicates inevitable crossings of 4 branches (a Dirac cone), enforcing $\nu = 8$.

$\xi_{x,\pi}^{(l)} \xi_{y,\pi}^{(l)} \xi_{z,\pi}^{(l)} = \pm 1$. Note that the sign ambiguity, originating from the phase difference between $\pm\pi$ rotations on spin-1/2's, is independent of l. We therefore require simultaneously

$$\begin{cases} (\xi_{x,\pi}^{(1)}\xi_{x,\pi}^{(2)})(\xi_{y,\pi}^{(1)}\xi_{y,\pi}^{(2)})(\xi_{z,\pi}^{(1)}\xi_{z,\pi}^{(2)}) = (-1)^3 = -1 \\ (\xi_{x,\pi}^{(1)}\xi_{y,\pi}^{(1)}\xi_{z,\pi}^{(1)})(\xi_{x,\pi}^{(2)}\xi_{y,\pi}^{(2)}\xi_{z,\pi}^{(2)}) = (\pm 1)^2 = +1 \end{cases}, \quad (1)$$

a contradiction. More generally, the two conditions imply each of the four 1D irreps at (π, π, π) appears the same number of times among the filled bands if the system is insulating, and therefore $\mathcal{S}_{73}^{\mathrm{BI}} \subseteq 4\mathbb{N}$ (Fig. 1).

To derive the tight bounds for $\mathcal{S}_{73}^{\mathrm{BI}}$, however, one must utilize the inversion symmetry P, which was not assumed in the previous analysis. As is well-known, for spinful electrons the combination of P and $\mathcal{T}$ leads to doubly degenerate bands everywhere in the Brillouin zone. In particular $P\mathcal{T}$ commutes with S_{α} at (π, π, π), and hence the bands paired by $P\mathcal{T}$ have the same $\xi_{\alpha,\pi}^{(l)}$. The previous argument can then be applied to half of the bands (one from each pair). Combined with the observation that $\mathcal{S}_{73}^{\mathrm{AI}} = 8\mathbb{N}$, we conclude $\mathcal{S}_{73}^{\mathrm{BI}} = 8\mathbb{N}$.

Band insulators on flat manifolds. — Here we present an alternative derivation of $\mathcal{S}_{\mathcal{G}}^{\mathrm{BI}}$ by defining the system on a nontrivial flat manifold. For simplicity we illustrate the main idea using $\mathcal{G} = $ *73* as an example, and a more general discussion is presented in Sec. VI of SM.

Suppose we are given a system of spinful electrons in $\mathbb{R}^3$ symmetric under $\mathcal{G} = $ *73*. Let us imagine putting the system on one of the 10 compact flat manifolds in 3D. The most familiar example of such manifolds is the torus, which can be obtained by imposing periodic boundary conditions. In doing so, we (implicitly) take a translation subgroup $\Gamma^{(0)}$ of *73* generated by $T_{\hat{\alpha}}^L = S_{\alpha}^{2L}$, and identify $\boldsymbol{r} \in \mathbb{R}^3$ by $\boldsymbol{r} \sim \boldsymbol{r} + L(l, m, n)$, with the two sides related by any $T_{\hat{x}}^{Ll} T_{\hat{y}}^{Lm} T_{\hat{z}}^{Ln} = T_{L(l,m,n)} \in \Gamma^{(0)}$. Here, L is the linear dimension of the torus $\mathbb{R}^3/\Gamma^{(0)}$ and should be chosen much larger than the microscopic lattice constant 1. To define the Hamiltonian on the torus, we also need to identify electronic creation operator $\hat{c}_i^{\dagger}(\boldsymbol{r})$ as $\hat{c}_i^{\dagger}(\boldsymbol{r}) \sim \hat{T}_{L(l,m,n)} \hat{c}_i^{\dagger}(\boldsymbol{r}) \hat{T}_{L(l,m,n)}^{-1} = \hat{c}_i^{\dagger}(\boldsymbol{r} + L(l, m, n))$, where the subscript i represents internal degrees of freedom.

Replacing $\Gamma^{(0)}$ by other fixed-point-free subgroups of **73** allows one to define the system on a nontrivial flat manifold. Here we choose a subgroup $\Gamma = \mathbf{19}$ generated by $\tilde{S}_\alpha \equiv T^L_{\tau_\alpha} R_{\alpha,\pi}$ with an odd integer $L \gg 1$. Note that, for instance, $\tilde{S}_x = T_{(\frac{L}{2},\frac{L}{2},0)} R_{x,\pi} = (S_y)^{L-1}(S_x)^L$. The spatial points are identified as before, i.e. $\boldsymbol{r} \sim \gamma(\boldsymbol{r})$ for all $\gamma \in \Gamma$, and this gives the flat manifold $\mathcal{M} = \mathbb{R}^3/\Gamma$. The identification of operators are, however, nontrivial:

$$\hat{c}^\dagger_i(\boldsymbol{r}) \sim \hat{\gamma}\hat{c}^\dagger_i(\boldsymbol{r})\hat{\gamma}^{-1} = \hat{c}^\dagger_j(\gamma(\boldsymbol{r}))(U_\gamma)_{ji}. \qquad (2)$$

Here U_g is a unitary representation of $g \in \mathcal{G}$, and in contrast to the torus case $U_\gamma \neq 1$ in general. What is slightly complicated here is that the electron spin transforms projectively under spatial symmetries, i.e., $U_g U_{g'} = \omega_{g,g'} U_{gg'}$ for $g, g' \in \mathcal{G}$, and U_g intrinsically possesses sign ambiguity. For example, π-rotation about the α-axis can be represented by either of $e^{\pm i\pi\frac{1}{2}\sigma_\alpha} = \pm i\sigma_\alpha$. To consistently identify operators, we need to fix the phase of U_g in such a way that U_γ ($\gamma \in \Gamma$) is a linear (non-projective) representation of $\Gamma \subset \mathcal{G}$. Such a choice of sign is always possible in 3D if Γ is fixed-point free [30]. For the current problem, one can freely choose $U_{S_\alpha} = \pm i\sigma_\alpha$, but consistency demands $U_{T_\alpha} = U^2_{S_\alpha} = -1$.

The argument presented so far uses only the Bieberbach subgroup Γ and does not rely on the non-interacting assumption. Indeed the interacting bounds we presented in [18] coincide with $\mathcal{S}^{\mathrm{BI}}_\Gamma/v_{\mathcal{G},\Gamma}$ for all SGs. As shown in Table I, however, $\mathcal{S}^{\mathrm{BI}}_\mathcal{G} \neq \mathcal{S}^{\mathrm{BI}}_\Gamma/v_{\mathcal{G},\Gamma}$ for 10 SGs including **73**. To derive the tight, non-interacting bounds for them one must utilize the other SG symmetries differentiating $\mathcal{G}$ from Γ.

Generally, an element g in $\mathcal{G}$ but not in Γ may not remain a symmetry on $\mathcal{M}$. The necessary and sufficient condition for g to remain a symmetry is that

$$\forall \gamma \in \Gamma, \quad g\gamma g^{-1} \in \Gamma \quad \text{and} \quad U_g U_\gamma U_g^{-1} = U_{g\gamma g^{-1}}. \qquad (3)$$

The first one is needed because $\boldsymbol{r}$ and $\gamma(\boldsymbol{r})$, the same point on $\mathcal{M}$, should be mapped to the same point again, i.e. $g(\gamma(\boldsymbol{r})) \sim g(\boldsymbol{r})$. Similarly, the second one is to ensure the operator identification is preserved: $\hat{g}\hat{c}^\dagger_i(\boldsymbol{r})\hat{g}^{-1} \sim \hat{g}\hat{\gamma}\hat{c}^\dagger_i(\boldsymbol{r})\hat{\gamma}^{-1}\hat{g}^{-1}$. For the problem at hand, both the rescaled body-centered translation $B = T_{(\frac{L}{2},\frac{L}{2},\frac{L}{2})}$ and the inversion P are remnant symmetries.

To derive a filling constraint, we focus on the commutation relation of B and P. They originally commute on $\mathbb{R}^3$ but here we claim they must satisfy $\hat{B}\hat{P} = (-1)^{\hat{F}}\hat{P}\hat{B}$ as operators acting on Hilbert space, where $\hat{F}$ is the fermion number operator. This follows from $BP = T_x T_y T_z PB$ and $U_{T_\alpha} = -1$. Or more explicitly,

$$\begin{aligned} \hat{B}\hat{P}\hat{c}^\dagger_i(\boldsymbol{r})\hat{P}^{-1}\hat{B}^{-1} &= \hat{c}^\dagger_i(-\boldsymbol{r} + (\tfrac{L}{2},\tfrac{L}{2},\tfrac{L}{2})); \\ \hat{P}\hat{B}\hat{c}^\dagger_i(\boldsymbol{r})\hat{B}^{-1}\hat{P}^{-1} &= \hat{c}^\dagger_i(-\boldsymbol{r} - (\tfrac{L}{2},\tfrac{L}{2},\tfrac{L}{2})), \end{aligned} \qquad (4)$$

and the identification rule (2) implies $\hat{c}^\dagger_i(-\boldsymbol{r} + (\frac{L}{2},\frac{L}{2},\frac{L}{2})) \sim (-1)^3 \hat{c}^\dagger_i(-\boldsymbol{r} - (\frac{L}{2},\frac{L}{2},\frac{L}{2}))$.

In addition to B and P, the TR symmetry $\mathcal{T}$ ($\hat{\mathcal{T}}^2 = (-1)^{\hat{F}}$) is also a remnant symmetry, and it still commutes with B and

P. This algebra requires a four-fold degeneracy in the single particle spectrum, and hence we need $4n$ electrons on $\mathcal{M}$ to realize a BI. Since the number of unit cells contained in $\mathcal{M}$ is $\frac{L^3}{|\Gamma/T_\Gamma|}v_{\mathcal{G},\Gamma} = \frac{L^3}{2}$ (see Sec. VI of SM), a BI is possible only if $\nu\frac{L^3}{2} \in 4\mathbb{N}$. Recalling L is odd, one concludes $\mathcal{S}^{\mathrm{BI}}_{73} = 8\mathbb{N}$. Note that the nontriviality of the algebra hinges on $(-1)^{\hat{F}} = -1$ when acting on single-particle states, and therefore the obstruction can in principle be circumvented in the presence of interaction.

Outlook. — In this work we have reported the full list of fillings for TR and SG symmetric BIs, with or without spin-rotation invariance. The results also apply to 2D systems, since any layer group can be viewed as a 'slice' of a SG [31]. Understanding the nature of the enforced band degeneracies, the symmetry-topology protection of the nodal Fermi surfaces, and the class of nontrivial BIs accessible by symmetry-lowering are interesting open problems, as is the actual prediction of new materials candidates using these insights. As pointed out above, for 12 SGs we could only prove tightness of the filling constraints in the non-interacting limit. It remains an interesting open problem whether interaction will enable trivial insulators at a lower filling in these systems. Another promising future direction is the extension to magnetic SGs, pertinent for systems with magnetic ordering.

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