# Closing the Gap in Band Theory

**Filling-Enforced Gaplessness in Band Structures of the 230 Space Groups**
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*Recommended with a Commentary by Liang Fu, Massachusetts Institute of Technology*

Band theory is a pillar of solid state physics, laid down by Felix Bloch nearly a century ago. Based on the quantum mechanics of an electron moving under a periodic potential, band theory gives a remarkably simple criterion regarding metals and insulators: a band insulator is only possible when the number of electrons in the unit cell is an even integer. This textbook counting rule only assumes the presence of translational symmetry of crystals. Now, by taking into account the full spatial symmetry of crystals, the work of Watanabe, Po, Zaletel and Vishwanath provides the ultimate list of allowed electron fillings for band insulators in each of the 230 space groups, finding stronger constraints in many cases. Besides completing the counting rule of band theory, this result is an important and practical guide to the material search of topological insulators and semimetals.

The original counting rule follows from the simple fact that filling a single band completely requires two electrons per unit cell, two accounting for the spin degeneracy. However, in certain crystals, multiple bands are stitched together by band crossings to form an inseparable unit. Then an insulator can only be obtained by completely filling units of bands so that a band gap is present, otherwise the system is forced to be gapless. This requirement gives a stronger bound on the allowed electron fillings. For example, in graphene the conduction and valence bands cross at the Dirac point. This band crossing makes graphene a gapless semimetal, despite having two electrons per unit cell.

It is known that band crossings are *inevitably* present in certain nonsymmorphic crystals. A nonsymmorphic symmetry such as glide can be thought of as the square root of a lattice translation. Glide symmetry then guarantees that bands are stitched into pairs to form double-valued representations of glide the square root, as illustrated in Fig. 1.

The authors made an admirable effort to work out the allowed electron fillings for band insulators in 230 space groups! This is achieved by exhaustively tabulating all band crossings of nonsymmorphic type, by taking advantage of various group-subgroup relations among space groups, by studying atomic insulators to obtain a subset of allowed fillings, and by case-by-case study when it becomes necessary.

Several outcomes of the study deserve highlight. First, the authors found that for four special space groups (no. 199, 214, 220 and 230) and at certain electron fillings, a band insulator is allowed, but an atomic insulator is forbidden. In other words, the ground state

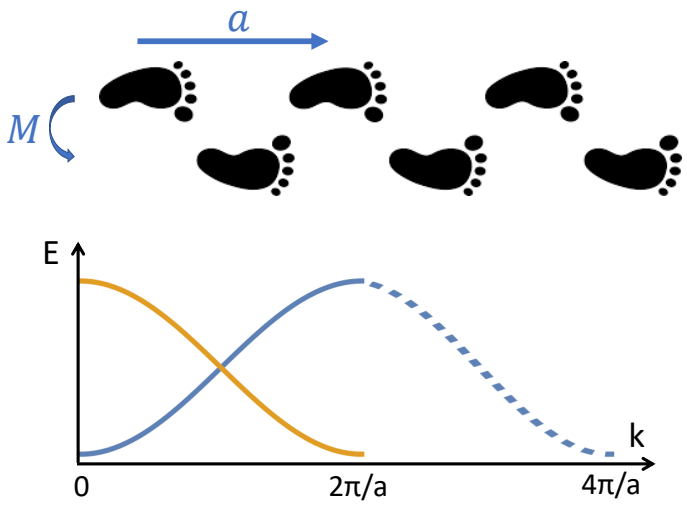


Figure 1: Glide symmetry leads to unavoidable band crossing. Top: glide symmetry $G$ in a one-dimensional periodic system, consisting of translation of $a/2$ followed by reflection $M$. Two consecutive glides amount to a primitive translation $T$. Bottom: band structure in the Brillouin zone $k \in [0, 2\pi/a]$. At a given wavevector $k$, every band is an eigenstate of $T$ with eigenvalue $e^{ika}$. Since $G^2 = T$, it must also be an eigenstate of $G$, with allowed eigenvalues $g_\pm = \sqrt{e^{ika}} = \pm e^{ika/2}$. Since $g_+(k + 2\pi/a) = g_-(k)$, the $g_+$ and $g_-$ bands must swap as $k$ advances by $2\pi/a$, leading to unavoidable band crossing.

of such band insulator cannot be a Slater determinant of any set of localized and orthogonal orbitals that conform with the symmetry of the crystal. Examples of these non-atomic band insulators are explicitly constructed in a follow-up study [1]. Whether they have topologically protected boundary states remains an interesting question.

Second, for the combinations of space groups and even-integer electron fillings that forbid a band insulator, the system is a natural candidate for topological semimetal—provided that the band crossing is close to the Fermi energy. This criterion serves as a general guide to search for topological semimetals.

Finally, in a lovely recent work [2], the same authors found a general constraint on the electron fillings in nonsymmorphic crystals, which permits a unique insulating ground state on closed manifolds. Importantly, this constraint is obtained by considering the many-body ground state degeneracy, hence is applicable to systems with and without interactions. Comparing this general constraint with the allowed fillings now established for band insulators, one finds that in almost all space groups, the constraint is saturated. However, for the few outliers, the possibility cannot be ruled out that at certain fillings, an insulating state is only allowed by interactions.

# References

[1] H. C. Po, H. Watanabe, M. P. Zaletel, and A. Vishwanath, Sci. Adv.2, e1501782 (2016).

[2] H.Watanabe, H.C.Po, A.Vishwanath, and M.P.Zaletel, Proc. Natl. Acad. Sci. U.S.A.112, 14551 (2015).