Letter

Noncompact atomic insulators

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We study the conditions for Bloch bands to be spanned by symmetric and strictly compact Wannier states that have zero overlap with all lattice sites beyond a certain range. Similar to the characterization of topological insulators in terms of an algebraic (rather than exponential) localization of Wannier states, we find that there may be impediments to the compact localization even of topologically "trivial" obstructed atomic insulators. These insulators admit exponentially localized Wannier states centered at unoccupied orbitals of the crystalline lattice. First, we establish a sufficient condition for an insulator to have a compact representative. Second, for $\mathcal{C}_2$ rotational symmetry, we prove that the complement of fragile topological bands cannot be compact, even if it is an atomic insulator. Third, for $\mathcal{C}_4$ symmetry, our findings imply that there exist fragile bands with zero correlation length. Fourth, for a $\mathcal{C}_3$-symmetric atomic insulator, we explicitly derive that there are no compact Wannier states overlapping with less than 18 lattice sites. We conjecture that this obstruction generalizes to all finite Wannier sizes. Our results can be regarded as the stepping stone to a generalized theory of Wannier states beyond dipole or quadrupole polarization.

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Introduction. In band theory, Wannier states are the Fourier transforms of Bloch states. They have multifold applications ranging from chemical bonding to *ab initio* calculations. The gauge freedom in defining Bloch states can be exploited to construct maximally localized Wannier states [1–4]. Recently, the notion of topological insulators was reformulated in terms of an obstruction to exponentially localized Wannier states, which allowed for a systematic classification of topological band structures in all symmetry classes [5–8]. In this Research Letter, we study Wannier states satisfying an even more stringent localization requirement. These are *compact Wannier states* that are strictly local and have zero overlap with all lattice sites outside of a finite domain. They are symmetric when they share the symmetries of the lattice restricted to the site-symmetry group that leaves their Wannier center invariant [5,6,9–13]. In the following, we assume that all Wannier states are symmetric. Moreover, we require that compact states originating from different unit cells are orthogonal [14]. This criterion was not enforced in previous works, which instead studied compact localized states (compact Wannier-type states) [15–25] that need not be orthogonal.

A Bloch band induced from a delta-function Wannier state at any atomic site of the unit cell—resulting in a trivial or *unobstructed* atomic insulator [5,6]—can always be adiabatically transformed to have compact Wannier states. Conversely, a topological band cannot—by definition—be written in terms of exponentially localized Wannier states, much less compact ones [6,26–30]. The same holds for fragile topological bands that can be trivialized upon mixing with nontopological bands [12,31–37].

There is so far one known category of insulators allowing for exponentially localized Wannier states which are necessarily not delta-function-like: delicate topological insulators [38], which are characterized by Hopf invariants and returning Thouless pumps. Here, we explore a second category of non-delta-function insulators that are *obstructed* atomic insulators (OAIs) [5,6,39–43], whose Wannier states may only be exponentially localized away from the atomic orbitals. Surprisingly, we find that not all OAIs have a compact representation: There are topological obstructions to compactness. We call the resulting phases noncompact atomic insulators. The condition of noncompactness is stronger than the "multicellularity" of delicate topological insulators, meaning that the Wannier states cannot be completely localized in a primitive unit cell: Noncompact Wannier states cannot be completely localized in any, potentially nonprimitive, unit cell. (Presently, it is not known if delicate topological insulators ultimately satisfy the stronger condition.) While the general theory of noncompact atomic insulators is still outstanding, this Research Letter proves their existence.

Compact Wannier states. We denote the atomic orbitals on a lattice with space group G by $|\boldsymbol{R} j\mu\rangle$. Here, $\boldsymbol{R}$ indicates the unit cell coordinate, while j labels the atomic site $\boldsymbol{t}_j \in A$ within the unit cell. We assume all atomic sites contained in A to be maximal Wyckoff positions [6,44]. The index μ labels the orbitals at a given site, which respect the site-symmetry group. To form Wannier states for an OAI, we construct obstructed orbitals at the positions $\boldsymbol{t}_\alpha \in B$:

$$|W_{\boldsymbol{R},\alpha}\rangle = \sum_{\boldsymbol{R}' j\mu} S_{j\mu,\alpha}(\boldsymbol{R}-\boldsymbol{R}')\,|\boldsymbol{R}' j\mu\rangle\,. \tag{1}$$

If $B \cap A = \emptyset$, the OAI has a *spatial* obstruction, in that its Wannier states are centered at empty positions of the

crystalline lattice. If $B \cap A \neq \emptyset$, the OAI has a *representation* obstruction, in that the transformation behavior of its Wannier states under the crystalline symmetry differs from that of all atomic orbitals present at the same site. While spatial and representation obstructions were treated on equal footing in previous works [5,6,12,31,34], we must distinguish between them when studying the real-space structure of Wannier states. The functions $S_{j\mu,\alpha}(\boldsymbol{R}-\boldsymbol{R}') \in \mathbb{C}$ must respect the space group symmetry. Furthermore, the states $|W_{\boldsymbol{R},\alpha}\rangle$ have compact support when $S_{j\mu,\alpha}(\boldsymbol{R}-\boldsymbol{R}')$ is strictly zero for all $|\boldsymbol{R}+\boldsymbol{t}_\alpha-\boldsymbol{R}'-\boldsymbol{t}_j|$ greater than a certain distance. For the obstructed orbitals $|W_{\boldsymbol{R},\alpha}\rangle$ to form a Wannier basis, they must also be orthonormal:

$$\langle W_{\boldsymbol{R},\alpha}|W_{\boldsymbol{R}',\beta}\rangle = \delta_{\boldsymbol{R}\boldsymbol{R}'}\delta_{\alpha\beta}. \tag{2}$$

The interplay between orthogonality, symmetry, and compact support is already nontrivial in two-dimensional systems where G contains a single $\mathcal{C}_n$ rotation (and translations), which we focus on in the following. Assuming spinless rotational symmetries, so that $(\mathcal{C}_n)^n = 1$, the rotation eigenvalues γ_μ take values

$$\gamma_\mu = e^{i\frac{2\pi}{n}l}, \quad l = 0\cdots n-1. \tag{3}$$

We call a *mobile cluster* a configuration of orbitals whose $\mathcal{C}_n$ eigenvalues exhaust all $l = 0\cdots n-1$, with each l appearing exactly once. These configurations are special in that they can be used to construct compact basis states at any Wyckoff position, not just at the atomic positions hosting the mobile cluster orbitals [6,44]. For instance, given that $|\boldsymbol{R}j\mu\rangle$, $\mu = 1\cdots n$ is a mobile cluster, there exists a strictly local unitary effecting

$$|\boldsymbol{R}j\mu\rangle \to |\boldsymbol{R}j'\mu'\rangle\,, \tag{4}$$

where j, j' label two Wyckoff positions with $\mathcal{C}_n$ symmetry and μ' labels a new set of orbitals that also forms a mobile cluster [45]. (See Fig. 1.)

Fragile phases are the band complements of other fragile phases or OAIs [12,31–37]. In the latter case, they are a difference of atomic insulators:

$$\text{FP} = \text{AI} \ominus \text{OAI}, \tag{5}$$

where FP denotes the fragile phase and AI is the (unobstructed) atomic insulator induced from the lattice. Now, let $N(\text{AI})$ count the number of mobile clusters in the unit cell. That is, for every group of n orbitals containing all eigenvalues in Eq. (3) present in the unit cell of AI, we increase $N(\text{AI})$ by 1, starting from zero. If only a part of the orbitals required for a mobile cluster is present (in addition to the orbitals already counted), $N(\text{AI})$ is unaffected and remains integer valued. For example, for the unit cell in Fig. 1(a), we have $N(\text{AI}) = 1$. Furthermore, let $\bar{N}(\text{OAI})$ count the minimal number of mobile clusters containing all orbitals of the OAI. That is, we envision an atomic limit $\tilde{\text{AI}}$ whose unit cell contains all orbitals of OAI just once *and* whose full set of orbitals can be grouped into mobile clusters without any missing or remaining orbitals: Then, $\bar{N}(\text{OAI}) = N(\tilde{\text{AI}})$. Now, for FP to be fragile, we need $N(\text{AI}) < \bar{N}(\text{OAI})$: Otherwise, the OAI could be built from a subset of the mobile cluster orbitals, potentially using Eq. (4), while the remaining orbitals form a compact and symmetric Wannier basis for FP. Conversely, we see that $N(\text{AI}) \geqslant \bar{N}(\text{OAI})$ is a sufficient condition for the OAI to be compact *and* to have an OAI (not fragile) complement. For instance, in wallpaper group $p2$, we have $N[((A)_{1a} \oplus (B)_{1a}) \uparrow G] = \bar{N}[(A)_{1b} \uparrow G] = 1$ [46], implying that the OAI $(A)_{1b} \uparrow G$ has a compact representative, and so does its complement $(B)_{1b} \uparrow G$.

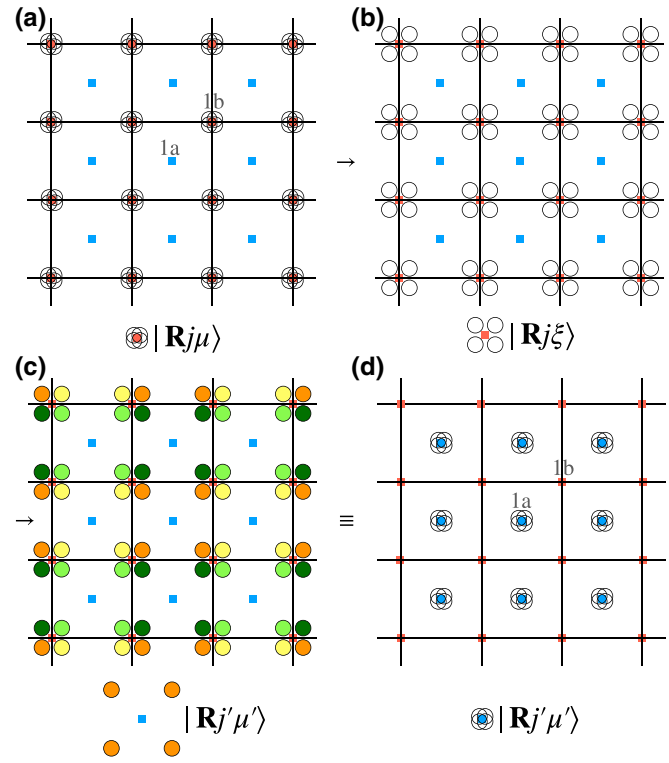

FIG. 1. Mobile clusters with $\mathcal{C}_4$ symmetry. A mobile cluster is a minimal set of physical orbitals $|\boldsymbol{R}j\mu\rangle$ whose transformation behavior under the crystalline symmetry is compatible with being located at any (possibly nonmaximal) Wyckoff position. For spinless $\mathcal{C}_4$ symmetry, the mobile clusters on maximal Wyckoff positions 1a and 1b contain four orbitals with $\mathcal{C}_4$ eigenvalues $\{1, -1, i, -i\}$. (a) We begin with mobile clusters centered at the 1b Wyckoff position. (b) Next, we locally change bases to obtain the states $|\boldsymbol{R}j\xi\rangle$ that do not have well-defined $\mathcal{C}_4$ eigenvalues, but instead are cyclically permuted by the action of $\mathcal{C}_4$. (c) and (d) These states can be used to construct new mobile clusters $|\boldsymbol{R}j'\mu'\rangle$ that are centered around Wyckoff position 1a.

$\mathcal{C}_2$ symmetry. OAIs with $\mathcal{C}_2$ symmetry and a fragile complement are noncompact. Consider the OAI induced from an s orbital on Wyckoff position 1a of wallpaper group $p2$ ($\boldsymbol{t}_{1a} = \boldsymbol{0}$), where the lattice hosts s orbitals located at Wyckoff positions 1b, 1c, and 1d [so that $\boldsymbol{t}_j \in \{(1/2, 0), (1/2, 1/2), (0, 1/2)\}$ is the position of the jth atomic s orbital]. The complement of the OAI is [46]

$$[(A)_{1b} \oplus (A)_{1c} \oplus (A)_{1d}] \uparrow G \ominus (A)_{1a} \uparrow G = \text{FP}. \tag{6}$$

We first note that $N[((A)_{1b} \oplus (A)_{1c} \oplus (A)_{1d}) \uparrow G] = 0$ (the unit cell does not contain a full mobile cluster) and $\bar{N}[(A)_{1a} \uparrow G] = 1$ (we need at least one mobile cluster to reproduce the OAI). Therefore the necessary condition $N(\text{AI}) < \bar{N}(\text{OAI})$ for a noncompact OAI with fragile complement is satisfied. Indeed, FP in Eq. (6) is the simplest possible fragile state, requiring the smallest crystalline symmetry (wallpaper group $p2$) and the smallest number of bands (two occupied and one

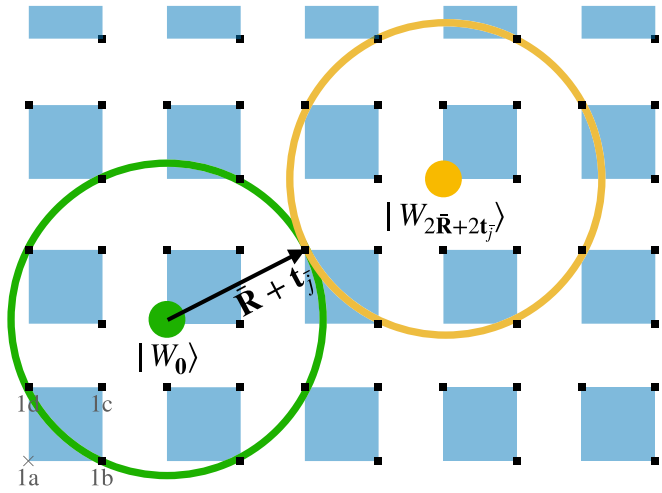

FIG. 2. Overlap of compact trial Wannier states with $\mathcal{C}_2$ rotational symmetry. For any compact state $|W_1\rangle = |W_{\mathbf{0}}\rangle$ of an OAI, there is another translated Wannier state $|W_2\rangle = |W_{2\bar{\mathbf{R}}+2\boldsymbol{t}_{\bar{j}}}\rangle$ that shares a single lattice site of nonzero overlap. Orthogonality $\langle W_1|W_2\rangle = 0$ is impossible when this site carries a single orbital. (Here, the OAI is centered at Wyckoff position 1a, while the atomic orbitals locate at positions 1b, 1c, and 1d.)

empty band) [34]. Equation (6) does not involve complex representations and is therefore compatible with (spinless) time-reversal symmetry (TRS). We will next show that the OAI $(A)_{1a} \uparrow G$ is noncompact. Let us assume that $|W_{\boldsymbol{R}}\rangle$ are compact Wannier states: Then, the overlap $\langle \boldsymbol{R}' j|W_{\boldsymbol{R}}\rangle$ is nonzero only for a finite number of separations $|\boldsymbol{R}-\boldsymbol{R}'-\boldsymbol{t}_j|$. Moreover, $\mathcal{C}_2$ symmetry implies $C_2|W_{\mathbf{0}}\rangle = |W_{\mathbf{0}}\rangle$, where C_2 represents a $\mathcal{C}_2$ rotation about Wyckoff position 1a of the unit cell at $\boldsymbol{R}=\mathbf{0}$. Now, consider an orbital $|\bar{\boldsymbol{R}}\bar{j}\rangle$ at maximal distance $|\bar{\boldsymbol{R}}+\boldsymbol{t}_{\bar{j}}|$ from the origin which still has a nonzero overlap $\langle\bar{\boldsymbol{R}}\bar{j}|W_{\mathbf{0}}\rangle \neq 0$ with $|W_{\mathbf{0}}\rangle$. Then, by $\mathcal{C}_2$ symmetry, it follows that

$$0 \neq \langle\bar{\boldsymbol{R}}\bar{j}|C_2^\dagger C_2|W_{\mathbf{0}}\rangle = \langle(-\bar{\boldsymbol{R}}-2\boldsymbol{t}_{\bar{j}})\bar{j}|W_{\mathbf{0}}\rangle \tag{7}$$

is also nonzero. However, this implies that $\langle W_{2\bar{\boldsymbol{R}}+2\boldsymbol{t}_{\bar{j}}}|W_{\mathbf{0}}\rangle \neq 0$, because these two Wannier functions have finite overlap on exactly one s orbital, located at $\bar{\boldsymbol{R}}+\boldsymbol{t}_{\bar{j}}$. (See Fig. 2.) We conclude that a compact set of Wannier states $|W_{\boldsymbol{R}}\rangle$ satisfying Eq. (2) cannot exist. This argument does not make any assumptions on the size of the Wannier states, as long as it is finite. Therefore the OAI $(A)_{1a} \uparrow G$ in Eq. (6) is noncompact. In the Supplemental Material (SM) [45], we show that in fact *all* $\mathcal{C}_2$-symmetric OAIs with fragile complement are noncompact.

$\mathcal{C}_4$ symmetry. Any OAI that is noncompact with $\mathcal{C}_2$ symmetry remains noncompact when the symmetry group is enlarged to contain $\mathcal{C}_4$ rotations: Because $(\mathcal{C}_4)^2 = \mathcal{C}_2$, $\mathcal{C}_4$-symmetric compact Wannier states inherit the constraints imposed by $\mathcal{C}_2$ and additionally need to form a representation under $\mathcal{C}_4$. In the SM [45], we moreover explicitly construct $\mathcal{C}_4$-symmetric compact Wannier states for all spatially obstructed OAIs that have a compact representation when $\mathcal{C}_4$ symmetry is relaxed to $\mathcal{C}_2$ symmetry. As a consequence, there exist $\mathcal{C}_4$-protected fragile phases—these are necessarily trivial with respect to $\mathcal{C}_2$ symmetry—that have a compact OAI complement. Consider the fragile state [48]

$$[(A)_{1b} \oplus (B)_{1b} \oplus ({}^2\mathrm{E})_{1b}] \uparrow G \ominus (A)_{1a} \uparrow G = \mathrm{FP}, \tag{8}$$

which is illustrated in Figs. 3(a) and 3(b). The one-band OAI $(A)_{1a} \uparrow G$ admits a compact Wannier basis $|W_{\boldsymbol{R}}\rangle$, with $|W_{\mathbf{0}}\rangle$ shown in Fig. 3(c). These compact states can be used to build a strictly local Hamiltonian whose ground state is FP, $H = \sum_{\boldsymbol{R}} |W_{\boldsymbol{R}}\rangle\langle W_{\boldsymbol{R}}|$. H has zero correlation length and a flat band spectrum [17,18,20–22,24,49–57]. We note that Eq. (8) involves the unpaired complex representation ${}^2\mathrm{E}$ and hence assumes broken TRS, implying that its realization requires magnetism.

In contrast, some *representation-obstructed* (not spatially obstructed) OAIs are noncompact only due to constraints imposed by $\mathcal{C}_4$ symmetry. Consider

$$[(A)_{1b} \oplus (B)_{1b} \oplus (B)_{1a}] \uparrow G \ominus (A)_{1a} \uparrow G = \mathrm{FP}, \tag{9}$$

which unlike Eq. (8) is compatible with TRS and therefore nonmagnetic. In the SM [45], we prove that the

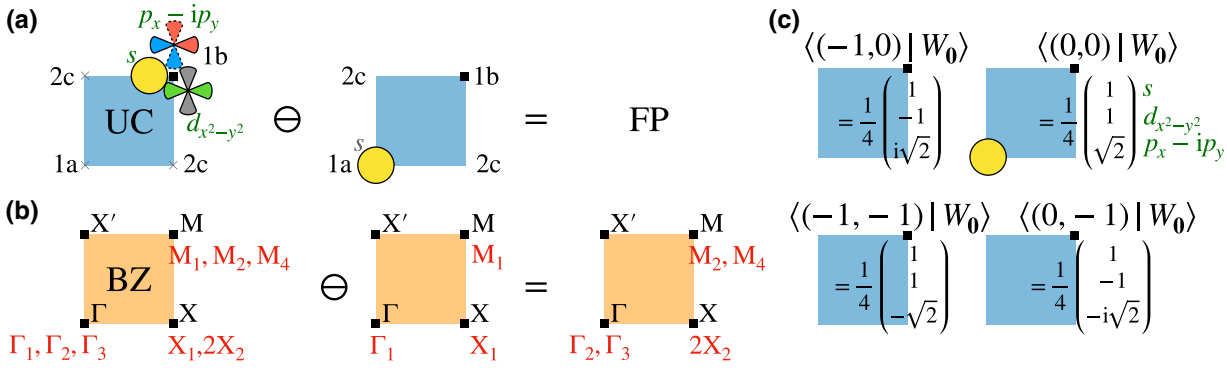

FIG. 3. Compact OAI with $\mathcal{C}_4$ rotational symmetry and fragile complement. (a) Real-space illustration of the fragile state. The unit cell (UC) contains three orbitals at Wyckoff position 1b (s, $d_{x^2-y^2}$, and $p_x - ip_y$ orbitals carry $\mathcal{C}_4$ eigenvalues 1, -1, and i, respectively). (b) Brillouin zone (BZ) decomposition of the corresponding Bloch bands into irreducible representations. (Representation labels follow the Bilbao Crystallographic Server [47].) (c) Compact Wannier state for the OAI, supported on four unit cells (blue) surrounding the 1a position (yellow) of the unit cell at $\boldsymbol{R}=\mathbf{0}$. The vectors $\langle\boldsymbol{R}|W_{\mathbf{0}}\rangle$ at each site contain the overlaps $(\langle\boldsymbol{R}|W_{\mathbf{0}}\rangle)_\mu \equiv \langle\boldsymbol{R}, 1\mathrm{b}, \mu|W_{\mathbf{0}}\rangle$ of the Wannier state $|W_{\mathbf{0}}\rangle$ with the on-site orbitals at Wyckoff position 1b, which are indexed by μ (orbital labels are shown in green).

representation-obstructed OAI $(A)_{1a} \uparrow G$ is noncompact. Nevertheless, it becomes unobstructed (and thereby compact) when $\mathcal{C}_4$ symmetry is relaxed to $\mathcal{C}_2$ symmetry: The $\mathcal{C}_4$ representations (A) and (B) both map into the same $\mathcal{C}_2$ representation (A).

$\mathcal{C}_3$ symmetry. All spatially obstructed one- and two-band OAIs with $\mathcal{C}_3$ symmetry are compact, irrespective of whether their band complement is another OAI or a fragile state. For lattices where $N(\mathrm{AI}) \geqslant \bar{N}(\mathrm{OAI})$, compactness of the OAI (and its complement) follows directly from the reasoning below Eq. (5). More nontrivially, consider the following TRS-broken fragile states in wallpaper group $p3$:

$$\left[(\gamma)_{1b} \oplus (e^{i\frac{2\pi}{3}}\gamma)_{1b} \oplus (e^{i\frac{2\pi}{3}}\gamma)_{1c}\right] \uparrow G \ominus (\gamma)_{1a} \uparrow G = \mathrm{FP}, \tag{10}$$

where $(\mu)_{1x}$ is an orbital with $\mathcal{C}_3$ eigenvalue μ at Wyckoff position 1x and $\gamma \in \{1, e^{i\frac{2\pi}{3}}, e^{-i\frac{2\pi}{3}}\}$ is a free parameter. The compact Wannier state for the OAI at $\boldsymbol{R} = \boldsymbol{0}$ is

$$|W_{\boldsymbol{0}\gamma}\rangle = \tfrac{1}{3}[|w_{\boldsymbol{0}\gamma}\rangle + \gamma^* C_3 |w_{\boldsymbol{0}\gamma}\rangle + (\gamma^* C_3)^2 |w_{\boldsymbol{0}\gamma}\rangle],$$
$$|w_{\boldsymbol{0}\gamma}\rangle = |\boldsymbol{0}, 1\mathrm{b}, \gamma\rangle + |\boldsymbol{0}, 1\mathrm{b}, e^{i\frac{2\pi}{3}}\gamma\rangle + |\boldsymbol{0}, 1\mathrm{c}, e^{i\frac{2\pi}{3}}\gamma\rangle, \tag{11}$$

where C_3 rotates about Wyckoff position 1a of the unit cell at $\boldsymbol{R} = \boldsymbol{0}$. Similarly, we construct the compact states of all further $\mathcal{C}_3$-symmetric one- and two-band OAIs with spatial obstruction in the SM [45] (there, we also discuss $\mathcal{C}_3$-symmetric OAIs with a representation obstruction).

In contrast, ascertaining the compactness properties of three-band OAIs with $\mathcal{C}_3$ symmetry is a challenging yet unsolved problem. Consider the TRS-broken fragile state [58]

$$[2(A_1)_{1b} \oplus ({}^2\mathrm{E})_{1b} \oplus 2(A_1)_{1c} \oplus ({}^2\mathrm{E})_{1c}] \uparrow G$$
$$\ominus [(A_1)_{1a} \oplus 2({}^2\mathrm{E})_{1a}] \uparrow G = \mathrm{FP}. \tag{12}$$

Here, FP is obtained as the complement of a three-band OAI built from Wannier states at Wyckoff position 1a that have $\mathcal{C}_3$ eigenvalues $\lambda_1 = 1$, $\lambda_2 = \lambda_3 = e^{i\frac{2\pi}{3}}$. [See Figs. 4(a) and 4(b) for an illustration.] To obtain a compact basis, we must impose the constraints in Eq. (2), where $\alpha = 1, 2, 3$ belongs to the obstructed orbital with $\mathcal{C}_3$ eigenvalue λ_α. For $\mathcal{C}_3$-symmetric trial Wannier states that have overlap with n lattice sites (located at the 1b and 1c Wyckoff positions and carrying three orbitals each), Eq. (2) is a system of coupled quadratic equations in $N = 6n$ complex variables. The problem of determining whether solutions to general systems of quadratic equations exist is NP-complete [59], and the runtime of all (currently known) algorithms scales exponentially in N. For OAIs with $\mathcal{C}_2$ and $\mathcal{C}_4$ symmetry, we were able to circumvent this difficulty: For $\mathcal{C}_2$-symmetric OAIs with fragile complement, a solution to Eq. (2) can be ruled out by a single translation (Fig. 2), proving noncompactness. For all spatially obstructed $\mathcal{C}_4$-symmetric OAIs, and likewise all spatially obstructed $\mathcal{C}_3$-symmetric OAIs with one and two bands, we found explicit solutions to Eq. (2), proving compactness. In the present case, however, both strategies fail [60]. Nevertheless, we prove in the SM [45] that Eq. (2) cannot be solved by states overlapping with $n < 18$ lattice sites [see Fig. 4(c)]. We conjecture that there is also no solution for $n \geqslant 18$.

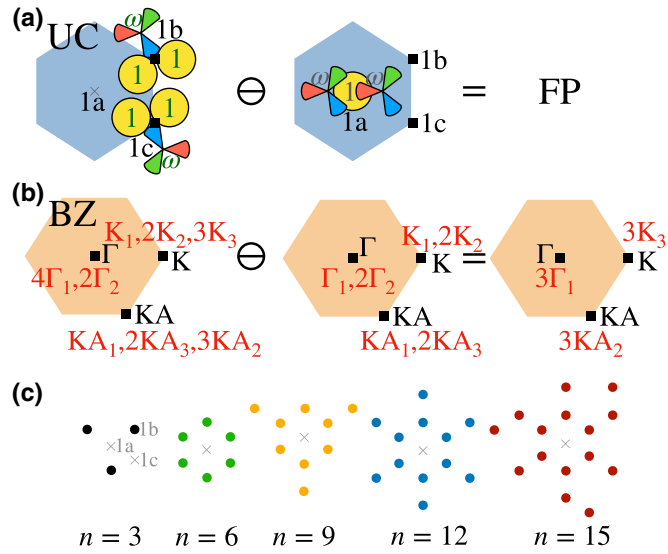

FIG. 4. Noncompact OAI with $\mathcal{C}_3$ rotational symmetry and fragile complement. (a) Real-space illustration of the fragile state. The unit cell (UC) contains three orbitals each at Wyckoff positions 1b and 1c (orbitals are labeled by their $\mathcal{C}_3$ eigenvalue, $\omega = e^{i\frac{2\pi}{3}}$). (b) Brillouin zone (BZ) decomposition of the corresponding Bloch bands into irreducible representations. (Representation labels follow the Bilbao Crystallographic Server [47].) (c) Trial state support for the OAI, labeled by size. Each colored atomic site indicates that the trial states for all three bands may have nonzero overlap with orbitals on that site. For all support sizes shown, there are no trial states that satisfy the requirements for an orthonormal Wannier basis [Eq. (2)].

Discussion. The existence of noncompact atomic insulators suggests to explore noncompactness as a new ordering principle for gapped phases. Promising directions of future study are the generalization of our analysis to arbitrary finite Wannier state sizes, larger symmetry groups, and higher dimensions. Moreover, it is fruitful to investigate the observable consequences of noncompactness. In particular, both the superfluid weight [61,62] and the conductivity in the presence of disorder [63] of a set of bands directly depend on Wannier spread. Hence we expect that both are enhanced in the noncompact case.

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