

Reduced Wannier Representation for Topological Bands

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We demonstrate a procedure for constructing a maximally localized Wannier basis for a subspace of bands with a non-zero Chern number. Bands with non-trivial topological indices have a topological obstruction preventing them from being represented by exponentially localized Wannier states. Here, we analyze the limits of using the projection procedure to obtain a Wannierizable subspace from a set of topologically obstructed bands. The Wannier functions from this subspace form what we refer to as a “reduced Wannier representation,” indicating that the Wannier functions necessarily do not span the full topological manifold. We consider the Haldane tight-binding model in the Chern phase as the platform for our investigation.

I. INTRODUCTION

Hamiltonians with translational invariance lead to a momentum space description in which the energy eigenstates take the form of Bloch waves labeled by crystal momentum. These states are inherently delocalized throughout the crystal, often obscuring properties that we expect to occur locally in insulators, such as electromagnetic responses and chemical bonding. On the other hand, Wannier functions provide a localized real-space representation of Bloch functions, offering additional insight into the chemical and electronic properties of materials [1–5]. They are frequently used to construct effective tight-binding models, particularly in strongly correlated systems, enabling a simplified yet accurate description of the electronic interactions [6–10]. In first-principles calculations, they facilitate the efficient interpolation of k -dependent quantities across the Brillouin zone, greatly enhancing computational efficiency [11, 12]. Moreover, Wannier functions have had a significant role in determining the topology of band structures, aiding in the discovery and characterization of topological materials [13–16].

In topological insulators, however, the construction of Wannier functions is inhibited by a “topological obstruction.” When the valence bands possess a nontrivial topological index, such as a Chern number in quantum-Hall insulators or \mathbb{Z}_2 invariant in spin-Hall insulators, the corresponding Wannier functions fail to be exponentially localized and instead exhibit power law decay [14, 16]. In reciprocal space, the obstruction arises from the inability to choose a gauge for the Bloch eigenstates that simultaneously respects the protecting symmetry and is a smooth and periodic function of wavevector. Specifically, a non-zero Chern number implies that the phase of the Bloch eigenstates winds non-trivially around the Brillouin zone (BZ), leading to vortices or singularities in the phase [13, 17]. Since Wannier functions are related to Bloch states through a Fourier transform, they require a smooth and periodic gauge to be well localized.

From a real-space perspective, this obstruction is rooted in the fact that topological insulators cannot be adiabatically connected to atomic insulators without closing the energy gap. The development of topologi-

cal quantum chemistry has recently provided a systematic framework for characterizing topological insulators in terms of elementary band representations derived from an atomic limit. In this context, elementary band representations can either form connected bands across the BZ, allowing them to be representable by localized Wannier functions respecting the crystal symmetries, or they can be disconnected, signifying the presence of a topological obstruction [14, 18, 19].

Despite these limitations, there have been efforts to construct a Wannier basis in the presence of topological obstructions. Soluyanov and Vanderbilt [13] showed that it is possible to construct localized Wannier functions for \mathbb{Z}_2 topological insulators in the topological (\mathbb{Z}_2 -odd) phase by choosing a gauge that breaks the protecting time-reversal symmetry such that the Wannier functions no longer form Kramers pairs.

There are systems whose topology is not classified by conventional K -theoretic topological indices but still exhibit an obstruction to being Wannier representable. These systems are said to have a “fragile topology” when the obstruction can be resolved by incorporating additional trivial bands corresponding to an atomic insulator [15, 16]. For instance, Song and Bernevig constructed a Wannier representation of two flat bands in magic-angle twisted bilayer graphene, possessing a fragile obstruction, by “borrowing” irreducible representations from higher-energy trivial bands at high-symmetry k -points [20]. Similarly, in studies of a kagome lattice model, Hu et al. [21] and Chen et al. [22] obtained a Wannier representation of an obstructed flat band by incorporating representations at high-symmetry momenta from a nearby wide band allowing for an elementary band representation associated with localized orbitals to be formed.

Here, we propose an alternative approach for constructing Wannier functions from a set of bands with a topological obstruction. We focus on the case of quantum anomalous Hall insulators, in which a non-zero Chern index characterizes the stable topological phase. Our approach is based on the methods of subspace selection for entangled energy bands via projection, as initially introduced by Souza, Marzari, and Vanderbilt [23]. We begin by selecting a subspace of the topological band space as the target manifold for Wannierization. This process may

involve band folding, i.e., breaking of translational symmetry in the gauge, to enlarge the population of starting bands. We then apply a standard projection method to this subspace to obtain well-localized Wannier functions, whose quadratic spread can be minimized using the methods discussed in the following section. To demonstrate this approach, we use the Haldane model in its Chern insulating phase as a prototypical example.

II. MAXIMALLY LOCALIZED WANNIER FUNCTIONS VIA PROJECTION

In this section, we review the standard approach for obtaining maximally localized Wannier functions guided by projection from a set of initial trial functions. This material constitutes a synopsis of the relevant material from the review by Marzari et al. [24]. The operations described below were implemented in an extension of the PYTHTB package [25], which was used to generate the results presented in Sec. III.

A. Wannier Functions

Wannier functions are related to Bloch functions through a Fourier transform,

$$|\mathbf{R}n\rangle = \frac{V}{(2\pi)^d} \int_{BZ} d\mathbf{k} e^{-i\mathbf{k}\cdot\mathbf{R}} |\psi_{n\mathbf{k}}\rangle, \quad (1)$$

where \mathbf{R} is a real-space lattice vector, V is the volume (or area) of the unit cell, d is the dimensionality of the BZ, and $|\psi_{n\mathbf{k}}\rangle$ are the Bloch states. The Bloch states have a gauge freedom, under which they can be transformed as

$$|\tilde{\psi}_{n\mathbf{k}}\rangle = e^{i\phi_n(\mathbf{k})} |\psi_{n\mathbf{k}}\rangle \quad (2)$$

without affecting the physical description of the system. This gauge freedom leads to a nontrivial modification of the Wannier functions, where a change in gauge results in Wannier functions with altered spreads and shapes.

Instead of a single band index n , consider a manifold of M bands that are separated in energy from any other bands, possibly with internal degeneracies. In this case, the notion of gauge freedom can be generalized to a unitary freedom that mixes the states within the manifold,

$$|\tilde{\psi}_{n\mathbf{k}}\rangle = \sum_{m=1}^M U_{mn}^{(\mathbf{k})} |\psi_{m\mathbf{k}}\rangle, \quad (3)$$

where $U_{mn}^{(\mathbf{k})}$ is periodic in \mathbf{k} . This unitary freedom is what allows for the construction of well localized Wannier functions.

The standard measure of localization of the Wannier functions is given by their quadratic spread,

$$\Omega = \sum_n [\langle \mathbf{0}n | r^2 | \mathbf{0}n \rangle - \langle \mathbf{0}n | \mathbf{r} | \mathbf{0}n \rangle]^2. \quad (4)$$

This functional can be decomposed into two separate terms,

$$\Omega = \Omega_I + \tilde{\Omega}, \quad (5)$$

where Ω_I is gauge-independent, reflecting the intrinsic spread of the chosen subspace, and $\tilde{\Omega}$ is gauge-dependent. The minimization of the spread is usually decomposed into two stages: first, identifying the optimal subspace of Bloch functions that minimize Ω_I , and then finding the unitary rotation within this subspace that minimizes $\tilde{\Omega}$. If the goal is to construct Wannier functions that span the entire set of isolated bands, minimizing Ω corresponds to minimizing only $\tilde{\Omega}$ using the methods of “maximal localization” [26].

B. Projection

One approach to initializing the gauge and subspace selection is to project the bands onto a set of localized trial orbitals $g_n(\mathbf{r})$. These trial functions are typically chosen based on chemical intuition for how the manifold’s localized states may behave. The resulting Wannier functions will tend to have the character of these trial orbitals and serve as a starting point for further minimization of the quadratic spread.

Suppose an isolated manifold of M Bloch states, called the “target manifold,” is to be Wannerized. The projection is carried out by projecting the target manifold onto the trial orbitals,

$$|\Phi_{n\mathbf{k}}\rangle = \sum_{m=1}^M |\psi_{m\mathbf{k}}\rangle \langle \psi_{m\mathbf{k}} | g_n \rangle. \quad (6)$$

In the summation, the Bloch states appear in both bra and ket forms so that any random phases they carry get canceled out, and the projected states $|\Phi_{n\mathbf{k}}\rangle$ have a smooth gauge in \mathbf{k} . From these projected states, one can construct a matrix of inner products,

$$(A_{\mathbf{k}})_{mn} = \langle \psi_{m\mathbf{k}} | g_n \rangle, \quad (7)$$

and define an overlap matrix,

$$(S_{\mathbf{k}})_{mn} = \langle \Phi_{n\mathbf{k}} | \Phi_{n\mathbf{k}} \rangle = (A_{\mathbf{k}}^\dagger A_{\mathbf{k}})_{mn}, \quad (8)$$

that can be used to construct a set of Löwdin-orthonormalized Bloch-like states that maintain a smooth gauge in \mathbf{k} ,

$$\begin{aligned} |\tilde{\psi}_{n\mathbf{k}}\rangle &= \sum_{m=1}^M |\Phi_{m\mathbf{k}}\rangle (S_{\mathbf{k}}^{-1/2})_{mn} \\ &= \sum_{m=1}^M |\psi_{m\mathbf{k}}\rangle (A_{\mathbf{k}} S_{\mathbf{k}}^{-1/2})_{mn}. \end{aligned} \quad (9)$$

These states are “Bloch-like” in that they transform like Bloch states under translation but are no longer eigenstates of the Hamiltonian.

When choosing a number of trial wave functions equal to the dimension of the target manifold, the Bloch-like states are related to the original Bloch energy eigenstates by a unitary transformation. This can be seen with the singular value decomposition (SVD) of the square matrix of inner products,

$$A_{\mathbf{k}} = V_{\mathbf{k}} \Sigma_{\mathbf{k}} W_{\mathbf{k}}^{\dagger}, \quad (10)$$

where $\Sigma = \text{diag}(\sigma_1, \sigma_2, \dots, \sigma_M)$ is a diagonal matrix of nonnegative singular values and V and W are unitary $M \times M$ matrices. From this decomposition, Eq. (9) can be recast as,

$$|\tilde{\psi}_{n\mathbf{k}}\rangle = \sum_{m=1}^M |\psi_{m\mathbf{k}}\rangle (V_{\mathbf{k}} W_{\mathbf{k}}^{\dagger})_{mn}, \quad n = 1, \dots, M. \quad (11)$$

It is now apparent that this transformation is unitary when A is square and non-singular, and the Bloch-like states are expected to retain the physical properties of the target manifold. If A is singular, then VW^{\dagger} becomes semi-unitary.

If the number of trial wave functions, J , is smaller than the dimension of the target manifold, M , the inner product matrix A becomes an $M \times J$ rectangular matrix. In this case, Σ is an $M \times J$ rectangular diagonal matrix, while V and W are $M \times M$ and $J \times J$ unitary matrices, respectively. Consequently, the matrix VW^{\dagger} appearing in Eq. (11) becomes an $M \times J$ semi-unitary matrix. Explicitly, it takes the form $V \mathbb{1}_{M \times J} W^{\dagger}$, projecting the target manifold onto a lower J -dimensional subspace as

$$|\tilde{\psi}_{n\mathbf{k}}\rangle = \sum_{m=1}^M |\psi_{m\mathbf{k}}\rangle (V_{\mathbf{k}} \mathbb{1}_{M \times J} W_{\mathbf{k}}^{\dagger})_{mn}, \quad n = 1, \dots, J. \quad (12)$$

C. Subspace Selection

In situations where the target manifold is not isolated from unwanted bands, or where one is interested in extracting an optimally smooth subspace from it, a procedure known as subspace selection, or disentanglement, can be used [23]. This allows for the extraction of a J -dimensional subspace of a generally momentum-dependent $M_{\mathbf{k}}$ -dimensional manifold containing the states to be Wannierized. The chosen subspace is the one that minimizes the gauge-invariant spread Ω_I . In the present context, we optionally use this technique to improve the smoothness and reduce Ω_I for the J -dimensional subspace initially spanned by the Bloch-like states of Eq. (12).

On a discrete mesh of N_k k -points, the gauge-invariant spread can be written as

$$\Omega_I = \frac{1}{N_k} \sum_{\mathbf{k}, \mathbf{b}} w_b \text{Tr} [P_{\mathbf{k}} Q_{\mathbf{k}+\mathbf{b}}] \quad (13)$$

where \mathbf{b} is a vector connecting neighboring k -points, w_b is the weight associated with a finite-difference shell [26], and $P_{\mathbf{k}} = \sum_{n=1}^J |\tilde{u}_{n\mathbf{k}}\rangle \langle \tilde{u}_{n\mathbf{k}}|$ is the projector onto the selected subspace. The $\tilde{u}_{n\mathbf{k}}$ are initialized as the cell-periodic versions of the Bloch-like states of Eq. (12), and $Q_{\mathbf{k}} = \mathbb{1} - P_{\mathbf{k}}$ is the complement of $P_{\mathbf{k}}$. From this relationship, it is clear that Ω_I is a measurement of the degree of subspace mismatch between neighboring k -points.¹ To minimize this part of the spread, the states at each \mathbf{k} must be chosen to be as close in character as possible to those at neighboring \mathbf{k} .

Typically, it is beneficial to obtain the initial subspace spanned by the J Bloch-like states from projection. This subspace is iteratively updated to move towards the minimum of Ω_I . Minimizing Ω_I is equivalent to solving the eigenvalue equation

$$\left[\sum_{\mathbf{b}} w_b P_{\mathbf{k}+\mathbf{b}}^{(i-1)} \right] |\tilde{u}_{n\mathbf{k}}^{(i)}\rangle = \lambda_{n\mathbf{k}}^{(i)} |\tilde{u}_{n\mathbf{k}}^{(i)}\rangle \quad (14)$$

for the i 'th iteration and selecting the J eigenvectors with the largest eigenvalues [23, 24]. At this point, it is appropriate to realign the final J Bloch-like functions $|\tilde{u}_{n\mathbf{k}}\rangle$ to the J trial states following the procedure of Sec. II B. That is, returning to Eq. (6), we use the current $|\tilde{\psi}_{m\mathbf{k}}\rangle$ in place of the $|\psi_{m\mathbf{k}}\rangle$ on the right-hand side, replace M by J , and repeat the procedure terminating in Eq. (11). These eigenvectors then form the J -dimensional manifold from which Wannier functions can be obtained.

D. Maximal Localization

As a final step, we may find a gauge that minimizes the gauge-dependent part of the spread $\tilde{\Omega}$. In practice, all one needs is the set of overlap matrices of the Bloch orbitals at neighboring k -points,

$$M_{mn}^{(\mathbf{k}, \mathbf{b})} = \langle u_{m\mathbf{k}} | u_{n, \mathbf{k}+\mathbf{b}} \rangle, \quad (15)$$

which encodes the information about first-order derivatives on a discrete k -mesh. The first-order change of the spread from an infinitesimal gauge transformation $U_{mn}^{(\mathbf{k})} = \delta_{mn} + dW_{mn}^{(\mathbf{k})}$, where dW is an anti-Hermitian matrix, can be written as [24, 26]

$$G^{(\mathbf{k})} \equiv \frac{d\Omega}{dW^{(\mathbf{k})}} = 4 \sum_{\mathbf{b}} w_b \left(\mathcal{A} \left[R^{(\mathbf{k}, \mathbf{b})} \right] - \mathcal{S} \left[T^{(\mathbf{k}, \mathbf{b})} \right] \right) \quad (16)$$

where $\mathcal{A}[\mathcal{O}] = (\mathcal{O} - \mathcal{O}^{\dagger})/2$ and $\mathcal{S}[\mathcal{O}] = (\mathcal{O} + \mathcal{O}^{\dagger})/2i$ are the anti-symmetric and symmetric superoperators re-

¹ This is evident from the relation $\text{Tr} [P_1 Q_2] = \|P_1 - P_2\|^2/2$.

spectively, and the quantities in the sum are defined as

$$R_{mn}^{(\mathbf{k},\mathbf{b})} = M_{mn}^{(\mathbf{k},\mathbf{b})} M_{nn}^{(\mathbf{k},\mathbf{b})*}, \quad (17)$$

$$T_{mn}^{(\mathbf{k},\mathbf{b})} = \frac{M_{mn}^{(\mathbf{k},\mathbf{b})}}{M_{nn}^{(\mathbf{k},\mathbf{b})}} \left(\text{Im} \ln M_{nn}^{(\mathbf{k},\mathbf{b})} - \mathbf{b} \cdot \frac{1}{N_k} \sum_{\mathbf{k}',\mathbf{b}'} w_b \mathbf{b}' \text{Im} \ln M_{nn}^{(\mathbf{k}',\mathbf{b}')} \right). \quad (18)$$

The gradient obtained from Eq. (16) can be used in a steepest-decent algorithm to find the global minimum. At each iteration, the step

$$dW^{(\mathbf{k})} = \epsilon G^{(\mathbf{k})} \quad (19)$$

is used, where ϵ is a small positive constant, and the unitary transformation on the Bloch manifold, initialized as the identity, is updated as

$$U^{(\mathbf{k})} \rightarrow U^{(\mathbf{k})} \exp [dW^{(\mathbf{k})}] \quad (20)$$

along with the nearest-neighbor overlap matrices

$$M^{(\mathbf{k},\mathbf{b})} \rightarrow U^{(\mathbf{k})\dagger} M^{(\mathbf{k},\mathbf{b})} U^{(\mathbf{k}+\mathbf{b})}. \quad (21)$$

The minimization is complete when the change in spread after subsequent iterations is below a small threshold. Once the minimum has been reached, the unitary transformation can be applied to the Bloch-like states to achieve an optimally smooth gauge.

E. Topological Obstruction

As discussed earlier, a Chern insulator has a topological obstruction preventing the construction of exponentially localized Wannier functions. In the context of the projection method, the topological obstruction manifests as a rank deficiency of the inner product matrix $A_{\mathbf{k}}$ defined in Eq. (10). As the system transitions from a trivial to a topological phase, a band inversion occurs, swapping the character of the highest occupied and lowest unoccupied bands. When attempting to Wannierize the n_{occ} -dimensional occupied manifold using a set of n_{occ} trial wave functions, the inner product matrix becomes rank deficient at certain points in the BZ due to this change in band character. This rank deficiency causes one or more singular values to drop to zero, making the normalization factor $S_{\mathbf{k}}^{-1/2} = W_{\mathbf{k}} \Sigma_{\mathbf{k}}^{-1} W_{\mathbf{k}}^{\dagger}$ in Eq. (9) diverge. Consequently, the projection fails to produce well-localized Wannier functions. The approach outlined below aims to address this issue.

III. AVOIDING THE TOPOLOGICAL OBSTRUCTION

To avoid the obstruction, we abandon the goal of generating a set of Wannier functions that fully spans the

topological manifold and instead aim to construct a set that spans “most of” the topological manifold. To do so, we reduce the number of trial functions such that the overlap matrix has full rank throughout the BZ, resulting in a set of Bloch-like states spanning a subspace of the topological manifold. This modification enables us to obtain exponentially-localized Wannier functions that can be further optimally localized using the methods of subspace selection and maximal localization.

A. Haldane Model

The Haldane model is a prototypical example of a Chern insulator and serves as the setting for testing our approach. The model is comprised of a two-dimensional honeycomb lattice, where, after setting the lattice constant $a = 1$, the lattice vectors can be chosen as $\mathbf{a}_1 = (1, 0)$ and $\mathbf{a}_2 = (1/2, \sqrt{3}/2)$. The primitive cell contains two spinless orbitals at positions $\tau_1 = (1/3)\mathbf{a}_1 + (1/3)\mathbf{a}_2$ and $\tau_2 = (2/3)\mathbf{a}_1 + (2/3)\mathbf{a}_2$, with onsite energies $\pm\Delta$. The tight-binding parameters consist of real nearest-neighbor hopping t_1 and complex next-nearest neighbor hopping $\pm it_2$. In the second quantized formalism, the tight-binding Hamiltonian is

$$H = \Delta \sum_i (-)^i c_i^{\dagger} c_i - t_1 \sum_{\langle i,j \rangle} (c_i^{\dagger} c_j + h.c.) + t_2 \sum_{\langle\langle i,j \rangle\rangle} (ic_i^{\dagger} c_j + h.c.). \quad (22)$$

A gap closure occurs at the \mathbf{K} and \mathbf{K}' points for $t_2 = \pm\Delta/3\sqrt{3}$ respectively. Henceforth, we set $\Delta = t_1 = 1$, in which case the topological transition occurs when the next-nearest neighbor hopping t_2 passes through $|t_2| = 1/3\sqrt{3} \approx 0.19$. We present results for the trivial phase at $t_2 = -0.1$ and the topological phase with Chern number $C = 1$ at $t_2 = -0.3$.

B. Reduced Wannier Functions

The Haldane model at half-filling has only one occupied band, which normally corresponds to one Wannier function per primitive cell. However, in the topological phase, we know it is impossible to construct a full set of Wannier functions of this density. As an example of our strategy, we consider the possibility of constructing three Wannier functions for every four primitive cells, thus representing $3/4$ of the occupied subspace. That is, we start from a 2×2 supercell, for which the construction of four Wannier functions would normally be straightforward, and instead attempt the construction of three Wannier functions in the topological phase.

Fig. 1 shows the band structure of the Haldane model computed using the PYTHTB package [25] with a 2×2 supercell on a 20×20 regular k -mesh. A band inversion occurs in going from the trivial phase of Fig. 1(a) to

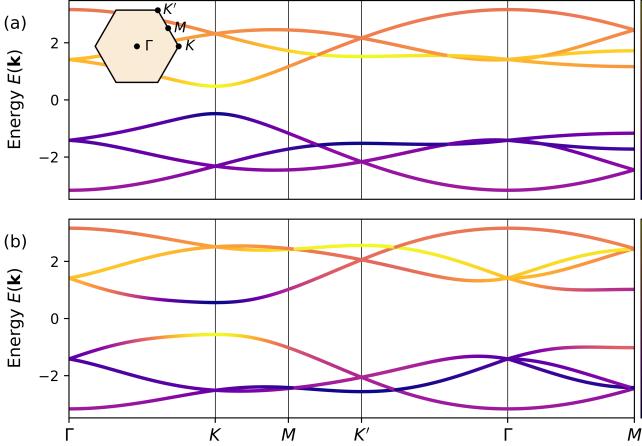


FIG. 1. Bands for the Haldane model on a 2×2 supercell. The color indicates the projection of the eigenstates onto sublattices, with purple and yellow representing the low- and high-energy sublattices, respectively. (a) The bands in the trivial phase ($C = 0$) where $t_2 = -0.1$. (b) The bands in the topological phase ($C = 1$) where $t_2 = -0.3$. In both cases, $\Delta = t_1 = 1$.

the topological phase of Fig. 1(b) at the \mathbf{K} point, which has been mapped from the \mathbf{K}' point after band folding. The color gradient indicates that the characters of the highest occupied and lowest unoccupied bands swap at \mathbf{K} ; the eigenstate of the highest energy valence band becomes fully localized on the high-energy sublattice, while the eigenstate of the lowest energy conduction band becomes fully localized on the low-energy sublattice. This inversion is a hallmark of the topological phase and signals the nontrivial nature of the band structure.

Consider that we attempt to apply the projection procedure to Wannierize the complete set of four topologically obstructed valence bands shown in Fig. 1(b). We use the natural choice of trial wave functions localized on the four low-energy sites in the 2×2 supercell, represented by delta functions. This yields a square 4×4 inner product matrix $A_{\mathbf{k}}$ that becomes singular at the \mathbf{K} point, where it has an entire column of zeros,

$$(A_{\mathbf{k}})_{4,n} = \langle \psi_{4,\mathbf{k}} | \delta_n \rangle = 0 \quad (23)$$

for all n . This results from the fact that the highest-energy occupied state $|\psi_{4,\mathbf{k}}\rangle$ has no support on the low-energy sublattice after the band inversion. Consequently, the inner-product matrix at this point is rank-deficient, with $\text{rank}(A_{\mathbf{k}}) = 3$, and has one singular value equal to zero, as shown in Fig. 2(a). As mentioned, this leads to a divergence in the normalization factor in the unitary projection, shown in Eq. (9). This rank deficiency reflects the presence of a topological obstruction preventing the construction of localized Wannier functions for the full set of valence bands. Even if we were to choose a different set of trial wave functions, altering the gauge of the Bloch-like states, the singularity would persist and shift to another point in the BZ.

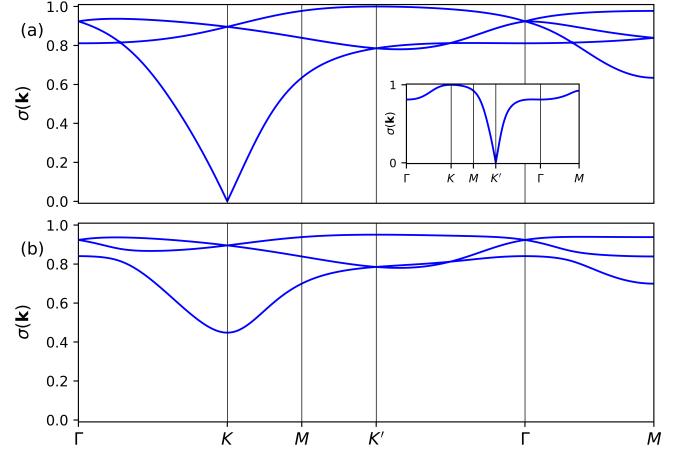


FIG. 2. The singular values plotted along a high-symmetry path in the BZ corresponding to the Haldane model in the $C = 1$ phase for a 2×2 supercell. (a) Four delta functions on the low-energy sites were used as trial wave functions. The inset shows the singular value in the case of a single primitive cell, with the trial wave function being a delta function on the sole low-energy site. (b) Three delta functions on a subset of low-energy sites are used as trial wave functions.

To resolve the singularity, we reduce the number of trial wave functions so as to make $A_{\mathbf{k}}$ a rectangular matrix with full rank at the problematic \mathbf{K} point.² In the present case, since $\text{rank}(A_{\mathbf{k}}) = 3$, removing one trial wave function makes $A_{\mathbf{k}}$ a 4×3 matrix with full rank even at \mathbf{K} , removing the singularity. However, in those regions of the BZ where the original $A_{\mathbf{k}}$ had full rank, $\text{rank}(A_{\mathbf{k}}) = 4$, the projection is no longer unitary but semi-unitary, projecting the original target bands onto a lower-dimensional subspace, as discussed in Sec. II B. Nonetheless, we can still construct a subset of Wannier functions spanning this subspace; we refer to these as “reduced Wannier functions.”

Specifically, we choose three trial wave functions to project onto the four topological bands in Fig. 1(b). These trial wave functions are represented by delta functions centered on three of the low-energy sites τ_i in the 2×2 supercell,

$$g_n(\mathbf{r}) = \delta(\mathbf{r} - \tau_i). \quad (24)$$

Figure 2(b) shows the resulting singular values from this projection, revealing that the singularity at the \mathbf{K} point that was present in Fig. 2(a) has been eliminated. The smoothness of the singular values suggests that the resulting trial wave functions $|\tilde{\psi}_{n\mathbf{k}}\rangle$ generated from Eq. (12) should be suitable for constructing well-localized Wannier functions.

Having obtained a trivial subspace spanned by these Bloch-like states, we use the methods of Sec. II to minimize the spread of the reduced Wannier functions within

² A matrix A with dimensions $(M \times N)$ has full rank if $\text{rank}(A) = \min(M, N)$.

Minimization Step	Ω	Ω_I	$\tilde{\Omega}$
P	0.265	0.229	0.036
P+ML	0.264	0.229	0.035
P+SS+P	0.202	0.190	0.012
P+SS+P+ML	0.201	0.190	0.011

TABLE I. Averaged spreads after each step of the minimization process for the three reduced Wannier functions of the $C = 1$ occupied bands for the Haldane model on a 2×2 supercell. The acronyms stand for projection (P), subspace selection (SS), and maximal localization (ML).

this subspace. After projection, we use subspace selection, followed by projection onto the same set of trial wave functions, and finally, maximal localization. This procedure yields three exponentially localized Wannier functions per 2×2 cell. Table I presents their averaged spreads after each step of the spread minimization, demonstrating the progressive minimization of the gauge-invariant and gauge-dependent spreads. Figure 3 shows the exponential decay of the density of one of the three Wannier functions away from its center. The other two reduced Wannier functions are related by C_3 rotations and show identical exponential decay and spreads. The centers of the three reduced Wannier functions, plotted in Fig. 4, are localized on the same low-energy sites as the trial wave functions.

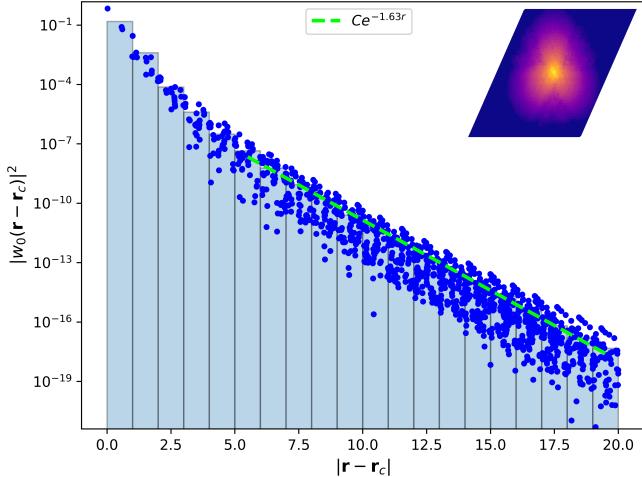


FIG. 3. Decay of the electron density (weights w_0) as a function of distance from the center of one of the three reduced Wannier functions. These Wannier functions were constructed by projecting onto the three trial functions of Eq. (24) in a 2×2 supercell, followed by subspace selection and maximal localization. The blue bars are the bin-averaged values of the weights. The inset shows the Wannier density plotted on a log scale in the supercell conjugate to the discrete k -mesh.

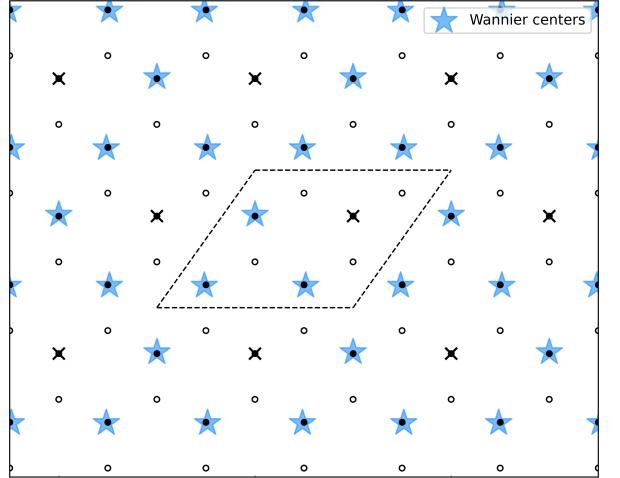


FIG. 4. The centers of the three reduced Wannier functions described in Sec. III B, indicated by stars. The high-energy and low-energy lattice sites are represented by open and filled circles, respectively. Crosses mark the low-energy site excluded from the set of trial wave functions in Eq. (24). Dotted lines delineate the supercell.

C. Wannier Fraction

In the trivial phase, the number of Wannier functions that can be constructed for the occupied bands is simply the number of occupied bands, n_{occ} . In the presence of an obstruction, however, the dimension of the subspace that can be spanned by exponentially localized Wannier functions is constrained by the maximum dimension of the null space of $A_{\mathbf{k}}$ at the (possibly multiple) singularities. For a two-band model, when we construct an $N \times N$ supercell, the dimension of the occupied manifold increases to $n_{\text{occ}} = N^2$. The Chern number of the occupied manifold remains invariant through band folding, along with the dimensionality of the null space at the singularities. Due to the obstruction, we cannot construct exponentially localized Wannier functions that span the entire N^2 bands. Instead, the largest subspace that permits exponentially localized Wannier functions has a dimension bounded by

$$\dim(\mathcal{R}) \leq N^2 - \max_{\mathbf{k}} [\dim(\mathcal{N}_{\mathbf{k}})], \quad (25)$$

where $\dim(\mathcal{R})$ represents the dimension of the reduced Wannier subspace, and $\max_{\mathbf{k}} [\dim(\mathcal{N}_{\mathbf{k}})]$ denotes the maximum dimension of the null-space of $A_{\mathbf{k}}$ across the BZ. We define the “Wannier fraction” as the ratio of the number of Wannier functions to the total number of bands in the topological manifold,

$$f_W = \frac{\dim(\mathcal{R})}{N^2}. \quad (26)$$

This fraction quantifies the extent to which the reduced Wannier functions span the topological manifold. Our first example presented in the preceding subsection was

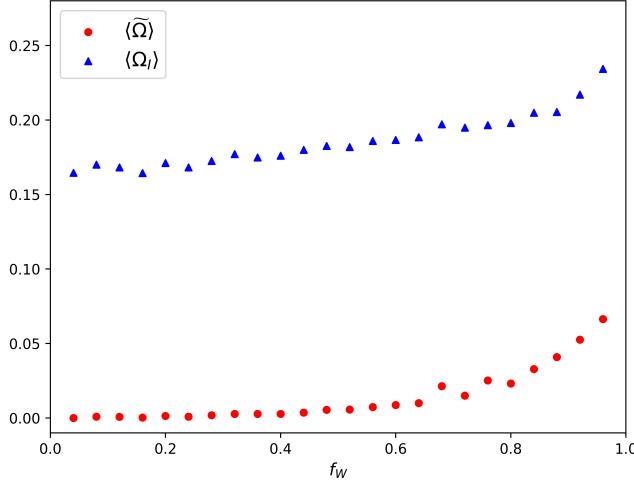


FIG. 5. The dependence of the gauge-invariant (blue triangles) and gauge-dependent (red circles) average Wannier spreads on the Wannier fraction corresponding to the Haldane model for a 5×5 supercell in its $C = 1$ phase. The plotted spreads are averaged over the Wannier functions.

for the case $f_W=3/4$. By applying the same procedure to larger supercells, we can construct reduced Wannier functions that span an increasing portion of the topological manifold.

To examine how the spread of the reduced Wannier functions varies with the dimension of the subspace they span, we compute different numbers of reduced Wannier functions for the Haldane model in the $C = 1$ phase on a 5×5 supercell. With band folding, the occupied manifold consists of 25 bands that, as a whole, are obstructed. We generated up to the permitted number of 24 exponentially localized Wannier functions using trial wave functions localized on randomly chosen subsets of low-energy sites in the home cell. Fig. 5 displays the averaged spreads of the reduced Wannier functions for varying Wannier fractions. Notably, the gauge-dependent part of the spread diminishes significantly at low Wannier fractions, while the gauge-independent spread reaches a finite value. As the Wannier fraction approaches saturation ($f_W = 1$), the spreads increase rapidly, highlighting the trade-off between the reduced Wannier functions spanning larger fractions of the topological manifold and their localization.

The Wannier centers corresponding to the largest Wannier fraction computed, $f_W = 24/25$, are depicted in Fig. 6. The low-energy site omitted from the trial wave functions is a center of C_3 symmetry, and also of an approximate C_6 symmetry from the perspective of the Wannier centers. The Wannier centers exhibit an apparent attraction towards this omitted site, resulting in a sizeable shift from their nominal locations. This reduction of symmetry is one of the consequences of the topological obstruction. The spreads of the centers closest to the omitted site, indicated by the sizes of the stars, are larger than those of the other centers. Heuristically,

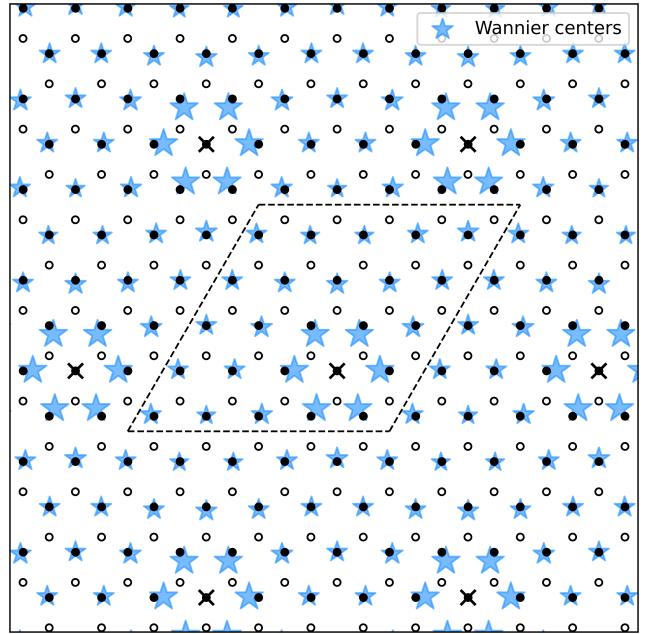


FIG. 6. Wannier functions (stars) at Wannier fraction $f_W = 24/25$. “X” denotes the sole low-energy site on which there is no trial wave function. The stars are centered on the Wannier centers, and their sizes reflect the Wannier spreads.

these observations are consistent with a picture in which the neighboring Wannier functions are uniformly “filling in” for the omitted one in order to minimize the total spread.

D. Disentangled Topological Subspace

In our construction of reduced Wannier functions, we partition the topological manifold into a subspace free from the obstruction spanned by the reduced Wannier functions and a complementary subspace that inherits the topological character of the original manifold. Symbolically, we have performed the operation

$$\text{topological} = \text{trivial} \oplus \text{topological}, \quad (27)$$

through careful use of the projection procedure. The trivial subspace is represented by the projector onto the reduced Wannier manifold, expressed in terms of the Bloch-like states as,

$$P_{\mathbf{k}}^{\text{triv}} = \sum_{n=1}^{\dim(\mathcal{R})} |\tilde{\psi}_{n,\mathbf{k}}\rangle\langle\tilde{\psi}_{n,\mathbf{k}}|. \quad (28)$$

These are the states obtained after the initial projection onto trial wave functions, followed by subspace selection and maximal localization. The complement of P^{triv} in the obstructed manifold is topological, obtained by taking the difference between the occupied and the trivial

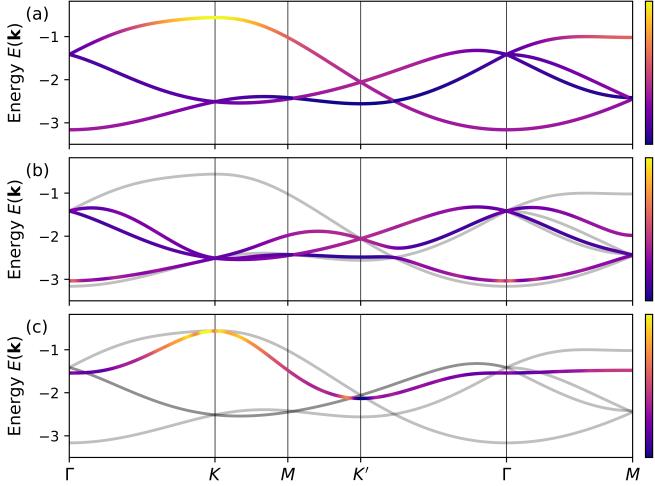


FIG. 7. (a) Folded bands of the topological occupied manifold for the Haldane model on a 2×2 supercell. (b) Wannier interpolated bands of the trivial subspace spanned by the reduced Wannier functions. (c) Interpolated bands of the topological subspace complementary to the reduced Wannier functions. As in Fig. 1, the color bars correspond to the projection onto low- and high-energy sublattices (purple and yellow respectively).

band projectors,

$$P_{\mathbf{k}}^{\text{topo}} = P_{\mathbf{k}}^{\text{occ}} - P_{\mathbf{k}}^{\text{triv}}. \quad (29)$$

This subspace retains the topological character of the occupied bands and inherits the obstruction. That is, we have segregated the obstruction into a one-dimensional subspace, leaving the rest of the occupied space free of any topological obstruction.

For each projector $P_{\mathbf{k}}^{\mathcal{M}}$ onto band manifold $\mathcal{M} = \text{'occ'}$, ‘triv’, or ‘topo’ in Eq. (29), we form the projected Bloch Hamiltonian

$$H_{\mathbf{k}}^{\mathcal{M}} = P_{\mathbf{k}}^{\mathcal{M}} H_{\mathbf{k}} P_{\mathbf{k}}^{\mathcal{M}}. \quad (30)$$

Diagonalizing these in the Haldane 2×2 supercell context at Wannier fraction $f_W = 3/4$, we find the projected band structures shown in Fig. 7. In Fig. 7(b), we show the Wannier interpolated band structure of the trivial subspace spanned by the reduced Wannier functions. These bands have a large degree of overlap with the lower-energy bands, but they avoid the high-energy band that underwent inversion at \mathbf{K} . Fig. 7(c) shows the interpolated band structure of the topological subspace. This band matches the highest energy occupied band at the inversion point and shows the same change in character, demonstrating that this state has inherited the topological features of the original energy eigenstates.

It is of interest to inspect the distribution of the Berry curvature and quantum metric in the Brillouin zone for each subspace $P_{\mathbf{k}}^{\mathcal{M}}$. The Berry curvature $\mathcal{B}_{\mu\nu}^{(n)}(\mathbf{k})$ and quantum metric $g_{\mu\nu}^{(n)}(\mathbf{k})$ of band $n \in \mathcal{M}$ are determined

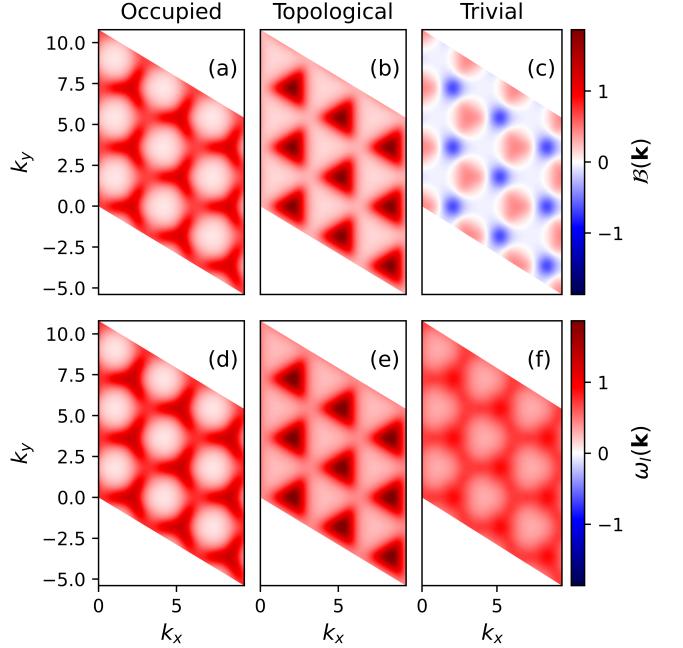


FIG. 8. (a)-(c) Berry curvature $\mathcal{B}(\mathbf{k})$ of (a) the occupied subspace, (b) the topological subspace, and (c) the trivial reduced Wannier subspace. (d)-(f) Trace of the quantum metric $\omega_I(\mathbf{k})$ of the same subspaces listed above. All plots extend over several reciprocal lattice unit cells.

respectively by the real and imaginary parts of the quantum geometric tensor [26–28]

$$F_{\mu\nu}^{(n)} = \langle \check{\partial}_\mu u_{n,\mathbf{k}} | \check{\partial}_\nu u_{n,\mathbf{k}} \rangle, \quad (31)$$

where $\check{\partial}_\mu = (1 - P_{\mathbf{k}}^{\mathcal{M}})\partial_\mu$ is the gauge-covariant derivative and $\partial_\mu = \partial_{k_\mu}$. Specifically,

$$\mathcal{B}_{\mu\nu}^{(n)} = -2\text{Im}F_{\mu\nu}^{(n)}, \quad g_{\mu\nu}^{(n)} = \text{Re}F_{\mu\nu}^{(n)}. \quad (32)$$

To simplify the presentation of the results, we focus on the band-traced curvature $\mathcal{B}(\mathbf{k}) = \sum_n \mathcal{B}_{xy}^{(n)}(\mathbf{k})$ and the band- and Cartesian-traced metric $\omega_I(\mathbf{k}) = \sum_n [g_{xx}^{(n)}(\mathbf{k}) + g_{yy}^{(n)}(\mathbf{k})]$, where the band sum runs over $n \in \mathcal{M}$. The notation $\omega_I(\mathbf{k})$ is chosen to emphasize the connection to the gauge-invariant spread of the Wannier functions in Eq. (13) through [26]

$$\Omega_I = \frac{1}{A_{\text{BZ}}} \int d\mathbf{k} \omega_I(\mathbf{k}), \quad (33)$$

where A_{BZ} is the Brillouin zone area. We have computed the Berry curvature $\mathcal{B}(\mathbf{k})$ and metric $\omega_I(\mathbf{k})$ in the Brillouin zone for the Haldane 2×2 supercell at Wannier fraction $f_W = 3/4$ in the topological phase. These are plotted in the topological phase for the entire occupied four-band subspace, the topologically obstructed one-band subspace, and the trivial three-band subspace in Figs. 8 and 9. The metric is largest in the vicinity of the band inversion point, where the character of the

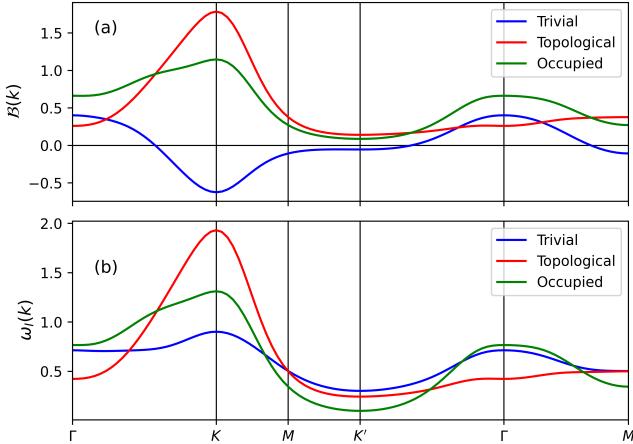


FIG. 9. The interpolation of (a) the Berry curvature and (b) the trace of the quantum metric along a path through high-symmetry points in the BZ.

bands is changing most rapidly. However, it remains finite throughout the BZ in the topological as well as the trivial phase, consistent with Ref. [29], which found that the gauge-invariant spread diverges at the topological phase transition but returns to being finite in the topological phase. Upon integrating the Berry curvatures, we confirm that the topological subspace carries a nontrivial Chern number $C = 1$, inheriting the Chern number of the occupied subspace, while the trivial subspace has $C = 0$. This must be the case since we have obtained exponentially localized Wannier functions for the reduced subspace.

IV. DISCUSSION

We have demonstrated a procedure for constructing a set of exponentially localized Wannier functions that span a subspace of an obstructed set of topological bands. Through this procedure, we have removed the obstruction and placed it in a one-band subspace, leaving the remaining part of the obstructed manifold topologically trivial and thus Wannierizable. From this trivial subspace, we obtain exponentially localized Wannier functions. Through band folding, we can increase the dimensionality of the trivial subspace, increasing the coverage of the reduced Wannier functions over the obstructed manifold at the cost of decreased localization. Of course, as the Bloch-like states corresponding to the reduced Wannier functions are not energy eigenstates, they cannot be used to compute spectral properties. However, expectation values of one-particle operators, such as energy or charge density, can still be written as a sum of traces over the trivial and topological subspaces, with the potential advantage that the trivial part can be computed in a Wannier basis.

Although we have illustrated our approach starting from a simplified tight-binding model, it can be extended

straightforwardly to first-principles calculations based on density functional theory (DFT). Modern first-principles workflows commonly involve constructing Wannier functions using tools like WANNIER90 [30, 31]. The projection and disentanglement procedure we describe are already integral parts of such workflows. As a result, it should be possible to isolate the topological obstruction and Wannierize the remaining subspace in a first-principles context, just as was done here for tight-binding models.

While we have demonstrated the approach for the specific case of a half-filled two-band Chern insulator with unit Chern number, it should be straightforward to apply this procedure to multiband systems or those with bands of higher Chern number. In the former case, it may not even be necessary to break translational symmetry in order to segregate the obstruction. In the latter case, it would be interesting to test whether the stronger obstruction can still easily be isolated to a single topological band.

In time-reversal invariant 2D and 3D systems with a nontrivial \mathbb{Z}_2 index, there is an obstruction that prevents the existence of a smooth gauge that respects the time-reversal symmetry and thus forbids the construction of Wannier functions that all take the form of Kramers pairs. Here, the corresponding procedure would be to decompose the $2N$ -dimensional occupied space into a $2(N-1)$ -dimensional trivial manifold represented by Kramers-pair Wannier functions, relegating one topological pair of bands to the remaining subspace. In the context of crystalline topological insulators, the corresponding issue is the inability to form Wannier functions that are permuted into one another by the crystallographic symmetry operations; again, it may be possible to do this for most, but not all, of the occupied bands.

In systems with fragile obstructions, such as those occurring in some moiré systems, obtaining a minimal Wannier representation of the obstructed bands is challenging due to the necessity of including additional trivial bands to trivialize the obstructed subspace [15]. Our approach would instead reduce the dimensionality of the band manifold containing the obstruction. It remains to be seen whether our approach, or a derivative of it, could be profitably applied to such systems.

Our work has been motivated in part by the recent flowering of interest in flat-band systems, often realized in moiré graphene or transition-metal dichalcogenide materials, where exotic correlated phases have been reported, including superconducting, Wigner crystal, quantum anomalous Hall, and fractional quantum anomalous Hall states [32–39]. In these systems, the flatness of the bands diminishes the kinetic energy, suppressing the tendency toward the formation of a Fermi liquid relative to more unusual many-body states. Depending on the microscopic details, the relevant correlated state may predominantly occupy either the trivial or topological subspace of the flat-band manifold. In any case, having a Wannier representation for the trivial portion of the

band manifold can be a valuable tool, potentially simplifying the construction and analysis of strongly correlated states in these flat-band settings.

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