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Real-Space Imaging of Band Topology via Wavefunction Zeros

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We prove that the wavefunction of a crystal at a high-symmetry momentum, $\Psi_{\mathbf{k}_*}(\mathbf{r})$, has symmetry-enforced zeros at certain positions in the unit cell, using a new invariant fixed uniquely by the symmorphic symmetry representation of the wavefunction. This allows one to infer the topology of an electronic band by probing zeros of the charge density, and in turn to connect scanning tunnelling microscopy to the group representation theory of bandstructure. We apply the theorem to 1H transition metal dichalcogenides, where it detects the obstructed atomic limit of WSe₂, the Haldane model, where it detects the Chern number modulo three, and the Bernevig–Hughes–Zhang model, where it detects the $\mathbb{Z}_2$ index. In addition, the zeros have important consequences for interaction effects: in kagome metals, they fix the sublattice structure of Van Hove wavefunctions, and in twisted bilayer graphene, they explain the qualitative interaction-induced reshaping of the flat bands.

Introduction—Band topology has revealed phases of matter whose electronic structure is expressed through robust conduction at edges and surfaces, and quantised or otherwise unconventional electronic responses. Electronic structure is usually described in terms of Bloch bands in momentum space, yet an equally fundamental description is possible in real space, where bands are built from Wannier orbitals [1]. This viewpoint underlies the theory of topological quantum chemistry, which connects the type and positions of orbitals to the global topology of bands across the Brillouin zone [2–7]. In real space, topologically trivial bands admit symmetry-respecting localised Wannier functions, whereas topological bands are characterised by a Wannier obstruction or, in the ‘obstructed atomic’ case, Wannier orbitals displaced away from the atoms to empty sites in the unit cell [8–12].

This real-space formulation hints that band topology should leave distinct signatures in the spatial organisation of a quantum state within the unit cell. Scanning tunnelling microscopy (STM) is especially well suited to explore this, since within the Tersoff–Hamann picture, the tunnelling current probes the local density of states $\text{LDOS}(eV, \mathbf{r}) = \sum_{\mathbf{k}} |\Psi_{\mathbf{k}}(\mathbf{r})|^2 \delta(eV - \varepsilon_{\mathbf{k}})$ with atomic spatial resolution [13, 14]. Yet, the quantities typically used to recognise topology are either indirect transport signatures, or momentum-space data sensitive to the phase of the wavefunction — such as Berry phases or symmetry characters. A local density probe seems to discard much of this information, retaining only $|\Psi_{\mathbf{k}}(\mathbf{r})|^2$. As the bias eV moves through a band, STM images how charge density reorganises within the unit cell, but without measuring the phase of the wavefunction. A fundamental question is whether such a phaseless real-space image can nevertheless reveal the topology of the band.

Recent experiments present a concrete clue [15, 16]: in monolayer WSe₂, the charge density is centred between the atoms near the valence band maximum at K , but shifts onto the atomic sites at Γ [15]. This shift was shown to imply that WSe₂ is an obstructed atomic insulator [17–20]. These developments suggest that the distribution of charge density in Bloch wavefunctions $|\Psi_{\mathbf{k}}(\mathbf{r})|^2$ contains symmetry information that survives the loss of phase.

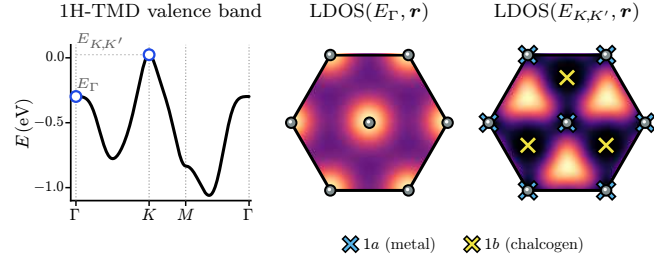


FIG. 1. Imaging the band topology of TMDs. Left: valence-band dispersion of 1H-TMDs. The band transforms with C_3 eigenvalues 1 and $e^{2\pi i/3}$ at Γ and K , indicating a topologically obstructed atomic insulator (OAI). Middle: $\text{LDOS}(E_{\Gamma}, \mathbf{r})$; Right: $\text{LDOS}(E_K, \mathbf{r})$. At K , symmetry-enforced zeros appear at the $1a$ and $1b$ positions (crosses); no zeros appear at Γ . The change in LDOS between these two energies is a real-space signature of an OAI.

This raises a natural question: how general is the connection between real-space STM images and band topology? Is the shift of spectral weight between sites, bonds, and hollow positions a material-specific feature, or the manifestation of a universal symmetry principle? The central claim of this paper is that there is a group-theoretic answer: the position of the charge within the unit cell is fixed by band representation theory. We derive a new real-space invariant [Eq. (4)] which proves that at high-symmetry momenta, Bloch wavefunctions must vanish at a set of positions we term the *dark set* of the band. The dark set appears as symmetry-enforced dark spots in the LDOS whenever the bias resolves the corresponding high-symmetry states.

We prove that for a fixed high-symmetry momentum $\mathbf{k}_*$, the zeros in the Bloch function $\Psi_{\mathbf{k}_*}(\mathbf{r})$ are fixed by the visible part of its irreducible representation (irrep); nonsymmorphic symmetry data are invisible to local density probes. In symmorphic crystals, *the dark set uniquely determines the representation content of a band*, up to complex-conjugate irrep pairs at time-reversal invariant momenta that no density measurement can distinguish. Symmetry indicators allow the inference of topological invariants from this data, such as the Chern number or $\mathbb{Z}_2$ invariant [11, 21–26].

Motivated by possible applications to STM, we focus on two-dimensional systems. We derive the general dark set selection rule, tabulate the symmetry-enforced dark sets across all 17 two-dimensional wallpaper groups, and apply the formalism to representative topological bands. For 1H transition metal dichalcogenides (TMDs), it diagnoses the obstructed atomic limit of the valence band [15, 16]. For the Haldane [27] and BHZ [28] models, we show how STM can diagnose a nonzero Chern number and $\mathbb{Z}_2$ index. The framework developed here suggests a new form of topological band spectroscopy, by which topology can be determined from the intracell structure of the bulk wavefunction.

The consequences of these zeros extend beyond STM, as the structure of charge density within the unit cell determines how electrons interact with one another. A symmetry-enforced zero can suppress certain interaction channels, or allow selected states to avoid an interaction-generated potential. On the kagome lattice, we show the zeros explain the sublattice texture of Van Hove wavefunctions — which promotes long-range Coulomb interactions known to stabilise exotic loop current orders. In twisted bilayer graphene (TBG), we show that the zeros explain the qualitative reshaping of the narrow bands by interactions: the Bloch states at Γ have a zero which allows them to avoid the Hartree potential created by the states at K . Thus, dark sets are not only STM signatures of topology; they are real-space constraints on the interacting physics of topological bands.

Derivation—Define a space-group element $h = \{\mathcal{R}|\mathbf{t}\}$, comprising a proper rotation or reflection $\mathcal{R}$ followed by a translation by $\mathbf{t}$. We define a high-symmetry momentum $\mathbf{k}_*$ and its little group $G_{\mathbf{k}_*}$, the subgroup of the crystal symmetries which leaves $\mathbf{k}_*$ invariant modulo a reciprocal lattice vector, $G_{\mathbf{k}_*} = \{h : \mathcal{R}\mathbf{k}_* = \mathbf{k}_* + \mathbf{G}\}$. We also define a high-symmetry real-space position $\mathbf{r}_*$ and the associated site symmetry group $G_{\mathbf{r}_*}$, i.e. those symmetries which leave $\mathbf{r}_*$ invariant modulo a lattice vector, $G_{\mathbf{r}_*} = \{h : \mathcal{R}\mathbf{r}_* + \mathbf{t} = \mathbf{r}_*\}$. For such h , we denote $\mathbf{t}_h(\mathbf{r}_*) = (1 - \mathcal{R})\mathbf{r}_*$.

An electronic band has a little group representation at $\mathbf{k}_*$, defined via matrices $\mathcal{D}_{\rho\mathbf{k}_*}(h)$ whose action encodes how the wavefunction transforms under the symmetry operation h (see the Appendix for a basic theoretical introduction), i.e. h acts as a unitary transformation U_h

$$U_h \Psi_{\mathbf{k}_*,a} = e^{-i\mathbf{k}_* \cdot \mathbf{t}} [\mathcal{D}_{\rho\mathbf{k}_*}(h)]_{ab} \Psi_{\mathbf{k}_*,b} \quad (1)$$

where ρ denotes the irrep, and a, b index the wavefunction components (summation over b is implicit).

Our goal is to find selection rules which force the amplitude of the wavefunction to vanish at certain points depending on its symmetry. Intuitively, these are positions in real space where the phases of nearby orbitals interfere destructively, as determined by their orbital character and positions. The single-orbital limit is familiar: the nodes of a spherical harmonic identify its angular momentum; the dark set generalises this from a single orbital to a crystal.

Consider the symmetry operations h contained in both

the site symmetry group $G_{\mathbf{r}_*}$ and the little group $G_{\mathbf{k}_*}$; we denote this intersection $H_{\mathbf{k}_*,\mathbf{r}_*} = G_{\mathbf{r}_*} \cap G_{\mathbf{k}_*}$. Evaluating Eq. (1) at a position left invariant by the symmetry, $\mathbf{r}_* = \mathcal{R}\mathbf{r}_* + \mathbf{t}$, we conclude

$$\Psi_{\mathbf{k}_*}(\mathbf{r}_*) = e^{-i\mathbf{k}_* \cdot \mathbf{t}} \mathcal{D}_{\rho\mathbf{k}_*}(h) \Psi_{\mathbf{k}_*}(\mathbf{r}_*) \quad (2)$$

Hence, *either* $e^{-i\mathbf{k}_* \cdot \mathbf{t}} \mathcal{D}_{\rho\mathbf{k}_*}(h)$ leaves the wavefunction invariant, *or else* $\Psi_{\mathbf{k}_*}(\mathbf{r}_*) = 0$.

To identify the vector space for which the matrix $e^{-i\mathbf{k}_* \cdot \mathbf{t}} \mathcal{D}_{\rho\mathbf{k}_*}(h)$ acts as a projector, we sum over the elements of $H_{\mathbf{k}_*,\mathbf{r}_*}$,

$$\mathcal{P}_{\mathbf{k}_*,\mathbf{r}_*} = \frac{1}{|H_{\mathbf{k}_*,\mathbf{r}_*}|} \sum_{h \in H_{\mathbf{k}_*,\mathbf{r}_*}} e^{-i\mathbf{k}_* \cdot \mathbf{t}_h(\mathbf{r}_*)} \mathcal{D}_{\rho\mathbf{k}_*}(h) \quad (3)$$

This object, known as a Reynolds operator [29, 30], projects onto the subspace left invariant by $e^{-i\mathbf{k}_* \cdot \mathbf{t}} \mathcal{D}_{\rho\mathbf{k}_*}(h)$ for all h . Taking the trace, we find that

$$m_{\mathbf{k}_*,\mathbf{r}_*} = \frac{1}{|H_{\mathbf{k}_*,\mathbf{r}_*}|} \sum_{h \in H_{\mathbf{k}_*,\mathbf{r}_*}} e^{-i\mathbf{k}_* \cdot \mathbf{t}_h(\mathbf{r}_*)} \chi_{\rho\mathbf{k}_*}(h) \quad (4)$$

must be nonzero, else the wavefunction vanishes at $\mathbf{r}_*$, where we introduced the characters of the irreducible representation ρ , $\chi_{\rho\mathbf{k}_*}(h) = \text{Tr}[\mathcal{D}_{\rho\mathbf{k}_*}(h)]$.

This formula determines the symmetry-enforced nodes in a Bloch wavefunction. The set of high-symmetry positions with $m_{\mathbf{k}_*,\mathbf{r}_*} = 0$ is the *dark set of the irrep* ρ : the orbital phases encoded in $\chi_{\rho\mathbf{k}_*}(h)$, dictated by the symmetry representation, interfere destructively and force $\Psi_{\mathbf{k}_*}(\mathbf{r}_*) = 0$. The positions of the dark set are gauge invariant: redefinition of the rotation axes, coordinate origin, or orbital embedding does not change the physical locations where $\Psi_{\mathbf{k}}(\mathbf{r})$ is forced to vanish (SM Sec. S2). The phase of the wavefunction, by contrast, is gauge dependent and experimentally inaccessible. Away from a high-symmetry momentum $\mathbf{k}_*$, the wavefunction does not transform as a single irrep; moving through the Brillouin zone, its charge density evolves between different irreps with different patterns of zeros. This enforces an energy dependence of the charge density across the band.

The differential current dI/dV measured in STM is proportional to the LDOS [31]; if the bias is chosen to intersect the band at a single high-symmetry momentum $\mathbf{k}_*$, then one can image $|\Psi_{\mathbf{k}_*}(\mathbf{r})|^2$ and hence probe the existence of the symmetry-enforced zeros. The selection rule acts irrep by irrep at $\mathbf{k}_*$; when an energy window contains several irreps, the only exact zeros are those shared by every contributing irrep. Two physical conditions control the visibility of these zeros. First, if a band is composed of tightly localised orbitals with minimal support off the atomic sites, then a significant fraction of the unit cell will appear dark simply because the density of states is small, as opposed to being strictly zero due to the selection rule. To discern regions which are forced-dark, the constituent orbitals must have considerable overlap with their neighbours, such that the density of states will

be large unless a zero is required by symmetry. Second, certain high-symmetry momenta will not be isolated energetically, but as we will show in model calculations, they can still dominate the LDOS at a fixed energy, allowing inference of the dark spots. In practice, the diagnostic is the position and symmetry of the LDOS minima.

The question naturally arises: at a given high-symmetry momentum $\mathbf{k}_*$, for a single isolated irrep ρ , does observation of the dark set suffice to determine the irrep of the wavefunction? The answer is the following:

Theorem. Probed over the high-symmetry positions of the unit cell, the symmetry-forced dark set of Eq. (4) determines ρ *exactly* up to complex conjugation $\rho \leftrightarrow \bar{\rho}$ at time-reversal invariant momenta (TRIM), and up to the character data of nonsymmorphic symmetries.

We tabulate the dark sets for all irreps in the 17 wallpaper groups in SM Sec. S1, verifying the theorem constructively; a non-constructive proof is given in SM Sec. S9. Conjugate pairs $E_{\pm}$ appear with identical dark sets at Γ in $p3$, $p4$, and $p6$, and at M in $p4$; in systems with (time-reversal or) mirror symmetries, ρ and $\bar{\rho}$ form degenerate components $E_{\pm}$ of a single (co)irrep, meaning the only remaining ambiguity in such systems is that due to nonsymmorphic symmetries.

Applications: Transition Metal Dichalcogenides—The first example we will consider is the semiconducting 1H transition metal dichalcogenides (1H-TMDs), a prototypical example of which is WSe_2 . The space group of this family is $P\bar{6}m2$, and the point group D_{3h} . Denoting the position $(a, b) = a\mathbf{R}_1 + b\mathbf{R}_2$ where $\mathbf{R}_1 = (1, 0)$ and $\mathbf{R}_2 = (-\frac{1}{2}, \frac{\sqrt{3}}{2})$, we consider the high-symmetry positions: the 1a position at the origin of the unit cell $(0, 0)$, the 1b position at $(\frac{1}{3}, \frac{2}{3})$, and the 1c position at $(\frac{2}{3}, \frac{1}{3})$. 1H-TMDs exhibit an atomically obstructed valence band, for which localised Wannier functions cannot be constructed if one insists on centring them at the atomic sites. This follows from the mismatch of the C_3 irreps at Γ and K : $\mathcal{D}_{\Gamma}(C_3) = 1$ and $\mathcal{D}_{\tau K}(C_3) = e^{2\pi i \tau/3}$ where $\tau = \pm$.

Consider first the τK point, at which the symmetry group is C_{3h} . At a C_3 centre defined by $\mathbf{r} = C_3\mathbf{r} + \mathbf{t}_{C_3}(\mathbf{r})$

$$m_{\tau K, \mathbf{r}} = \frac{1}{3} [1 + \vartheta_{\tau K, \mathbf{r}} \xi_{\tau K} + (\vartheta_{\tau K, \mathbf{r}} \xi_{\tau K})^2], \quad (5)$$

where $\vartheta_{\tau K, \mathbf{r}} = e^{-i\tau \mathbf{K} \cdot \mathbf{t}_{C_3}(\mathbf{r})}$, and $\xi_{\tau K}$ is the C_3 eigenvalue of the Bloch state. Hence the state is bright at precisely the centre for which $\vartheta_{\tau K, \mathbf{r}} \xi_{\tau K} = 1$. For the three C_3 centres, the phases at K are $\vartheta_{K, \{1a, 1b, 1c\}} = \{1, \omega, \omega^2\}$. The valence band of the TMD has $\xi_{\Gamma} = 1$ and $\xi_{\tau K} = \omega^{\tau}$, so it is nodeless at Γ and bright only at 1c at K (Fig. 1); the calculation is elaborated in the Appendix. An unobstructed valence band would have $\xi_{\Gamma} = \omega^{\pm}$, whose dark set includes all three C_3 centres (see SM Sec. S3C).

Haldane model—The next example we consider is the Haldane model of a honeycomb lattice Chern insulator [27]. For any C_3 -symmetric two-dimensional insulator, the Chern number mod 3 is fixed by the C_3 eigenvalues at the C_3 -invariant momenta $\xi_{\Gamma}, \xi_K, \xi_{K'}$; for a single occupied band, $e^{2\pi i C/3} = \xi_{\Gamma} \xi_K \xi_{K'}$ [22]. For a honeycomb lattice

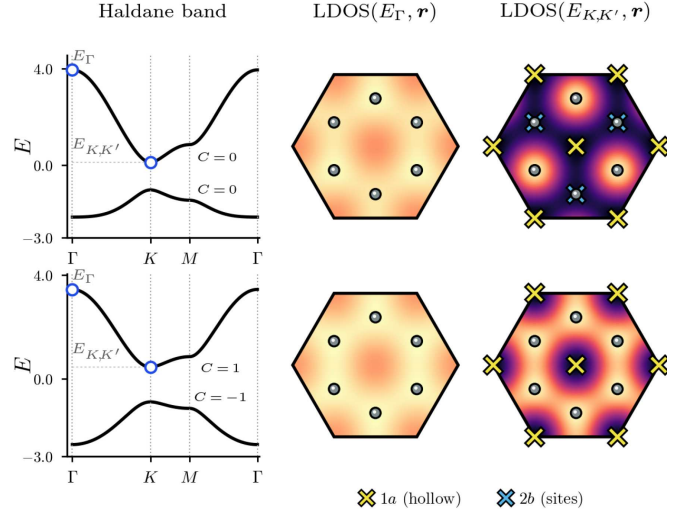


FIG. 2. Imaging the Chern number of the Haldane model. Top row: trivial phase, $C = 0$; bottom row: Chern phase, $|C| = 1$. In the trivial phase, the K/K' states have zeros on the same sublattice. In the Chern phase the two valleys have zeros (crosses) on opposite sublattices, leaving only the hexagon centre dark in the total LDOS. The distinct dark sets allow inference of the Chern number modulo three.

of s orbitals, $\xi_{\Gamma} = 1$, and so it remains to determine the characters at the K/K' points to infer the Chern number mod 3. We find (Appendix) that $\xi_K = e^{\pm 2\pi i/3}$ implies the wavefunction at K is dark on the A/B sublattice, while $\xi_{K'} = e^{\pm 2\pi i/3}$ implies the wavefunction at K' is dark on the B/A sublattice. Hence, a single centre bright at both K and K' implies $C = 0$, whereas two centres bright, each originating from K and K' , imply $|C| = 1$. We demonstrate this with numerical LDOS simulations for $|C| = 0, 1$ (Fig. 2 top, bottom). The key observation is that for $C = 0$, one sublattice is dark at K/K' ; for $C = \pm 1$, only the origin is dark. When K and K' are not degenerate, the selection rule is even more transparent: in the trivial case only one sublattice is bright as the bias is varied, whereas in the topological case a second sublattice suddenly turns bright when the bias energy intersects the second valley (SM Sec. S4).

Prior theory work on indenene [32] has proposed a connection between the characters at K and the charge density — specifically, that s orbitals at the honeycomb positions produce the same maxima of charge density near K as $p_{x,y}$ orbitals at the triangular position [33]. Our formalism makes rigorous those results.

Bernevig-Hughes-Zhang model—The next example we consider is the BHZ model, a minimal example of a square lattice $\mathbb{Z}_2$ topological insulator [28]. The topologically nontrivial phase is characterised by a finite spin Hall conductivity, and is diagnosed by a $\mathbb{Z}_2$ invariant. The presence of time-reversal symmetry ensures the Chern number vanishes, yet a $\mathbb{Z}_2$ topology remains, characterised by the Kane–Mele invariant ν [34, 35]. For a single occupied Kramers pair such as the lower band of the BHZ model, inversion symmetry implies $(-1)^{\nu} = \zeta_{\Gamma} \zeta_X \zeta_Y \zeta_M$,

where ζ are the inversion eigenvalues at the TRIM [21]. The resulting dark sets are calculated in the Appendix.

Let $\mathbf{r}_*$ be an inversion centre, i.e. $I\mathbf{r}_* = \mathbf{r}_*$. Then, $\mathbf{t}_I(\mathbf{r}_*) = 2\mathbf{r}_*$, and if no other symmetries are present, $m_{\mathbf{k}_*, \mathbf{r}_*} = 1 + e^{-i\mathbf{k}_* \cdot \mathbf{t}_I} \zeta_I(\mathbf{k}_*)$. A simple rule follows: the number of zeros mod 2 across all TRIM, at an inversion centre *with no other symmetry*, equals the $\mathbb{Z}_2$ invariant (SM Sec. S6). With C_4 symmetry, the rule becomes simpler: the bonds have the same (opposite) contrast if $\nu = 1$ ($\nu = 0$). We demonstrate this with LDOS simulations for the BHZ valence band in Fig. 3: in the topological case (bottom) the bonds are bright at both Γ and M , yet in the trivial case (top) they are dark at M .

Kagome Van Hove wavefunctions—In the following examples, we move beyond the application of STM and explore the consequences the dark set has when interactions are included. Intuitively, the arrangement of charge density within the unit cell should strongly influence how electrons interact. A paradigmatic example is the kagome lattice — the wavefunctions near the Van Hove singularities (VHS) at the M -point exhibit an unusual structure known as the *sublattice interference effect*, whereby the wavefunction resides on only one or two of the three sublattices [36, 37]. We show how this sublattice texture originates from the particular band representations at the M -point, i.e. the dark set of $\Psi_{M_i}(\mathbf{r})$.

The three sublattices are located at the $3c$ Wyckoff positions of the group $p6mm$, inducing the M -point irreps $A_1 \oplus B_1 \oplus B_2$ (see SM Sec. S7). Calculation of the dark sets reveals that at M_1 , the A_1 wavefunction vanishes on both the B and C sublattices, while the $B_{1,2}$ wavefunctions vanish on the A sublattice (Fig. 4); cyclic permutation gives the result at the other two M points. In the nearest-neighbour kagome model, the middle (so-called p -type) Van Hove state is the A_1 irrep, while the lower (so-called m -type) Van Hove state is the B_2 irrep; the flat band at M transforms as B_1 , and is distinguished from B_2 by a node on the bonds. Therefore, the sublattice texture of the kagome Van Hove states is a consequence of the dark sets of the M -point irreps A_1 and B_2 .

Hence, the dark set gives insight into the spatial structure of wavefunctions, which in turn has striking consequences for interaction effects [36–47]. At the p -type VHS, different M -points live on strictly distinct sublattices — scattering between M -points therefore has zero projection onto onsite interactions, enhancing the effect of longer-range couplings which stabilise exotic loop current orders. This example highlights how symmetry-enforced zeros can produce fascinating correlation effects.

Twisted Bilayer Graphene—A second example of this is found in magic-angle TBG, where Coulomb interactions strongly reshape the nominally flat bands in a highly momentum-selective way [48]; the dark set explains the origin of this selectivity. Computation of the dark sets (SM Sec. S8) reveals that the states near K have no zeros common to both layers, whereas the states at Γ have a C_3 -enforced zero at the AA stacking regions (Fig. 5). This zero and its connection to the Chern number have

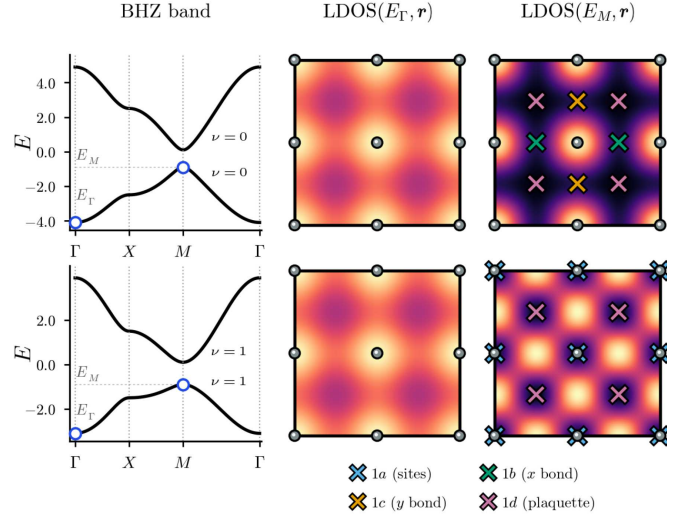


FIG. 3. Imaging the $\mathbb{Z}_2$ invariant of the BHZ model. Top row: trivial phase, $\nu = 0$; bottom row: quantum spin Hall phase, $\nu = 1$. In the trivial phase the bonds and plaquette centre have zeros (crosses) at M ; in the quantum spin Hall phase the bonds are bright. The Kane-Mele $\mathbb{Z}_2$ invariant can be diagnosed simply by whether the bonds have the same ($\nu = 1$) or opposite ($\nu = 0$) contrast at Γ and M .

previously been observed by Ledwith et al. [49], who have shown that its existence prevents the formation of a fully gapped Mott state, producing a so-called ‘Mott semimetal’. The zero has profound consequences for how the bands are renormalised [50–53]: the Hartree potential is strong at the AA regions, due to the concentrated density from the K states, which consequently shift upwards in energy sharply. However, the Γ states have a zero at the AA regions, allowing them to avoid the Hartree potential, and so do not shift significantly. It is worth emphasising that this zero is a non-perturbative consequence of representation theory, and cannot be removed by interactions unless they close the gap to remote bands or break symmetries. The difference in symmetry irreps at Γ and K therefore explains the qualitative reshaping of the flat bands.

Discussion—The examples above show that symmetry-enforced zeros give a local way to connect momentum-space irreps to real-space wavefunction structure, in the spirit of real-space invariants [54]. A classic momentum-space counterpart is Kohmoto’s result that the Hall conductance is determined by the total vorticity of wavefunction zeros across the Brillouin zone [55]. The dark set interchanges momentum and position in this construction: at fixed $\mathbf{k}_*$, the irrep pins zeros to definite locations in real space. Previous works have also considered formulations of topology in real space using the projected position operator or Hamiltonian, retaining phase information absent from the charge density [56–62].

As the bias moves through a band, the LDOS samples different regions of the Brillouin zone and can track how spectral weight is reorganised among sites, bonds and hollow positions. Such bias-dependent textures are a real-

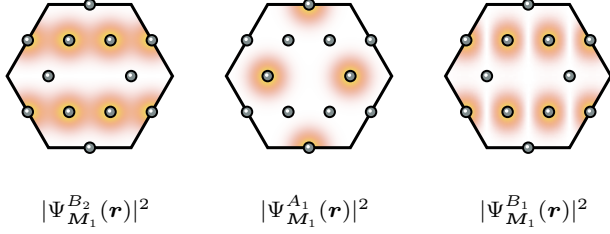


FIG. 4. **Kagome Van Hove dark sets.** The wavefunctions at the VHS of an s orbital kagome lattice correspond to irreps A_1 and $B_{1,2}$. At the momentum M_1 , the A_1 irrep is forced-dark on B and C , while the $B_{1,2}$ irreps are forced dark on A .

space window onto the momentum dependence of Bloch wavefunctions, and hence onto the wavefunction data from which quantum geometry is built [63–65]. STM studies of kagome metal CoSn have visualised energy-dependent redistribution of intracell spectral weight between flat and dispersive bands [66]; the symmetry-enforced part of such a texture is the dark set structure developed here.

Spectral geometry asks the question “*Can one hear the shape of a drum?*”; can the shape of a vibrating surface be inferred from its sound [67]? This paper poses a variation: “*Can one see the band topology of a wavefunction in its charge density?*” Naïvely, the wavefunction amplitude should be agnostic to the phase information from which band topology is built. But the amplitude of a complex function is fixed by its phase near vortices or domain walls, where it is forced to vanish. The dark set makes this intuition precise, demonstrating that crystal symmetry converts band topology into exact zeros of the wavefunction. These zeros are the crystalline analogue of atomic nodes; Bloch states can be viewed as many-atom molecular orbitals, and the dark set comprises their generalised nodes. This represents a surprising result in group representation theory, and might be of broader relevance to the study of irreducible representations of finite groups.

The dark set allows symmetry-indicated topology to be read from the organisation of charge within the unit cell, but also determines the form factors through which electrons interact. In kagome metals, M states near a p -type VHS avoid each other by living on different sublattices, promoting the relevance of long-range Coulomb interactions, known to stabilise loop current orders [36–

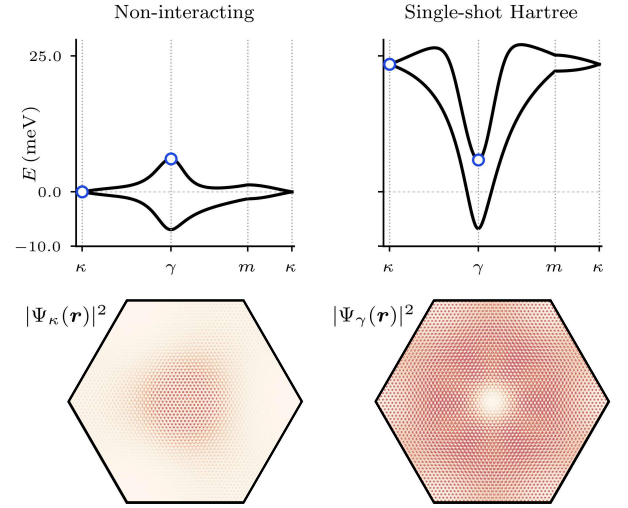


FIG. 5. **Band renormalisation in moiré graphene.** Top: non-interacting and Hartree-renormalised narrow bands of TBG near $\theta = 1.05^\circ$. The Γ states (bottom right) are forced-dark at the AA-stacked regions, where the K states (bottom left) are bright. The Hartree potential is strongest at the AA regions, strongly increasing the energy at K , but not at Γ where the wavefunction avoids the Hartree potential.

Similarly, the Γ and K states in TBG live in different regions of the unit cell as a consequence of their C_3 irreps, causing the Γ states to avoid the Hartree potential from the K states [53]. Thus, the same real-space structure that makes band topology visible can decide which interaction channels survive in topological materials. Wavefunction zeros therefore provide a bridge between three views of quantum materials that are usually separated: momentum-space topology, real-space spectroscopy, and correlated electronic order.

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Appendix

INTRODUCTION TO BAND REPRESENTATION THEORY

A symmetry g acts on a wavefunction $|\alpha\rangle$ via

$$\hat{U}_g|\alpha\rangle = \sum_{\beta} D_{\beta\alpha}(g)|\beta\rangle.$$

An *irreducible representation* (irrep) is the “smallest symmetry-closed space of states”; no change of basis can split it into smaller independent spaces which are each closed under all symmetries — equivalently, $D_{\beta\alpha}(g)$ cannot be block-diagonalised. A familiar example is the atomic $s, p, d, \dots$ orbitals: an s orbital is invariant under rotations, the p orbitals form a three-dimensional space mixed by rotations, and the d orbitals form a five-dimensional space. In group theory language, each such symmetry type is an irrep.

In a crystal, the continuous rotation group is reduced to a *point group*, so the symmetry labels become coarser than atomic angular momentum labels — e.g. on a triangular lattice, angular momentum is only conserved mod 3, and so an orbital transforming trivially under C_3 may contain both s - and f -wave components. The general statement is that functions can be classified as irreps of the point group, which are often denoted with *Mulliken notation* using a letter and subscript — e.g. A_{2g}, E_{1u} .

Bloch states can be understood using representation theory in both momentum and real-space; we begin by discussing the former. A *space group* operation $g = \{R_g|\mathbf{t}\}$ sends a Bloch state at crystal momentum $\mathbf{k}$ to $R_g\mathbf{k}$. Whereas in a translationally invariant system the only momentum invariant under rotations is $\mathbf{k} = 0$, in a crystal, momenta differing by a reciprocal lattice vector are equivalent. Hence, at *high-symmetry momenta* for which $R_g\mathbf{k}_* = \mathbf{k}_* + \mathbf{G}$, the wavefunction can be simultaneously diagonalised with the symmetry g , and the Bloch eigenstates transform as irreps of the symmetries which leave $\mathbf{k}_*$ invariant — referred to as the *little group*, $G_{\mathbf{k}_*}$,

$$\hat{U}_g|\psi_{\mathbf{k}_*,a}\rangle = e^{-i\mathbf{k}_*\cdot\mathbf{t}} \sum_b D_{ba}^{\rho}(g)|\psi_{\mathbf{k}_*,b}\rangle, \quad g \in G_{\mathbf{k}_*}.$$

The label ρ specifies the type of irrep; irreps can be fully classified by the *characters* $\chi_{\rho}(g) = \text{Tr } D^{\rho}(g)$ of the symmetry matrices which act on them.

Band-representation theory relates these momentum-space irreps to the real-space irreps and locations of the atomic orbitals which give rise to them. A *Wyckoff orbit* is a set of *Wyckoff positions* $\mathbf{r}_*$ which map to themselves under a subset of the symmetries, referred to as the *site-symmetry group* $G_{\mathbf{r}_*}$. A local orbital placed at $\mathbf{r}_*$ therefore transforms as an irrep of $G_{\mathbf{r}_*}$ — e.g. an s orbital at a C_3 centre transforms trivially, whereas a chiral p_+ orbital transforms with a factor $e^{2\pi i/3}$.

From orbitals $|\phi_{\mathbf{R},\alpha}\rangle$ one forms Bloch states,

$$|\psi_{\mathbf{k},\alpha}\rangle = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot(\mathbf{R}+\mathbf{r}_{\alpha})} |\phi_{\mathbf{R},\alpha}\rangle, \quad (\text{E1})$$

where $\mathbf{r}_{\alpha}$ is the position of the orbital within the unit cell. At $\mathbf{k}_*$, a symmetry operation $g \in G_{\mathbf{k}_*}$ acts on Eq. (E1) through two ingredients. First, it rotates or reflects the local orbital $|\phi_{\mathbf{R},\alpha}\rangle$ according to its $G_{\mathbf{r}_*}$ irrep. Second, it may move the orbital to an equivalent position in a neighbouring unit cell, contributing a Bloch phase via $e^{i\mathbf{k}_*\cdot(\mathbf{R}+\mathbf{r}_{\alpha})}$. This allows one to determine the $G_{\mathbf{k}_*}$ irrep implied by Eq. (E1) when $\mathbf{k} = \mathbf{k}_*$.

To take a simple example, consider s orbitals on two honeycomb sublattices located at positions $\mathbf{r}_{\pm}$. The s orbitals transform trivially under C_3 , i.e. transform trivially under the site symmetry group. However, under a C_3 rotation about the hexagon centre, the Bloch sum acquires a phase $e^{i\mathbf{k}_*\cdot(1-C_3)\mathbf{r}_{\pm}}$. At K , the phase is $e^{i\mathbf{K}\cdot(1-C_3)\mathbf{r}_{\pm}} = \omega^{\pm}$. Hence the two s orbital Bloch sums transform at K as the one-dimensional C_3 irreps with characters ω and ω^2 . At the opposite valley $\mathbf{K}' = -\mathbf{K}$ the phases are complex conjugated, while at Γ both phases are unity. Thus, when only C_3 is present, the induced band representation has irrep content $\Gamma : 1 \oplus 1, K : \omega \oplus \omega^2$, and $K' : \omega^2 \oplus \omega$. Another example — of s orbitals on a kagome lattice — is detailed in SM Sec. S7B.

This is the organising principle behind topological quantum chemistry and band-representation theory [5]. A set of localised Wannier orbitals generates a constrained pattern of irreps at high-symmetry momenta such as Γ, K, M . Comparing the irrep content of a group of bands with the catalogue of band representations gives information about their parent real-space description.

The irreps at high-symmetry momenta imply constraints on the ability to construct the band as a Fourier transform of some local orbital as in Eq. (E1). If the high-symmetry irreps of a group of bands cannot be obtained from symmetric exponentially localised Wannier orbitals, the bands have a *Wannier obstruction*, and are otherwise said to possess an *atomic limit*. If they can be obtained from localised Wannier orbitals only by placing the Wannier centres at positions displaced from the atoms, the bands have an *obstructed atomic limit*.

Symmetry-based indicators compare the observed irreps at high-symmetry momenta with those obtained from atomic limits, allowing inference of topological invariants such as the Chern number — e.g. in a C_3 symmetric two-dimensional insulator with a single occupied band,

$$e^{2\pi i C/3} = \xi_{\Gamma} \xi_K \xi_{K'},$$

where $\xi_{\mathbf{k}_*}$ is the C_3 eigenvalue of the occupied band at $\mathbf{k}_*$; thus $\xi_{\mathbf{k}_*}$ determine $C \bmod 3$. For an inversion-symmetric time-reversal invariant insulator with one occupied Kramers pair, the inversion eigenvalues $\zeta_{\mathbf{k}_*}$ at the time-reversal invariant momenta (TRIM) give

$$(-1)^{\nu} = \prod_{\mathbf{k}_* \in \text{TRIM}} \zeta_{\mathbf{k}_*},$$

where ν is the Kane-Mele $\mathbb{Z}_2$ index. The main text proves that momentum space irreps can be determined from *zeros of the wavefunction*, thus allowing inference of topological invariants via symmetry-based indicators.

DARK SETS OF 1H-TMDS

Let $\omega = e^{2\pi i/3}$ and denote the three C_3 centres by $1a = (0, 0)$, $1b = (\frac{1}{3}, \frac{2}{3})$, and $1c = (\frac{2}{3}, \frac{1}{3})$. The states retained in the three-band model of 1H-TMDs are even under the horizontal mirror, so the C_{3h} projector reduces to its C_3 part. At K , the local phases $(e^{-i\mathbf{K}\cdot\mathbf{t}_{C_3(1a)}}, e^{-i\mathbf{K}\cdot\mathbf{t}_{C_3(1b)}}, e^{-i\mathbf{K}\cdot\mathbf{t}_{C_3(1c)}})$ are $(1, \omega, \omega^2)$; at K' they are the complex conjugates $(1, \omega^2, \omega)$. For a state with C_3 eigenvalue ξ_K at the K -point,

$$m_{K,\mathbf{r}} = \frac{1}{3} \sum_{n=0}^2 (\vartheta_{K,\mathbf{r}} \xi_K)^n \quad (\text{E2})$$

Hence, $\mathbf{r}$ is symmetry-allowed precisely when $\vartheta_{K,\mathbf{r}} \xi_K = 1$. The TMD valence band has C_3 eigenvalues $\xi_\Gamma = 1$, $\xi_K = \omega$, and $\xi_{K'} = \omega^2$. Therefore

$$D_\Gamma = \emptyset, \quad D_K = \{1a, 1b\}, \quad D_{K'} = \{1a, 1b\}. \quad (\text{E3})$$

Thus the valley states are allowed only at the hollow centre $1c$, whereas the Γ state has no symmetry-enforced zero at the three C_3 centres.

For comparison, a chiral E' doublet at Γ would have

$$D_\Gamma(E') = \{1a, 1b, 1c\}. \quad (\text{E4})$$

DARK SETS OF THE HALDANE MODEL

Let O be the hexagon centre and A, B the two honeycomb sublattice centres. Their local C_3 phases at K $(e^{-i\mathbf{K}\cdot\mathbf{t}_{C_3(O)}}, e^{-i\mathbf{K}\cdot\mathbf{t}_{C_3(A)}}, e^{-i\mathbf{K}\cdot\mathbf{t}_{C_3(B)}})$ are $(1, \omega, \omega^2)$; at K' the phases are $(1, \omega^2, \omega)$.

As in the TMD case, a valley state with C_3 eigenvalue ξ has $\mathbf{r}$ symmetry-allowed precisely when $\vartheta_{K,\mathbf{r}} \xi = 1$. The dark sets are therefore

$$\begin{aligned} D_K(1) &= \{A, B\}, \quad D_K(\omega) = D_{K'}(\omega^2) = \{O, A\}, \\ D_{K'}(1) &= \{A, B\}, \quad D_{K'}(\omega) = D_K(\omega^2) = \{O, B\}, \end{aligned} \quad (\text{E5})$$

Hence, a honeycomb s orbital band has no symmetry-enforced C_3 -centre zero at Γ . At K , the hexagon centre is dark and exactly one atomic sublattice is bright. If the same sublattice is bright at K and K' , the total LDOS is dark on the opposite sublattice, and O . If different sublattices are bright at the two valleys, their total LDOS has only O dark.

DARK SETS OF THE BHZ MODEL

We evaluate the four Wyckoff positions $\mathbf{r}_{1a} = (0, 0)$, $\mathbf{r}_{1b} = (\frac{1}{2}, \frac{1}{2})$, $\mathbf{r}_{2c_x} = (\frac{1}{2}, 0)$, and $\mathbf{r}_{2c_y} = (0, \frac{1}{2})$ at $\Gamma = (0, 0)$, $X = (\pi, 0)$, $Y = (0, \pi)$, and $M = (\pi, \pi)$. The points $1a$

and $1b$ are C_4 centres — namely, they contain C_4 in their site symmetry group — at Γ and M , while $2c_x$ and $2c_y$ are only C_2 centres. When C_4 symmetry is broken, the notation changes as $2c_x \rightarrow 1b$, $2c_y \rightarrow 1c$, $1b \rightarrow 1d$.

For a Kramers pair with inversion eigenvalue $\zeta(\Lambda)$,

$$m_{\Lambda,\mathbf{r}_i} = 1 + e^{-2i\Lambda\cdot\mathbf{r}_i} \zeta(\Lambda) \quad (\text{E6})$$

at the C_2 centres $\mathbf{r}_i$, which are therefore dark when $e^{-2i\Lambda\cdot\mathbf{r}} \zeta(\Lambda) = -1$. In the BHZ model, $\zeta(\Gamma) = \text{sgn}(m+2)$, $\zeta(X) = \zeta(Y) = \text{sgn}(m)$, and $\zeta(M) = \text{sgn}(m-2)$. The C_2 phases $(e^{-2i\Lambda\cdot\mathbf{r}_{1a}}, e^{-2i\Lambda\cdot\mathbf{r}_{2c_x}}, e^{-2i\Lambda\cdot\mathbf{r}_{2c_y}}, e^{-2i\Lambda\cdot\mathbf{r}_{1b}})$ at X, Y, M are $(1, -1, 1, -1)$, $(1, 1, -1, -1)$, and $(1, -1, -1, 1)$.

At the C_4 centres $1a$ and $1b$, the selection rule depends on the C_4 characters. If the two members of the Kramers pair have C_4 eigenvalues χ_1, χ_2 , then

$$m_{\Lambda,\mathbf{r}} = \frac{1}{4} \sum_{a=1}^2 \sum_{j=0}^3 (\varphi_{\Lambda,\mathbf{r}} \chi_a)^j. \quad (\text{E7})$$

where $\varphi_{\Lambda,\mathbf{r}} = e^{-i\Lambda\cdot(1-C_4)\mathbf{r}}$. The s -like pair has $(\chi_1, \chi_2) = (1, 1)$, while the $p_\pm$ pair has $(\chi_1, \chi_2) = (i, -i)$. We find $\varphi_{\Gamma,1a} = \varphi_{\Gamma,1b} = 1$, while $\varphi_{M,1a} = 1$ and $\varphi_{M,1b} = -1$. Therefore the C_4 centres are dark at Γ for the $p_\pm$ irrep; at M , the plaquette centre $1b$ is always dark, and the site centre $1a$ is dark only for the $p_\pm$ irrep.

Combining the C_2 and C_4 projectors gives

$$D_\Gamma = \begin{cases} \emptyset, & m > -2, \\ \{1a, 1b, 2c_x, 2c_y\}, & m < -2, \end{cases} \quad (\text{E8})$$

$$D_M = \begin{cases} \{1b, 2c_x, 2c_y\}, & m > 2, \\ \{1a, 1b\}, & m < 2. \end{cases} \quad (\text{E9})$$

At X/Y the result is determined only by the sign of m :

$$m > 0: \quad D_X = \{1b, 2c_x\}, \quad D_Y = \{1b, 2c_y\}, \quad (\text{E10})$$

$$m < 0: \quad D_X = \{1a, 2c_y\}, \quad D_Y = \{1a, 2c_x\}. \quad (\text{E11})$$

Restricting to the two bond centres gives the inversion-clean reduction used in the main text. For $|m| < 2$, neither bond centre is dark at Γ or M . For $m > 2$, $D_\Gamma^{\text{bond}} = \emptyset$ and $D_M^{\text{bond}} = \{2c_x, 2c_y\}$; for $m < -2$ the two are exchanged, so $D_\Gamma^{\text{bond}} = \{2c_x, 2c_y\}$ and $D_M^{\text{bond}} = \emptyset$. At X and Y , the bond-centre dark sets depend only on the sign of m : for $m > 0$ one has $D_X^{\text{bond}} = \{2c_x\}$ and $D_Y^{\text{bond}} = \{2c_y\}$, while for $m < 0$ one has $D_X^{\text{bond}} = \{2c_y\}$ and $D_Y^{\text{bond}} = \{2c_x\}$.

For the two regimes plotted in the main text, both bond centres are dark at M in the trivial phase $m > 2$, while neither bond centre is dark at M in the quantum spin Hall phase $0 < m < 2$. The site and plaquette centres are not inversion-clean probes at Γ and M , because their stabiliser contains C_4 .

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