Substrate-induced topological minibands in graphene

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The honeycomb lattice sets the basic arena for numerous ideas to implement electronic, photonic, or phononic topological bands in (meta-)materials. Novel opportunities to manipulate Dirac electrons in graphene through band engineering arise from superlattice potentials as induced by a substrate such as hexagonal boron-nitride. Making use of the general form of a weak substrate potential as dictated by symmetry, we analytically derive the low-energy minibands of the superstructure, including a characteristic 1.5 Dirac cone deriving from a three-band crossing at the Brillouin zone edge. Assuming a large supercell, we focus on a single Dirac cone (or valley) and find all possible arrangements of the low-energy electron and hole bands in a complete six-dimensional parameter space. We identify the various symmetry planes in parameter space inducing gap closures and find the sectors hosting topological minibands, including also complex band crossings that generate a valley Chern number atypically larger than one. Our map provides a starting point for the systematic design of topological bands by substrate engineering.

I. INTRODUCTION

The hunt for materials with topological properties, originally rooted in two-dimensional quantum Hall systems [1], has been fueled by numerous proposals for materials with electronic topological bands [2–4] and has recently sparked ideas for engineered meta-materials hosting topological bands for electromagnetic [5–7] (photonic) or elastic [8, 9] (phononic) modes. Many of these proposals are based on the honeycomb lattice, which provides a natural host for topological phenomena through various types of engineering, from the (dynamical) Haldane model [10, 11] and cold atomic [13] systems, to designer dielectrics holding topological photons [14]. The topological properties in these systems arise from band crossings or Dirac cones. In time-reversal-symmetric systems, such cones appear in compensating pairs and topological features cancel out. Nevertheless, topological properties manifest in individual valleys or cones and are brought forward in the field of valleytronics [15–17]—as with topological materials, valleytronics can be engineered in non-electronic systems [18].

In this paper, we investigate a generic valleytronic system where the Dirac electrons of the cone are engineered via a weak hexagonal substrate potential, with a well-known realization of such a system given by placing graphene on hexagonal boron nitride (G-hBN). Symmetry considerations on the substrate potential then define a six-dimensional parameter space that describes all possible arrangements of minibands and their topological properties. Focusing on the six lowest electron and hole bands, the threefold symmetry of the scattering potential leads to a characteristic “1.5” Dirac cone deriving from three crossing bands as well as two strongly anisotropic two-band crossings. We discuss several pertinent examples for new topological band arrangements resulting from the atypical Berry curvatures generated by these crossings, including also situations with high valley Chern number.

While depositing graphene on a substrate can improve the electrical properties of the film [19–21], such simple manipulation also allows for the (deliberate) tuning of its spectral properties. An example that has received much attention recently is bilayer graphene with its flat bands at “magic twist-angles” [22–26], domain-wall induced edge states [27–30], and superconducting properties [31–33]. In this situation, the Dirac cones of both graphene layers contribute equally to the physical phenomena. In contrast, when graphene is placed on an insulating substrate, e.g., silicon-carbide (SiC) or boron-nitride (BN), the electronic states of the latter are separated far in energy. Consequently, only the Dirac cones of graphene have to be considered, with corrections induced by the substrate, such as a gap opening in the Dirac spectrum [34, 35]. In particular, including the misfit between the graphene lattice and the substrate lattice leads to a (“Moiré”) superstructure that generates more complex reconstructions of the Dirac cones into minibands [29, 36–38]: the scattering of the graphene electrons on such a threefold symmetric and weak substrate potential (e.g., G-hBN) naturally leads to the hybridization of backfolded cones that results in secondary gap openings. The latter give birth to conventional or even topological minibands [29, 39, 40] and constitute the main focus of the present work. The shape and character of these band arrangements depends sensitively on the substrate-induced potential; here, rather than focusing on specific lattice–substrate arrangements [29, 37, 39, 40], we provide a complete map relating the miniband structure with the scattering parameters of the substrate potential under weak coupling conditions.

Similar multiband engineering has attracted interest in recent years, starting with proposals to hybridize three (one Dirac cone plus a flat band) [41, 42] and four bands (a double-Dirac cone) [43] in photonic [14] or phononic [44, 45] metamaterials by exploiting properly tuned accidental degeneracies. While these degenerate multiband configurations reside at the Γ point, our three-band mixing occurs near the K-points of a Dirac material and involves three linear bands, corresponding
to what we call a 1.5 Dirac cone, in allusion to the double-Dirac cone of Refs. [14, 43–45]. Alternatively, the formation of what we call the 1.5 Dirac cones by the scattering of a Dirac fermion on a hexagonal substrate potential can be understood in terms of the formation of the new “three-fermions” of Ref. [46].

Depositing graphene on a substrate with hexagonal symmetry generates both (incommensurate) Moiré [47, 48] or (commensurate) grain-boundary [49, 50] superstructures. Below, we analyze how such a superstructure splits an individual Dirac cone into minibands, see Fig. 1(a). Exploiting that such a cone maps onto itself under the combined action of inversion (I) and time reversal (T), we can use symmetry arguments [36] to characterize the scattering potential. The latter then is described by six parameters that can be grouped into two sets of three TI symmetric (TIS) and three TI antisymmetric (TIAS) amplitudes, defining two three-dimensional parameter spaces. The main goal of the present work then is to find a systematic and complete map between the six-dimensional parameter space of symmetry-allowed scattering potentials and the ensuing miniband structure including its topological properties.

The three lowest electron and hole minibands derive from three backfolded cones that mix at the \( \kappa \) and \( \kappa' \) points of the mini-Brillouin zone, see Fig. 1(a). A purely TI-symmetric potential then splits the threefold degeneracies at the \( \kappa \) and \( \kappa' \) points into combinations of a single cone and a parabolic band—the mutual arrangement of the latter depends on the chosen parameters. Turning on a TI-antisymmetric component of the substrate potential leads to a splitting of the remaining degeneracy of the cones and frees the Berry curvatures previously hidden in the degeneracy points [51]. The Berry curvatures deriving from the 1.5 cone sum up to values \( \pm 1/4 \) for the top and bottom bands and averages to zero for the middle band, cf. numerical results in Ref. [39], quite different from the usual weight \( \pm 1/2 \) characterizing a conventional Dirac-like cone. Our analytic derivation provides deeper insights into the origin of these reduced contributions to the Chern number. Finally, by proper tuning of parameters, we find values generating electron or hole bands that are gapped away from other bands—appropriate placement of the chemical potential within the minigap then allows for realizing topological valley physics [15, 16] with minibands. Furthermore, we find substrate configurations that generate such isolated bands with a network of Berry curvature with a higher-than-one Chern number.

In the following Sec. II, we set up our phenomenological model Hamiltonian describing an isolated cone of Dirac-like particles subject to a weak substrate potential with TI-symmetric \( D_3 \) and more general \( C_3 \) symmetries. We solve the problem analytically for the six low-energy electron and hole bands by folding back the neighboring unit cells in the Brillouin zone; more exact band-structure calculations are done numerically with 62 bands, i.e., including higher-order reciprocal vectors. In Sec. III, we analyze the miniband geometries for the \( D_3 \) and \( C_3 \) symmetric potentials, emphasizing the geometric arrangements of the bands with singlets and doublets at the \( \kappa \) and \( \kappa' \) points in the high symmetry \( D_3 \) case and the Berry-curvature maps characteristic of the low-symmetry \( (C_3, \text{TI-symmetry broken}) \) situation. The latter derive from multiple band crossings and we present an analytic calculation for the curvatures associated with the various bands. In Sec. IV, we present specific examples where the substrate potential produces isolated minibands (with well defined gaps separating bands) characterized by nontrivial Chern numbers. We summarize our work and conclude in Sec. V.

II. DIRAC-LIKE PARTICLES IN \( C_3 \) AND \( D_3 \) SYMMETRIC POTENTIALS

We study an effective model describing the low-energy physics of Dirac electrons subject to a weak hexagonal periodic potential. This situation is realized by the triangular Moiré pattern resulting when graphene is deposited on an insulating hexagonal substrate, such as boron-nitride. To do so, we consider a spinless Dirac-like particle described by a

FIG. 1. (a) High- and low-energy description of Dirac-like particles subject to a substrate potential. The large Brillouin zone (BZ) of the host material (left) generates Dirac cones at the \( K \)- and \( K' \)-points (dark orange). Selecting one of the latter (here a \( K \)-point) defines the new \( \gamma \) point of the mini-BZ (right) generated by the triangular substrate potential. The scattering of the Dirac-like particle by the substrate produces a periodic mirroring (light gray cones) of the original Dirac cone and leads to band-hybridization at the boundary of the first mini-BZ (light shaded red). The high-symmetry points \( \kappa \) and \( \kappa' \) of the mini-BZ produce threefold degeneracies and the hybridization of the associated bands through the substrate generates bands with tunable topological properties. (b) Electronic dispersion along the lines \( \gamma \rightarrow \kappa \rightarrow \mu \rightarrow \kappa' \rightarrow \gamma \rightarrow \mu \), with dotted orange lines referring to pristine graphene (dispersion backfolded to the mini-BZ; numbers indicate degeneracies) and black solid lines showing the dispersion for a finite scattering potential \( V(x) \) that lifts the degeneracies and opens gaps (we have chosen parameters \( \Delta = 0.1e_0 \) and \( m_0 = 0.13e_0m_0 \), \( m_s = 0.03e_0m_0 \); the red square delimits the region for the dispersions shown in Figs. 2 and 5). (c) The band energies near the \( \kappa \) and \( \kappa' \) points appear as projections of three equidistant points (shaded red triangle) on a circle of radius \( \delta \epsilon \) centered at \( \epsilon \) and rotated by \( \phi \); see Eq. (8).
pseudospinor with linear dispersion $T(k)$ moving in two dimensions in the presence of a weak periodic potential $V(x)$,

$$H = v \hbar k \cdot \sigma + \Delta \sigma_3 + \sum_{\ell = 1, \ldots, 5} V_G \epsilon^\ell \mathbf{G}^\ell \cdot x,$$  \hspace{1cm} (1)

where $\sigma_j$ denote Pauli isospin matrices, $v$ is the Fermi velocity, and we allow for a finite mass (or spectral gap) $\Delta$ which constitutes a TIAS parameter. We assume a smooth, threefold rotational-symmetric potential with only one set of long-wavelength amplitudes $V_G$, for the six reciprocal lattice vectors $G_\ell = G \left[ \cos(2\pi \ell/6), \sin(2\pi \ell/6) \right]$, $\ell = 0, \ldots, 5$. The reciprocal lattice constant $G = 4\pi/3L$, with $L$ the real-space periodicity, defines an energy scale $\epsilon_0$ via the minimal recoil momentum $G$ for elastic scattering,

$$\epsilon_0 = v \hbar G/2.$$  \hspace{1cm} (2)

We assume the lattice to be much larger than the mass $\Delta$ and the amplitudes $V_G$, of the potential. In building the Moiré pattern in the G-hBN system, the (approximate) periodicity $L(\theta) = [(r - 1)^2 - 4r \sin^2(\theta/2)]^{1/2}$ is determined by the ratio $r \geq 1$ of the lattice constants of graphene and the substrate, and their misfit angle $\theta$ [36, 37]; note, that we deal with a slightly incommensurate situation where the lattices do not match exactly on the distance $L$. An exact match can be obtained in twisted bilayer graphene and requires fine-tuning of the angle $\theta$ [52]. In the following, we ignore effects arising due to the quasi-periodicity appertaining to a Moiré pattern.

The eigenmodes of the kinetic part $T(k) + \Delta \sigma_3$ in the Hamiltonian (1) describe particles with dispersion

$$\epsilon^\pm(k) = \pm \sqrt{\hbar^2 k^2 + \Delta^2}$$  \hspace{1cm} (3)

and associated momentum eigenstates

$$|k, \pm\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{1 + \Delta/\epsilon^\pm(k)} e^{i \varphi(k)/2} \\ \pm \sqrt{1 - \Delta/\epsilon^\pm(k)} e^{i \varphi(k)/2} \end{pmatrix} |k\rangle,$$  \hspace{1cm} (4)

where $|k\rangle$ is a plane wave state with wave vector $k = (k_1, k_2)$. The phase $\varphi(k) = \arg(k_1 + i k_2)$ and signs $\pm$ refer to particle (+) and hole (−) bands, in the following specified by the index $s = \pm 1$.

The most general expression for the small scattering amplitudes $V_G$, respecting threefold rotational symmetry takes the form [36]

$$V_G = u_\ell + m_\ell \sigma_3 + a_\ell (\hat{\mathbf{z}} \times \mathbf{G}_\ell) \cdot \sigma_,$$  \hspace{1cm} (5)

where $u_\ell = u_s + (-1)^\ell i u_s$, $m_\ell = m_s + (-1)^\ell i m_s$, and $a_\ell = a_s + (-1)^\ell i a_s$, define three complex parameters with the hat $\hat{\cdot}$ referring to normalized units of unit amplitude. The real (imaginary) parts of the parameters define a potential that is even (odd) under real space inversion. While $u_\ell$ quantifies the overall amplitude of the potential landscape, $m_\ell$ describes a periodic modulation of the Dirac mass $\Delta$. The parameters $a_\ell$ are associated with a spatially periodic vector potential describing the action of an out-of-plane pseudomagnetic field with the same spatial periodicity as the (substrate) potential; in graphene, such a term can arise due to nonuniform strain [20]. Note that local $U(1)$ symmetry in the Hamiltonian allows one to eliminate the longitudinal component of this vector potential via a proper transformation of the wavefunction (see Appendix A); the parameters $a_\ell$ then describe the transverse component of the vector potential after fixing the gauge.

The various components of the Hamiltonian can be grouped into two sets that are defined through their transformation properties under the combined action of time-reversal and spatial inversion, the TI-symmetric (TIS) parameters $u_s, m_s, a_s$, and the TI-antisymmetric (TIAS) parameters $\Delta, u_s, m_s, a_s$ [36], the latter picking up a minus sign under the action of TI. Dropping the TIAS parameters enhances the structural symmetry group from $C_3 \times D_3$. Note that $T$ and $I$ by themselves are not good symmetries of the Hamiltonian (1), unless we include the host material’s second Dirac cone (e.g., at the time-reversed point $K'$, with the parameters $(-\Delta, u_s, -m_s, -m_s, -a_s, -a_s)$ for the case of a time-reversal-symmetric mass and potential).

Including the scattering by the potential $V(x)$, the free Dirac-like spectrum is folded back in reciprocal space, defining the Brillouin zone (BZ) shown on the right of Fig. 1(a). The band structure is obtained from diagonalizing the Bloch Hamiltonian

$$H(k) = \sum_{i,j} |k_{ij}\rangle T(k_{ij}) \langle k_{ij}| + \sum_{\ell = 0}^{5} |k_{ij} + G_\ell\rangle V_G \langle k_{ij}|,$$  \hspace{1cm} (6)

with $k$ restricted to the first Brillouin zone and $k_{ij} \equiv k + i G_0 + j G_1$, with $i, j$ integers, denoting the original position in reciprocal space; see top right in Fig. 1. Given a choice of scattering amplitudes, Eq. (6) can be diagonalized numerically [36] including a sufficiently large set of bands $(i, j) \in \mathbb{Z}^2$; see Fig. 1(b).

Alternatively, focusing on the lowest bands, useful insights can be gained from an analytic solution involving only mixing of the three neighboring cells sharing the $k$ point and the $k'$ point (equivalently, we denote the latter by $\zeta \kappa$, points, $\zeta = \pm 1$, with $k'$ equivalent to $-k$). Including scattering induced by the potential (5) between the unperturbed states $|\zeta \kappa + q, \pm\rangle$, $|\zeta (\kappa - G_0) + q, \pm\rangle$, and $|\zeta (\kappa - G_1) + q, \pm\rangle$, the many-band Bloch Hamiltonian (6) can be truncated to the lowest three electron ($s = 1$) and hole ($s = -1$) bands described by

$$H^\zeta_\kappa(q) = \begin{pmatrix} e_{\xi_0} & e_{\xi_1} & e_{\xi_s} & e_{\xi_j} \\ e_{\xi_2} & e_{\xi_3} & e_{\xi_*} & e_{\xi_j} \\ e_{\xi_4} & e_{\xi_5} & e_{\xi_*} & e_{\xi_j} \\ e_{\xi_6} & e_{\xi_*} & e_{\xi_*} & e_{\xi_j} \end{pmatrix},$$  \hspace{1cm} (7)

with the unperturbed energies $e_{\xi_j} = \epsilon^\zeta(\zeta \kappa + q_j)$ and matrix elements $V^\zeta_\kappa = (\zeta \kappa + q_j, \zeta [V \xi_0\zeta^* (\zeta (\kappa - G_0) + q_j, s), s)$, where $q_j = 2\pi j/3$, $j = 0, 1, 2$, are $2\pi/3$-rotated q-vectors.

Such a three-band degenerate perturbation theory provides a reliable analytical solution near the BZ boundary, while the band structure is given by the Dirac-like spectrum (3) near the $y$ point. By diagonalizing (7), we find that the energies for electrons and holes can be written in the form of projections of three points on a circle of radius $\delta \epsilon_\xi(q)$ centered around
the mean energy $\bar{\epsilon}_\zeta(q)$,

$$\bar{\epsilon}_\zeta(q) = \bar{\epsilon}_\zeta(q) + \delta\epsilon_\zeta(q) \cos[\phi_\zeta(q) + 2\pi\epsilon^{\text{sn}}/3]$$ (8)

for the three bands $n = 1, 2, 3$ arranged in ascending order of excitation energy; see Fig. 1(c). Here, the mean $\bar{\epsilon}_\zeta(q) = \Sigma_j \epsilon_\zeta/j/3$ derives from the unperturbed energies averaged over the $2\pi/3$-rotated $q$ vectors, while the radius $\delta\epsilon_\zeta(q) = 2(\Sigma_j(2(\Delta\epsilon_\zeta)^2 + |V_{ij}|^2)/3)^{1/2}$ involves the energy disbalance $\Delta\epsilon_\zeta = [\epsilon_\zeta - \bar{\epsilon}_\zeta]/2$. The offset angle $0 \leq \phi_\zeta \leq \pi/3$ is given by

$$\phi_\zeta(q) = \frac{1}{3} \cos^{-1} \left[ \frac{\text{Re}(\Pi_j V_{ij}) + 4 \Pi_j \Delta\epsilon_\zeta - \Sigma_j \Delta\epsilon_\zeta |V_{ij}|^2}{[\delta\epsilon_\zeta(q)/2]^3} \right]$$ (9)

and the integer $\epsilon^{\text{sn}} = s(n - 1/2) + 1/2$ ensures the proper band ordering. While the radius $\delta\epsilon_\zeta(q)$ defines the magnitude of the splittings, the phase $\phi_\zeta(q)$ determines their relative arrangements. The associated eigenfunctions can be found in a closed analytic form as well; see Appendix B.

The three-band mixing described by (7) determines the structure of the minibands near the corresponding edge of the Brillouin zone. In the absence of a scattering potential $V$, the three energies in Eq. (8) collapse to a triplet at $\zeta\kappa$ (i.e., $q = 0$). Deviations away from $\kappa$ are linear in $q$ and locally define three planes that derive from the cutting of the three original cones—these three planes define our 1.5 Dirac cone. A finite scattering potential $V$ lifts the threefold degeneracy near the $\zeta\kappa$ points; at the high-symmetry points, the splitting derives from the Hamiltonian (7) at $q = 0$.

$$H_\zeta^s = \begin{pmatrix}
\epsilon^s(\kappa) & -\frac{2}{\sqrt{3}} \Delta_{\zeta}^s & -\frac{1}{\sqrt{3}} \Delta_{\zeta}^s \\
\frac{2}{\sqrt{3}} \Delta_{\zeta}^s & \frac{1}{\sqrt{3}} \Delta_{\zeta}^s & \frac{2}{\sqrt{3}} \Delta_{\zeta}^s \\
-\frac{1}{\sqrt{3}} \Delta_{\zeta}^s & \frac{2}{\sqrt{3}} \Delta_{\zeta}^s & \epsilon^s(\kappa)
\end{pmatrix},
$$

with

$$\Delta_{\zeta}^s = 3/2 \text{Re}V_{\zeta}^s = \frac{3}{4}(-u_s + \zeta \sqrt{3} m_s + \zeta s \lambda_{20}),$$

$$\Delta_{\zeta}^{s*} = \sqrt{3} \text{Im}V_{\zeta}^s = \frac{\sqrt{3}}{2}(\zeta u_s + \sqrt{3} m_s + \zeta 2 a_s)$$ (10)

derived from the scattering amplitudes $V_{\zeta}^s(q = 0)$ (we assume a vanishing Dirac mass $\Delta = 0$, see Sec. III C for results with a finite $\Delta$). Diagonalizing $H_\zeta^s$, we find the energy splittings

$$\epsilon^{s\text{sn}}_{\zeta} |_{\text{singlet}} = \epsilon^s(\kappa) + \frac{2}{3} \Delta_{\zeta}^s,$$

$$\epsilon^{s\text{sn}}_{\zeta} |_{\text{doublet}} = \epsilon^s(\kappa) - \frac{1}{3} \Delta_{\zeta}^s \pm \frac{1}{2} \Delta_{\zeta}^{s*},$$ (11)

where the splittings $\Delta_{\zeta}^s$ and $\Delta_{\zeta}^{s*}$ are associated with the TIS parameters $u_s, m_s,$ and $a_s$ and the TIAS parameters $u_\Delta, m_\Delta,$ and $a_\Delta$, respectively.

In a TI-symmetric situation, we have $\Delta_{\zeta}^{s*} = 0$ and the original triplet splits into a singlet and a doublet separated by $\Delta_{\zeta}^s$. If $\Delta_{\zeta}^s > 0 (< 0)$, the singlet will be higher (lower) in energy than the doublet, which is equivalent to an offset angle $\phi_\zeta(0) = 0$ ($\pi/3$); in the following, we will denote these arrangements by $\Delta(\triangledown), \triangledown(\triangledown)$, corresponding to the red shaded triangles in Fig. 1(c). In the opposite case with only finite TIAS parameters, we find that $\Delta_{\zeta}^{s*} = 0$ and the triplet fully splits into singlets in a symmetric fashion. This splitting is controlled by $\Delta_{\zeta}^s$ and comes with the offset phase $\phi_\zeta(0) = \pi/6$ and thus will be denoted with the symbol $\triangledown$. A general TI-symmetry broken case will involve all parameters and leads to an interplay between the singlet-doublet splitting $\Delta_{\zeta}^s$ and the doublet splitting $\Delta_{\zeta}^{s*}$. In such a situation, the angle $\phi_\zeta(0)$ can assume any value. We summarize the above discussion in Table I.

A similar analysis can be done at the $\mu$ point, where it is sufficient to consider two bands only; the Hamiltonian mixing the corresponding states $|\mu, \pm\rangle$ and $|\mu, \pm\rangle$ takes the form

$$H_\mu^s \approx \left( \epsilon^s(\mu) \frac{1}{2} \hat{\Delta}^s \right),$$ (12)

where $\hat{\Delta}^s$ is the band gap at $\mu$ induced by the potential,

$$\hat{\Delta}^s = 2 s (a_s - i a_s) - 2 (m_s - i m_s).$$ (13)

Diagonalizing (12), we obtain the energy splitting at the $\mu$ point in the form

$$\epsilon^{s\text{sn}}_{\mu} |_{\text{doublet}} = \epsilon^s(\mu) \pm \frac{1}{2} |\hat{\Delta}^s|.$$ (14)

### Table I. Parameters driving the energy splittings $\Delta_{\zeta}^s$ and $\Delta_{\zeta}^{s*}$ at the $\zeta\kappa$ points. The symbols $\Delta, \triangledown, \triangledown$ indicate the arrangement of split energies, doublet below singlet when $\Delta_{\zeta}^s > 0$, doublet above singlet for $\Delta_{\zeta}^s < 0$, and full symmetric splitting for $\Delta_{\zeta}^s = 0$ and $\Delta_{\zeta}^{s*} \neq 0$, respectively. These arrangements are dictated by the offset angle $\phi_\zeta(0)$ [Eq. (9)].

| Parameters | $\Delta_{\zeta}^s$ | $\Delta_{\zeta}^{s*}$ | $\phi_\zeta(0)$ |
|------------|------------------|------------------|----------------|
| TIS $u_s, m_s, a_s$ | $> 0, < 0$ | $0$ | $0 (\Delta), \pi/3 (\triangledown)$ |
| TIAS $u_\Delta, m_\Delta, a_\Delta, \Delta$ | $0$ | $\neq 0$ | $\pi/6 (\triangledown)$ |
III. BLOCH BANDS ALONG $\kappa-\mu-\kappa'$

As illustrated in Figs. 2 and 5, the TI symmetric parameters split the triplet at $\kappa$ and $\kappa'$ into a doublet (with the doublet degeneracy protected by the TI symmetry) and an additional singlet, while the antisymmetric terms in $V$ additionally split the remaining doublet—it is the latter splitting that generates the topological properties of the minibands by breaking the TI symmetry.

A. $D_3$ symmetry

We first focus on the TI-preserving situation with $u_A = m_A = a_A = \Delta = 0$. The remaining TIS parameters define the 3D parameter space $(u_s, m_s, a_s)$ shown in Fig. 2. The four planes mark parameters for which residual triplet degeneracies remain at $\kappa$ and $\kappa'$, i.e., they signal singlet–doublet gap closures ($\Delta^\ast = 0$). These planes compartmentalize the three-dimensional parameter space into $n = 14$ regions with different characteristic band arrangements, seven of which are shown in the maps A to G in Fig. 2. Each of these maps is characterized by a different arrangement of singlets and doublets in the four $(\zeta, s)$ sectors ($\kappa$ versus $\kappa'$, electrons versus holes), with the singlet either above the doublet ($\Delta^\ast > 0$), $\Delta^\ast < 0$, $\Delta^\ast = 0$ or vice versa. The maps A to G show the situation with an arrangement $\nabla$ for positive energies at $\kappa'$ ($\Delta^\ast < 0$); the configurations with a $\Delta$ instead appear for $\Delta^\ast > 0$.

For a given point in the TIS parameter space, the $\nabla$ and $\Delta$ configurations at $\kappa$ and $\kappa'$ are smoothly related through the evolution of the angle $\phi^s$ (see Fig. 3). Configurations with the same singlet–doublet arrangement at $\kappa$ and $\kappa'$ ($\nabla$ or $\Delta$) as in case B have an intermediate level crossing with the phase $\phi^s$ continuously changing either from $\phi^s(0) = 0$ to $\pi/3$ and back to $\phi^s(0) = 0$ or from $\phi^s(0) = \pi/3$ and back to $\phi^s(0) = \pi/3$. Configurations that change the singlet–doublet arrangement as in case G ($\nabla$ or $\Delta$) have no intermediate level crossing and the phase evolves unidirectionally from $\phi^s(0) = 0$ to $\phi^s(0) = \pi/3$ or from $\phi^s(0) = \pi/3$ to $\phi^s(0) = 0$.

Tuning the TIS parameters across the plane associated with a given $\zeta$, $s$ inverts the corresponding singlet–doublet configuration ($\nabla \leftrightarrow \Delta$) by going through a gap closing and reappearing. As the gap vanishes at $\Delta^\ast = 0$, the radius $\delta \epsilon_0(0)$ of the circle in (8) goes through zero and the offset phase $\phi^s(0)$ flips by $\pi/3$. An example for such a gap closure and reappearing when going from the maps B to G in Fig. 2 is shown in Fig. 4. Note that the configuration $\nabla$ or $\Delta$ of B features an intermediate band crossing along $k-\mu-\kappa'$ while the configuration to $\Delta$ or $\nabla$ in G does not. Hence, while moving across the plane in parameter space, this intermediate crossing must continuously move into a higher band when passing through the triple degeneracy.

B. $C_3$ symmetry

Next, we address the TI-antisymmetric case, i.e., with finite TIAS parameters $u_A, m_A, a_A$ and vanishing TIS parameters $u_s = m_s = a_s = \Delta = 0$. This defines a second 3D space of antisymmetric parameters $u_A, m_A, a_A$ describing spectra at $\kappa$ and $\kappa'$ points, where the singlet in Eq. (11) remains unchanged while the doublet is split symmetrically away; see Fig. 5. Most interestingly, this gap opening induces finite Berry curvatures (see Sec. III D for a detailed analysis) in the $1.5$ cone and generates the curvature maps A to G shown in Fig. 5. Shown are the configurations with equivalent Berry curvatures in the $(\zeta, s) = (+, +)$ sector, i.e., for $\Delta^\ast \sim (u_A + 2a_A + \sqrt{3}m_A) > 0$; configurations with reverse...
Berry curvatures are realized for negative values $\Delta^{+,''} < 0$. Again, the four planes crossing at the origin define the locations of triple-degenerate bands at the $\kappa$ and $\kappa'$ points where bands rearrange when $\Delta^{+,''} = 0$. As before, the evolution of the spectra when moving between $\kappa$ and $\kappa'$ points and when changing the antisymmetric parameters across one of the four triplet-degenerate planes can be understood in terms of the rotation and inflation/deflation of the circle defining the energies in (8).

In general, we deal with the situation that is neither purely symmetric nor purely antisymmetric with respect to TI symmetry and thus we have to cope with all six TIS and TIAS parameters assuming finite values. We then have to consider the interplay of the two cases. As we have seen, the TIS terms give rise to doublet–singlet gaps, while the TIAS terms control the splitting of the doublet. The magnitude of both splittings is determined by the distance of the configuration point to a particular plane in the respective parameter space. Knowing the two points in the parameter spaces of Fig. 2 and Fig. 5 allows one to quickly determine the band configurations at the $\kappa$ and $\kappa'$ points as well as their associated Berry curvatures.

### C. Finite mass $\Delta$

In the above discussions of $D_3$- and the $C_3$-symmetric cases, we have assumed a vanishing Dirac mass $\Delta$. Relaxing this assumption to a situation where $\Delta$ is finite and of similar or smaller magnitude as the other $3 + 3$ parameters, we find two effects: first, a gap opening at the $\gamma$ point, freeing additional Berry curvature and allowing one to define an (Abelian) Berry curvature for each band (see Sec. III D). The periodic potential can perturbatively modify this mass gap, $\Delta \to \hat{\Delta} \approx \Delta + \Delta^{(3)}$; as the correction appears only in the third order of the scattering parameters,

$$\Delta^{(3)} = -3m_\rho \frac{m_\alpha^2 - 3m_\alpha^2 - (u_\alpha^2 - u_\mu^2) + 4(a_\alpha^2 - a_\mu^2)}{\epsilon_0^2} - 3m_\mu \frac{2u_\alpha u_\mu + 8u_\alpha a_\mu}{\epsilon_0^2},$$

the renormalization of the mass gap at $\gamma$ is small and can usually be neglected. Second, a finite mass $\Delta$ produces a (again small) correction in the band arrangement at the Brillouin zone edge. Interestingly, the previous classification of Figs. 2 and 5 remains quantitatively correct under proper replacement of the bare TIS and TIAS parameters with their (slightly) renormalized counterparts

$$\bar{u}_\alpha = u_\alpha + \alpha m_\alpha, \quad \bar{u}_\mu = u_\mu + \alpha m_\mu, \quad \bar{m}_\alpha = m_\alpha + \alpha u_\alpha, \quad \bar{m}_\mu = m_\mu + \alpha u_\mu,$$

and

$$\bar{a}_\alpha = a_\alpha \sqrt{1 - \alpha^2}, \quad \bar{a}_\mu = a_\mu \sqrt{1 - \alpha^2},$$

FIG. 3. Band structure for the lowest three conduction bands ($s = +$) near the BZ edge ($\kappa - \mu - \kappa'$) with TIS-symmetric parameters corresponding to the maps B and G in Fig. 2. (a) Band energies deriving from projections of three points on the circle (8); the corresponding triangle (light red shading) rotates with the offset angle $\phi(0)$, see Eq. (9), along the path $\kappa \to \mu \to \kappa'$ in reciprocal space. Two inequivalent situations are shown, with the same arrangement $\bigcirc$ between $\kappa$ and $\kappa'$ as featured in B and with an opposite arrangement $\bigtriangledown$ as in G. In the former case, the triangle undergoes a rotation from $\pi/3 \to 0 \to \pi/3$ along $\kappa \to \mu \to \kappa'$, while in the latter case it evolves unidirectionally $0 \to \pi/3$. (b) 3D illustration of the band structure near the BZ edge showing the nontrivial geometries of the band touchings at $\kappa$ and $\kappa'$ (light red open circles) and at $\mu$ (black open circle) for parameters as in the maps B and G of Fig. 2.

FIG. 4. Evolution of the lowest three conduction bands ($s = +$) near the BZ edge ($\kappa - \mu - \kappa'$) when going from the TIS-symmetric parameter map B to G via a straight line as shown in Fig. 2. The single–doublet splitting at $\kappa$ (inverted red triangle) shrinks to zero upon approaching the point X and opens up in an inverted geometry upon continuing towards G (red triangle). At the same time, the band crossing at $\mu$ in B (blue open circle) moves towards the $\kappa$ point (see cyan arrows). Passing through the triple degeneracy at $\mathbf{X}$, the band crossing moves further to higher bands as the parameters approach G.
FIG. 5. Doublet splittings at the $\kappa$ and $\kappa'$ points depending on the parameters $u_\alpha, m_\alpha, a_\alpha$ for the massless TI-antisymmetric situation and with vanishing parameters $\Delta, u_3, m_3, a_3$. Colored segments describe the local Berry curvature $\Omega^{sn}(k)$ [see Sec. III D] of the $n$-th electron and hole bands, with red (blue) denoting positive (negative) values, see $\Omega^{sn}$ color scale. The four planes in the central figure mark the points of threefold degeneracy at the $\kappa$ and $\kappa'$ points where gap closures allow for band rearrangements and exchange of Berry curvature (see color-code in A relating the four $(\zeta, s)$-sectors with the relevant planes for gap closure). The same color code as in Fig. 2 has been chosen, e.g., blue for $(\zeta, s) = (\nu, +)$, implying a corresponding exchange of the Berry curvature when going from B to D. The fractions $\delta C^n$ denote the integrated Berry curvatures for the lowest $(n = 1)$ electron and hole bands arising from the vicinity of the $\kappa - \mu - \kappa'$ points; adding the contribution $\delta C^n_\text{q} = \pm 1/2$ from the vicinity of the $\gamma$ point (not shown) provides the Chern number $C^n_\kappa = \delta C^n_\kappa + \delta C^n$ for the lowest bands. In B, the bands cross at $\mu$ and the Abelian Berry curvature is not well-defined.

where $\alpha \equiv \Delta/\epsilon^\kappa(k) \ll 1$. This result can be obtained by evaluating Eq. (10) with a finite but small $\Delta$. It should be noted, however, that in such a case the $D_\omega$-symmetry for states near the BZ boundary holds only approximately: while the doublet is no longer symmetry protected, the $\Delta$-induced splitting near the BZ edge will be at least an order of magnitude smaller than any other discussed gap contribution.

### D. Berry curvatures and Chern numbers

The breaking of either inversion or time-reversal symmetry in our single-valley model (1) allows for a finite Abelian 2D Berry curvature [54]

$$\Omega^{sn}(k) = i \sum_{s' \neq sn} \frac{(sn) \partial H \langle s'n' | \langle s'ns| \partial H |sn\rangle - (1 \leftrightarrow 2)}{[\epsilon^{sn} - \epsilon^{s'n}]/2}, \quad (17)$$

where $sn$ is the band index with associated energy $\epsilon^{sn}$ and wave function $|ksn\rangle$ and $\partial_{k}H$ denote derivatives along $k_1$ and $k_2$; we have suppressed the variable $k$ in the right-hand side of Eq. (17). When bands do not cross, their Berry curvature is well-defined and we can assign a Chern number

$$C^{sn} = \frac{1}{2\pi} \int_{BZ} d^2 \kappa \Omega^{sn}(k) \in \mathbb{N} \quad (18)$$
to each separate band $sn$. In the following, we determine the local Berry curvatures near the high-symmetry points $\gamma$, $\kappa$, $\mu$, and $\kappa'$ in reciprocal space and integrate their contributions to the Chern number. For that matter, the contribution for the lowest electron and hole bands at the $\gamma$ point involves a standard calculation [54]; the result is dominated by the Dirac mass $\Delta$ and results in a local Berry curvature

$$\Omega^\gamma_\kappa(q) = \frac{\hbar v_a}{2 \Delta} \frac{(\hbar v)^2 \Delta}{[\Delta^2 + (\hbar v)^2 q^2]^{3/2}} \quad (19)$$

where the wavevector $q$ denotes the deviation from the $\gamma$ point. The result (19) describes a smeared (by $\Delta/\hbar v$) $\delta$-function in 2D with weight 1/2 and hence contributes to the Chern number with

$$\delta C^{\gamma}_\kappa = (s/2) \text{sign} (\Delta) \quad (20)$$

1. Three-band crossings at $\kappa$ and $\kappa'$: 1.5 Dirac cones

In order to determine the Berry curvatures near the $\kappa$ and $\kappa'$ points, we study the three-band Hamiltonian (7) for a purely TIAS situation. A small-momentum expansion (with polar coordinates $q = (q \cos(\phi), q \sin(\phi))$) around $\kappa$ or $\kappa'$ provides the Hamiltonian

$$H^\kappa_\phi(q) \approx \begin{pmatrix} \hbar v q \cos(\phi) & \frac{i}{\sqrt{3}} \Lambda'' & -\frac{i}{\sqrt{3}} \Lambda'' \\ -\frac{i}{\sqrt{3}} \Lambda'' & \hbar v q \cos \left( \phi + \frac{2\pi}{3} \right) & \frac{i}{\sqrt{3}} \Lambda'' \\ \frac{i}{\sqrt{3}} \Lambda'' & -\frac{i}{\sqrt{3}} \Lambda'' & \hbar v q \cos \left( \phi + \frac{4\pi}{3} \right) \end{pmatrix}.$$  \quad (21)

where $z'' = \Delta^z''$ is the magnitude of the TIAS band splitting and we choose the zero of energy at the high-symmetry point $\epsilon^\kappa$, see Eq. (11). We restrict the sums in (17) to the three
minibands constituting the 1.5 Dirac cone and make use of the eigenenergies and eigenfunctions of the Hamiltonian (21); see Appendix B. With proper arrangement of terms and using symmetries, one arrives at the Berry curvatures

\[
\Omega^{\phi}(q) = \frac{\hbar^2 v^2}{\left[\left(\frac{2}{\sqrt{3}} \Delta''\right)^2 + (\hbar v)^2 q^2\right]^{3/2}} \Phi[\phi(q) + 2\pi s n/3],
\]

(22)

for the bands \( n = 1, 2, 3 \) with \( \phi(q) \) and \( s n \) defined above; see Eq. (9) (we suppress the indices \( \xi \) and \( s \)). The factor

\[
\Phi(\phi) = \frac{4}{\sqrt[3]{3}} \cos(\phi) / [1 + \cos(2\phi)]^3
\]

(23)
describes a threefold \( \varphi \)-dependent modulation of the Berry curvature. Furthermore, given the simpler form of Eq. (21), the angle \( \phi(q) \) reduces to

\[
\phi(q, \varphi) = \frac{1}{3} \arccos \left[ \frac{(\hbar v q)^3 \cos(3\varphi)}{\left[\left(\frac{2}{\sqrt{3}} \Delta''\right)^2 + \hbar^2 v^2 q^2\right]^{3/2}} \right].
\]

(24)
The integration of \( \Phi[\phi(q, \varphi) + 2\pi s n/3] \) over the angle \( \varphi \) generates the dependence of the Berry curvature on \( n \),

\[
\int_{0}^{2\pi} d\varphi \Phi(\phi(q, \varphi)) = \varepsilon^n \left[ (2\Delta'')^2 / 3 + (\hbar v)^2 q^2 \right],
\]

(25)

with \( \varepsilon^n = \text{sign}([1 + 2n \pi] n/3) \in \{-1, 0, 1\} \). As a result, the Berry curvature (22) assumes the form of a broadened (by \( \Delta'' / \hbar v \)) and warped 2D \( \delta \)-function of weight 1/4 (with the index \( s \) reinstalled),

\[
\delta C^\varepsilon \xi = (\varepsilon^n / 4) \text{ sign}(\Delta'' \xi)
\]

(26)

In Fig. 6, we show the dispersions of the three bands \( n = 1, 2, 3 \) at the \( \kappa \) point together with a Berry curvature map exhibiting a \( C_3 \) symmetric angular dependence. Such a Berry curvature map with total weights \( \pm 1/4 \) and zero for the top/bottom and middle bands has been found numerically [39]. Our analytical result provides additional insight on the origin of these weights: the distribution of the 1.5 Dirac cone Berry curvature can be understood as splitting the zero curvature at degeneracy into two parts \( 1/2 \) and \( -1/2 \) attributed to the top \( (n = 2, 3) \) and bottom \( (n = 1, 2) \) pairs of bands. The weight \( \pm 1/2 \) is again equally split between the pair constituents, such that the middle band ends up with a zero integrated curvature \( \delta C^\varepsilon_\xi = 1/4 - 1/4 = 0 \), while the top and bottom bands remain with a weight \( \delta C^\varepsilon_\xi = \pm 1/4 \) and \( \delta C^\varepsilon_\xi = \mp 1/4 \).

Above, we have discussed the novel situation of emergent Berry curvatures when splitting the 1.5 Dirac cones at the \( \kappa \) and \( \kappa' \) points. A different situation arises when the three bands crossing at these points is first split with a finite TIS parameter, see Fig. 3(b), leaving a singlet and a doublet at the \( \kappa \) and \( \kappa' \) points. The doublet then is associated with a conventional (warped) Dirac cone where a finite TIS parameter frees a conventional Berry curvature of integrated weight \( \pm 1/2 \).

FIG. 6. Band structures and associated Berry curvatures calculated in a small-momentum expansion around the high-symmetry points. (a) The 1.5 Dirac cone, deriving from three cutting cones at the \( \kappa \) and \( \kappa' \) point (see Fig. 1), contribute with \( \delta C^\varepsilon_\mu = (\varepsilon^n / 4) \text{ sign}(\Delta'' \xi) \) to the Berry curvature of the miniband; see also Ref. [39] for equivalent results found numerically. (b) The two bands (deriving from two cutting cones; see Fig. 1) approaching one another near the \( \mu \) point contribute with \( \delta C^\varepsilon_\mu = (\varepsilon^n / 2) \text{ sign}(\Delta'' \xi) \) to the Berry curvature of the Bloch band.

2. Two-band crossings near \( \mu \): anisotropic Dirac cone

The second nontrivial contribution to the Berry curvature arises from the two-band splitting near the \( \mu \) point; see Fig. 6. While in Fig. 5 B the two bands \( n = 1, 2 \) (in ascending order of excitation energy) cross in \( \mu \), in a more general situation, these bands split and free a Berry curvature that resides a finite distance \( \delta q \) away from the \( \mu \) point; see Figs. 5 A, C, D, F as well as Fig. 6. In order to derive the Berry curvature for this situation, we again employ a small-momentum expansion with \( q = (q_1, q_2) \) measured with respect to the point \( \mu = G_0 / 2 = (G / 2, 0) \) in reciprocal space. Including both TIS and TIS parameters, we find the characteristic two-band anisotropic
Dirac Hamiltonian

\[ H^I_\mu(q) = \frac{\hbar}{2} \left( q_1 + q_2^2/G \right) + \frac{1}{2} \Delta + \hbar q_2 \epsilon e^{i\phi} \left( q_1 + q_2^2/G \right) \]  

(27)

where \( G \) is again the reciprocal lattice constant and we chose the zero of energy at \( \epsilon' = 0 \). We see that the substrate potential defines the gap \( \Delta \) and the renormalized velocity \( \tilde{v} \) along \( q_2 \) via \[ \tilde{\Delta} = 2s(a_s - i a_s + 2(m_s - i m_a), \quad \hbar \tilde{v} \epsilon e^{i\phi} = 2i(u_s + i u_a). \]

A straight-forward evaluation of Eq. (17) using the eigenenergies and eigenfunctions of (27), see Appendix B, results in the Berry curvatures \[ \Omega^{\mu}(q) = \frac{\epsilon^n}{2} \frac{\hbar v \hbar \tilde{\Delta}}{\left( \tilde{\Delta}^2 + (\hbar v)^2 q_1^2 + (\hbar \tilde{v})^2 (q_2 - \delta q)^2 \right)^{3/2}} \]  

(28)

where \( \tilde{\Delta} = \tilde{\Delta}' = (sa_s - m_s) \sin \theta - (sa_s - m_s) \cos \theta \) is the minimal gap displaced from the \( \mu \) point by \( \hbar \tilde{v} \delta q = (sa_s - m_s) \sin \theta - (sa_s - m_s) \cos \theta \) along the \( q_2 \)-direction, i.e., towards the \( \kappa \) or \( \kappa' \) point. The Berry curvature Eq. (28) assumes the form of an anisotropically broadened 2D \( \delta \)-function with weight \( n/2 \), see Fig. 6; in the limit \( \Delta \to 0 \), it approaches the 2D \( \delta \)-function \[ \Omega^\mu(q) \to (\epsilon^n/2) \sin(\tilde{\Delta}) \delta(q_1) \delta(q_2 - \delta q). \]

The integration of (28) thus contributes a term \[ \delta C^\mu_\gamma = (\epsilon^n/2) \sin(\tilde{\Delta}). \]  

(29)

As \( \delta q \) becomes large, the curvatures at \( \kappa \) and \( q_2 - \delta q \) start overlapping and our approximations break down. Nevertheless, the contributions still add, until a gap closure intervenes when \( \delta q = G/2 \sqrt{3} \) (i.e., the minimal gap from \( \mu \) passes through the \( \kappa \) point) and the Berry curvatures originating from the \( \mu \) point get redistributed between the second and third band.

The Chern number of the individual minibands is obtained by adding the contributions from the \( \gamma, \kappa, \kappa' \), and \( \mu \) points. Focusing on the lowest electron and hole bands (with \( n = 1 \)), we first define the contribution \( \delta C^\gamma = \delta C^\mu_\gamma + \delta C^\mu_\kappa + \delta C^\mu_\kappa' \) arising from the vicinity of the \( \kappa \) \( \kappa' \) points, with \( \delta C^\mu_\kappa = \pm 3/2 \) and \( \delta C^\mu_\kappa' = \pm 1/4 \) and the factor 3 arising from the three \( \mu \) points in the first BZ. These contributions then add up to values \( \delta C^\gamma \in \{ \pm 1/2, \pm 3/2 \} \) and are shown in Fig. 5 for the various maps \( A \to G \). Adding the contribution \( \delta C^\mu_\gamma = \pm 1/2 \) from the \( \gamma \) point, we can reach values \( C^\gamma \in \{ 0, \pm 1, \pm 2 \} \) for the Chern numbers of the lowest excitation bands.

In the above discussion, we have focused on a single Dirac cone deriving, e.g., from an original \( K \)-point; adding a time-reversed cone at \( K' \) then adds the same bands but with opposite Berry curvatures such that the total Berry curvatures add up to zero (note that for a graphene derived system it is always the inversion symmetry that breaks the Tl symmetry). In this situation, nontrivial topology manifests itself in valley physics [15, 16]; only upon breaking of time-reversal symmetry can the Berry curvatures of separate cones be decoupled and overall topological effects be realized.

\[ \begin{array}{c|c|c|c|c|c|c|c} \hline \text{(T+I)-symmetric} & \text{(T+I)-antisymmetric} \\
\hline u_s & m_s & a_s & u_s & m_s & a_s & [e_0] & C^+ \ \\
\hline (a) & 0 & 0 & 0 & -0.1 & 0 & 0 & 0 \ \\
(b) & 0 & 0 & 0 & 0 & 0.1 & 0 & 1 \ \\
(c) & 0 & 0 & 0.1 & -0.05 & 0 & 0 & 1 \ \\
(d) & 0.2 & 0 & 0 & -0.12 & 0 & 0 & 2 \ \\
\hline \end{array} \]

TABLE II. TIS and TIAS parameters for several topological band insulators involving the lowest electron and hole-type minibands and resulting Chern numbers \( C^+ \) and \( C^- \). The \( \gamma \) point is gapped with a mass \( \Delta = 0.1 e_0 > 0 \). The associated Berry curvatures are shown in Fig. 7.

IV. TOPOLOGICAL VALLEY INSULATOR FROM FILLED MINIBANDS

In order to realize topological (valley) physics [15, 16] with surface-induced minibands, we have to tune the \( 3 \times 3 \times 1 \) TIS, TIAS, and mass parameters in (1) such as to generate isolated bands with finite Chern numbers and place the Fermi level near the \( \mu \) point. The flatness of the bands along the \( \mu \) point get redistributed between the second and third band.

The Chern number of the individual minibands is obtained by adding the contributions from the \( \gamma, \kappa, \kappa' \), and \( \mu \) points. Focusing on the lowest electron and hole bands (with \( h = 1 \)), we first define the contribution \( \delta C^\gamma = \delta C^\mu_\gamma + \delta C^\mu_\kappa + \delta C^\mu_\kappa' \) arising from the vicinity of the \( \kappa \) \( \kappa' \) points, with \( \delta C^\mu_\kappa = \pm 3/2 \) and \( \delta C^\mu_\kappa' = \pm 1/4 \) and the factor 3 arising from the three \( \mu \) points in the first BZ. These contributions then add up to values \( \delta C^\gamma \in \{ \pm 1/2, \pm 3/2 \} \) and are shown in Fig. 5 for the various maps \( A \to G \). Adding the contribution \( \delta C^\mu_\gamma = \pm 1/2 \) from the \( \gamma \) point, we can reach values \( C^\gamma \in \{ 0, \pm 1, \pm 2 \} \) for the Chern numbers of the lowest excitation bands.

In the above discussion, we have focused on a single Dirac cone deriving, e.g., from an original \( K \)-point; adding a time-reversed cone at \( K' \) then adds the same bands but with opposite Berry curvatures such that the total Berry curvatures add up to zero (note that for a graphene derived system it is always the inversion symmetry that breaks the TI symmetry). In this situation, nontrivial topology manifests itself in valley physics [15, 16]; only upon breaking of time-reversal symmetry can the Berry curvatures of separate cones be decoupled and overall topological effects be realized.
and thereby generates the curvature network illustrated in Fig. 7 (d). Note that, with this choice of parameters, the Berry curvature near the $\kappa$ and $\kappa'$ points derives from the $\mu$ point and accumulates a total valley Chern number $C^+ = 2$. An alternative realization of such a Berry curvature network with $C^+ = 2$ has been found in Ref. [29] for spontaneously strained graphene on hBN, however, without a protecting minigap. Within our formulation, such a strain-induced situation is captured by an additional finite $a_\kappa$ parameter, e.g., for parameters $\Delta = 0.1 \epsilon_0$, $u_s = 0.2 \epsilon_0$, $a_\kappa = 0.12 \epsilon_0$, we obtain a similar Berry curvature network as in Fig. 7(d) for an isolated band with a Chern number $C^+ = -2$.

V. SUMMARY AND CONCLUSION

In the present paper, we have subjected a Dirac-like particle to a periodic substrate potential and have calculated the ensuing band structure as well as its topological properties. Within our phenomenological approach, the model Hamiltonian involves the Fermi velocity $v$ of the Dirac-like particle, possibly a finite (TI-antisymmetric) mass $\Delta$ opening a gap at the $\gamma$ point, and $3 + 3$ TI-symmetric (TIS) and TI-antisymmetric (TIAS) parameters opening up gaps at the $\kappa$, $\kappa'$, and $\mu$ points. While TIS parameters leave a cone at the $\kappa$ and $\kappa'$ points, these band touchings are lifted by the TIAS parameters and a finite Berry curvature emerges at the $\gamma$ (due to a finite $\Delta$) as well as at the $\kappa$, $\kappa'$, and $\mu$ points (due to the TI-antisymmetric potential part). Such a system opens the possibility for deliberate miniband engineering and tuning of the Dirac material between different (valley) topological phases.

The phenomenological Dirac-like model described in this paper involves a single Dirac cone—in reality, such a model originates from a microscopic bandstructure where the microscopic lattice generates the effective low-energy Dirac-like dispersion, while the periodic substrate potential defines a secondary or miniband structure. Microscopic time-reversal symmetry then generates a partner valley that compensates the Berry curvatures of the original Dirac cone. The topological properties of the Dirac material then are reduced to valley-specific features that have to be brought to manifest through special measures [17], e.g., via exploiting the valley Hall effect in a nonlocal conductance measurement as proposed in Refs. [16 and 39] and measured in Refs. [56]. While this type of (bulk) measurement probes the valley Berry curvature, other techniques, such as scanning tunneling spectroscopy, attempt to image topological edge states; this latter technique has been successfully applied to states associated with the main gap in graphene bilayers [28, 30]. In photonic systems [7] designing the edge and boundary termination is easier such that (valley) edge states can be imaged directly [57–60].

The realization of valley-topological physics through substrate-assisted miniband engineering involves proper tuning in a high-dimensional parameter space. Not only does one require a proper set of TIAS parameters bringing forward Berry curvatures with finite Chern numbers, in addition, the topological minibands have to be isolated from the other bands through proper gaps. Our analysis of TIS and TIAS parameter-spaces summarized in Figs. 2 and 5 provides a systematic overview of possible arrangements of miniband structures for the lowest bands in the vicinity of the $\kappa$, $\kappa'$, and $\mu$ points. Our specific examples in Fig. 7 demonstrate that isolated mini-bands with nontrivial Chern numbers can be achieved in principle. The next important step in a program aiming at substrate-assisted topological mini-band engineering then has to establish the connection between the phenomenological and microscopic parameters describing real band electrons subject to a substrate potential. Inspiration for the solution of this task can be gained from several principles: the TIS mass parameter $\Delta$ derives from sublattice asymmetry [34] breaking inversion symmetry, the potential parameters $u$ can be engineered with an electrostatic top-gate pattern [61, 62], finite mass parameters $m$ derive from a modulated sublattice asymmetry [36, 37], and gauge field parameters $a$ are induced by bond modulations, e.g., through strain [20, 29, 63]. More detailed analysis then involves realistic bandstructure calculations that pose a challenging problem given the large supercell of Moiré or grainboundary structures in real systems. Alternatively, optically engineered atomic crystals [13, 64] and optical waveguide arrays [7, 60] may provide another arena for
the implementation of topological minibands.

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Appendix A: Local $U(1)$ symmetry and transverse gauge

For the reader’s convenience, we briefly elaborate on the role of gauge freedom and gauge fixing in the model of a Dirac-like particle elastically scattered on a static potential [36]. For this purpose, let us consider the Dirac particle minimally coupled to a vector potential $A(x) = (A_1(x), A_2(x))$, i.e.,

$$H = v \left[ \hbar k + A(x) \right] \cdot \sigma + \Delta \sigma_3,$$  \hspace{1cm} (A1)

where $v$, $k$, $\sigma$ and $\Delta$ are defined in the main text, see Eq. (6). The vector potential can always be decomposed into longitudinal and transverse parts, i.e., $A(x) = A_\parallel(x) + A_\perp(x)$ with $\nabla \times A_\parallel(x) = 0$ and $\nabla \cdot A_\perp(x) = 0$. We can furthermore express these components through scalar functions, i.e.,

$$A_\parallel(x) = \nabla a_\parallel(x), \quad A_\perp(x) = \hat{\xi} \times \nabla a_\perp(x).$$  \hspace{1cm} (A2)

The vector potential $A(x)$ can have different physical origins, such as the presence of electromagnetic fields. However, in G-hBN it arises due to the proximity of the substrate layer even in absence of external fields. The (pseudo) magnetic field associated with the vector potential is given by

$$B_{\text{pseudo}} = \nabla \times A(x) = \nabla^2 a_\perp(x) \hat{\xi}. \hspace{1cm} (A3)$$

We are allowed to make the unitary transformation $U(x) = e^{-i a_\parallel(x)}$ without changing the physics of our system. This is our local $U(1)$ gauge freedom. The identity

$$U^\dagger(x) [-i \nabla] \cdot \sigma \ U(x) = [-i \nabla - \nabla a_\parallel(x)] \cdot \sigma$$  \hspace{1cm} (A4)

then readily implies that the transformation $U(x)$ removes the longitudinal component $A_\parallel(x)$ of the vector potential from the Hamiltonian,

$$U^\dagger(x) \ H \ U(x) = v [ \hbar k + A_\perp(x)] \cdot \sigma + \Delta \sigma_3$$  \hspace{1cm} (A5)

We conclude that whenever a term of the form $A(x) \cdot \sigma$ is present in the Hamiltonian of spinless non-interacting Dirac-like particles, we can remove its longitudinal part through a suitable gauge transformation.

Appendix B: Topological minibands

1. 2D Abelian Berry curvature

For a given Hamiltonian $H(k)$ parametrized by the crystal momentum $k = (k_1,k_2)$ with eigenfunctions $|n(k)\rangle$ and eigenenergies $\epsilon^n(k)$, we can define the 2D Abelian Berry curvature as

$$\Omega^n(k) = \left[ \nabla \times A^{\parallel}(k) \right]_3$$

$$= \left[ \nabla \times (n(k) \nabla n(k)) \right]_3$$

$$= \partial_1(n(k)\partial_2|n(k)\rangle) - \partial_2(n(k)\partial_1|n(k)\rangle).$$  \hspace{1cm} (B1)

However, a major drawback of this expression is that it involves taking derivatives of the wavefunctions. In practice, this way of calculating the Berry curvature quickly becomes intractable. In some cases, this difficulty can be overcome by trading the derivatives for sums over all bands containing matrix elements with derivatives of the Hamiltonian and an energy denominator. [54]

$$\Omega^n(k) = i \sum_{n' \neq n} \frac{\langle n | \partial_{k_j} H(k)|n'\rangle \langle n'| \partial_{k_j} H(n)|n\rangle - (1 \leftrightarrow 2)}{[\epsilon^n - \epsilon^{n'}]^2},$$  \hspace{1cm} (B2)

where we have suppressed the $k$ dependence on the right-hand side in our notation and we have made use of the identity $\langle n | \partial_{k_j} H(k)|n'\rangle = (\partial_{k_j} n|n'\rangle (\epsilon_n - \epsilon_{n'})$ for $n \neq n'$.

2. Three-band crossing: 1.5 Dirac cone

The three energy bands $(n = 1, 2, 3)$ of the effective Hamiltonian (21) describing a fully hybridized three-band crossing can be obtained by solving the cubic characteristic equation. In this case, we find

$$\epsilon^n(q, \varphi) = \sqrt{2(\Delta'v)^2/3 + (\hbar v q)^2 \cos(\phi^n(q, \varphi))},$$

$$\phi^n(q, \varphi) = \frac{1}{3} \arccos \frac{[\hbar v q]^2 \cos(3\varphi)}{[(2\Delta'v)^2/3 + (\hbar v q)^2]^{3/2}} + 2\pi \ell^n/3, \hspace{1cm} (B3)$$

where $\ell^n = s(n-1/2)+1/2$ (as in the main text). The associated unnormalized eigenvectors can be found to be

$$|n(q, \varphi)\rangle = \left( 1 + \chi^n(q, \varphi + 2\pi/3) \right) / \left( 1 - \chi^n(q, \varphi) \right),$$  \hspace{1cm} (B4)

where $\chi^n(q, \varphi) = i [\hbar v q \cos(\varphi) - \epsilon^n(q, \varphi)] / (\Delta'/\sqrt{3})$. The Berry curvature (22) for each band can then be obtained by evaluating Eq. (17), which requires some care in how to arrange the various terms and the exploitation of symmetries.

3. Two-band crossing: Anisotropic Dirac cone

A simple two-spinor rotation

$$U = e^{i(\pi/2+\theta) \sigma_1/2} . e^{i(\pi/2) \sigma_2/2} \hspace{1cm} (B5)$$
and substraction of $\hbar v q^2 / G$ (irrelevant for the discussion of band topology) brings the effective Hamiltonian (21) into a form where the anisotropic Dirac Hamiltonian becomes manifest,

$$U^\dagger H(q)U = \begin{bmatrix} \tilde{\Delta} & \hbar v q_1 - i \hbar (q_2 - \delta q) \\ \hbar v q_1 + i \hbar (q_2 - \delta q) & -\tilde{\Delta} \end{bmatrix}, \quad (B6)$$

where $\theta$, $\tilde{\Delta}$, $\tilde{v}$ and $\delta q$ are defined in the main text before and after Eq. (28). The corresponding energy bands ($n = 1, 2$) can be readily found to be

$$e^n(q) = e^n s(2n - 3) \sqrt{\tilde{\Delta}^2 + (\hbar v q_1)^2 + (\hbar \tilde{v})^2 (q_2 - \delta q)^2}, \quad (B7)$$

where $e^n = s(2n - 3)$ (as in the main text). In the rotated basis of Eq. (B6), the associated normalized eigenvectors are

$$|n(q)\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} \sqrt{1 + \Delta/\epsilon_\pm(q)} e^{-i \varphi(q)/2} \\ \epsilon^{n} \sqrt{1 - \Delta/\epsilon_\pm(q)} e^{i \varphi(q)/2} \end{bmatrix}, \quad (B8)$$

where $\varphi(q) = \text{Arg}(q_1 + i (\tilde{v}/v) q_2)$, similar to Eqs. (3) and (4). The Berry curvature (28) for an anisotropic cone can then be obtained by evaluating Eq. (17).

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