Designer Spin-Orbit Superlattices: Symmetry-Protected Dirac Cones and Hot Spots of Spin Berry Curvature in 2D van der Waals Metamaterials

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The emergence of strong relativistic spin-orbit effects in low-dimensional systems provides a rich opportunity for exploring unconventional states of matter. Here, we present a route to realize highly tunable relativistic band structures based on the lateral patterning of proximity-induced spin-orbit coupling (SOC). The concept is illustrated on a 1D patterned graphene heterostructure, where the periodic spatial modulation of SOC is shown to give rise to a rich mini-band structure with massless and massive Dirac bands carrying large Berry curvature. The envisaged systems support robust spin Hall responses driven by the quantum geometry of mini-bands, which can be tailored through metasurface fabrication methods and twisting effects. These findings suggest new pathways to 2D quantum material design and low-power spintronic applications.

The intertwining of orbital and spin degrees of freedom underpin a wealth of phenomena, from the formation of topological insulators to the spin Hall effect of light [1–7]. In condensed matter systems, spin-orbit coupling (SOC) is a relativistic interaction due to the motion of electrons in the electric field of the crystal lattice, which can yield spin-dependent band structures and Berry-curvature effects that strongly influence the electrodynamics of quasiparticles [8, 9]. Because the Berry curvature flux encodes global topological invariants (such as the Chern number for quantum anomalous Hall insulators), SOC is also a key mechanism behind quantized transport in 2D and 3D topological phases of matter [10, 11].

Broken symmetries alter the spin-orbital character of electronic states [12, 13], and therefore provide pathways by which to realize novel spin phenomena. Among these, the emergence of spin textures in spin-orbit-coupled systems with broken spatial inversion symmetry has generated enormous excitement in the fields of spintronics and magnonics recently [14, 15]. Owing to a close interplay of spin, lattice (pseudospin), and orbital degrees of freedom, SOC manifests both in real and momentum spaces—spinmomentum locking of spin-split Fermi surfaces [16–18], magnetic skyrmions [19–21], and persistent spin helices [22–24] are prominent examples—and forms the basis of several transport effects of fundamental and practical interest. Chief among these is the current-driven spin polarization that occurs in non-magnetic conductors with nontrivial spin textures, such as spin-momentum-locked Rashba interfaces and topological surfaces [25-27]. The ensuing net spin polarizations are often large (allowing current-induced magnetization switching of ferromagnets [28–30]) and tend to lie perpendicularly to the applied electric field owing to the tangential nature of conventional Rashba-type spin textures. Moreover, recent studies have found that the net spin orientation can be tuned in chiral materials boasting more exotic spin textures due

to fully broken reflection symmetries [31–34], which has the potential to unlock unconventional spin-orbit torques [35–37].

Likewise, the rich landscape of spin Hall effects (SHEs) reflects the symmetries underlying spin-orbit-coupled matter [38]. Of recent and growing interest is the SHE in vertical heterostructures built from graphene and 2D semiconductors [39]. In these systems, the interfacial breaking of point-group symmetries leads to two main types of SOC that can be either induced or greatly enhanced via proximity effects: the sublattice-staggered SOC (responsible for the valley-Zeeman effect) and the more familiar Rashba SOC [40–42]. Beyond featuring an exceptionally high degree of SOC tunability via strain and twisting effects [43–48], proximitized 2D crystals support a robust extrinsic SHE driven by scalar impurities, having no counterpart in other, non-Dirac 2D systems [49] (for a recent review see Ref. [42]). Such symmetrybreaking effects are also of ubiquitous importance for 2D quantized transport [50-53], as well as for metallic anomalous Hall and magnetic spin Hall phases [54, 55].

Despite this, most theoretical work so far has focused on *translation invariant* spin-orbit fields that reflect the periodicity of the underlying crystal structure, since this is the most conspicuous case. An interesting exception is the modulation of the strength of Rashba and Dresselhaus SOC induced in quantum-wire setups, previously explored in the context of spin-transistor devices [56–58]. Inspired by recent advances in the realization of artificial Dirac band structures in graphene with 1D superlattice potentials [59-61], the purpose of this work is to show that the quantum geometry and electrodynamic response of 2D materials can be engineered via synthetic spin-orbit fields created by a metasurface. Our proposal, outlined in Fig. 1(a), leverages proximity-induced effects between atomically thin crystals to engender effective spin-orbit fields with periodicity $a_{\rm S}$ much greater than the lattice scale, which we call *super-spin-orbit fields* (SSOFs). We envision that the long-wavelength modulation of the spinorbit field acting on charge carriers can be achieved by placing graphene on a patterned high-SOC substrate, akin to the patterning of electrostatic potentials in a lateral graphene superlattice [59–61] (other possibilities are discussed below). As we shall see, the envisaged synthetic SSOFs not only lead to the formation of mini-bands, but remarkably also impact their underlying quantum geometry, yielding a number of interesting and useful effects.

Setting the scene.—To model the electronic properties of a graphene sheet subject to a proximity-induced SSOF, we employ a continuum low-energy description based on the Weyl-Dirac Hamiltonian [62], supplemented with a 1D periodic perturbation comprising a scalar potential U(x) [59] and SOC terms allowed by symmetry [40–42]. We focus exclusively on long-period perturbations, hence suppressing intervalley scattering [59]. The Hamiltonian in the valley-isotropic basis is

$$H = v \left(\boldsymbol{\sigma} \cdot \mathbf{p} \right) \otimes s_0 + U(x) \sigma_0 \otimes s_0 + H_{\rm so}(x), \quad (1)$$

where v is the bare Fermi velocity of 2D massless Dirac fermions ($v = 10^6$ m/s), σ_a and s_a (a = x, y, z) are Pauli matrices acting on the pseudospin and spin subspaces, respectively, σ_0 and s_0 are 2×2 identity matrices, and $\mathbf{p} = -i\hbar \nabla$ is the momentum operator. For the broad class of effective Dirac Hamiltonians that are locally invariant under the C_{3v} point group [41, 42], the SSOF receives up to 3 contributions, namely, a spin-flip Rashba term $[H_R(x) = \lambda_R \Phi(x) (\sigma_x \otimes s_y - \sigma_y \otimes s_x)]$, a valley-Zeeman term due the broken sublattice symmetry $[H_{vz}(x) = \tau \lambda_{vz} \Phi(x) \sigma_0 \otimes s_z$, where $\tau = \pm 1$ is the valley index], and a Kane-Mele (KM) term $[H_{\rm KM}(x) =$ $\lambda_{\rm KM} \Phi(x) \sigma_z \otimes s_z$]. Here, $\lambda_{\rm R}$, $\lambda_{\rm vz}$ and $\lambda_{\rm KM}$ denote the nominal strength of Rashba, valley-Zeeman and intrinsiclike SOC, respectively, while $\Phi(x)$ describes the spatial profile of the SOC modulation $[\Phi(x + m a_S) = \Phi(x)]$ with m an integer]. An example of a graphene system subject to a SSOF with a square-wave profile is depicted in Fig. 1(a). Recent measurements [45-47] have shown that proximity-induced Rashba SOC in graphene/WSe₂ attains giant values of up to 15 meV [46], which is more than 350 times larger than graphene's intrinsic SOC [63], and makes group VI dichalcogenides ideal high-SOC substrates for our proposal. Lastly, we assume that the superlattice potential, when present, is designed to track the SSOF modulation (e.g. via a patterned bottom gate), and thus write $U(x) = u \Phi(x)$, where u is the scalar potential amplitude.

The most striking scenario, on which we will focus our attention, concerns Rashba SSOFs with a zero-mean profile [that is, $\langle \Phi(x) \rangle = (1/a_{\rm S}) \int_0^{a_{\rm S}} dx \, \Phi(x) = 0$]. For example, this can be accomplished through encapsulation of a graphene sheet between identical dielectric layers with a relative offset of $a_{\rm S}/2$. More exotic experimental routes,



FIG. 1. (a) 1D periodic modulation of the proximity-induced SOC. In this example, the SSOF is imprinted on graphene via the use of a dielectric metasurface decorated with 2D semicondutors (labelled TMD). (b) Energy dispersion of low-lying states around the K point for a zero-mean square-wave profile with $a_{\rm S} = 100$ nm, $\lambda_{\rm KM} = 20$ meV, and u = 0. (c) Same as (b) but with u = 15 meV. As a guide to the eye, the bare energy dispersion of graphene is shown in red (inner cones).

yet viable, include metal intercalation [64], periodic folding of graphene [65], proximity coupling to rippled group-VI dicalcogenides [66, 67] and deposition of graphene on stepped surfaces [68]. The low-energy physics in all these routes are captured by Eq. (1) (or simple generalizations thereof) with a suitable choice of parameters.

Results.—To build intuition, we first consider a SSOF with zero spatial average $(\langle \Phi(x) \rangle = 0)$ that locally preserves all the spatial symmetries of the honeycomb lattice, i.e. with a single term $(H_{\rm KM})$. The energy spectrum is two-fold spin degenerate in this case and exhibits the typical mini-band structure due to a synthetic periodic perturbation. In Fig. 1(b), we show numerically exact results for a long-period square-wave modulation of type KM. The most striking feature of the low-energy spectrum is the band touching at zero energy, i.e. the SOC spatial modulation precludes the opening of a topological gap [3]. (Higher-energy mini-bands are located at energies $\approx \pm 2\pi v \hbar/a_{\rm S} \approx \pm 40$ meV and thus lie outside the energy range of Fig. 1.) Importantly, the linearly dispersing zero energy states in our system cannot be gapped out without breaking the global average condition of the periodic perturbation. In other words, the Dirac point degeneracy survives SSOFs with $\langle \Phi(x) \rangle = 0$. What is more, the emergent 2D Dirac fermions unveiled here remain massless even for SSOFs that *locally* break one or more spatial symmetries, such as a spatially modulated Rashba SOC. The robustness of the crossing point

between the electron and hole mini-bands hints at interesting quantum geometry effects to be discussed shortly.

Next, we observe that the KM-SSOF renormalizes the group velocity along the modulation direction, \hat{x} , while it produces no change perpendicularly to it. This is the opposite behavior of graphene under a periodic (scalar) potential [59], and provides a simple mechanism to fine tune charge carrier propagation. This possibility is highlighted in Fig. 1(c), showing that the combined action of a SSOF and a periodic potential squeezes the Dirac cones along *both* parallel and perpendicular directions to the reciprocal superlattice vector. Perturbation theory provides further insights [69]. In the limit $u, \lambda_{\rm KM} \ll \hbar v/a_{\rm S}$, the component of the group velocity parallel to the wavevector **k** of the low-lying Dirac states is found to be

$$v_{\hat{\mathbf{k}}} \cong v \left[1 - \mu \, \frac{u^2 \sin^2 \theta_{\mathbf{k}} + \lambda_{\rm KM}^2 \cos^2 \theta_{\mathbf{k}}}{\hbar^2 v^2 (2\pi/a_{\rm S})^2} \right], \qquad (2)$$

where $\theta_{\mathbf{k}}$ is the wavevector angle and μ is a geometric factor ($\mu \approx 1.645$ for a square-wave SSOF). Equation (2) shows that the periodic perturbation can be tuned to yield an isotropic group velocity. Indeed, setting $u = \pm \lambda_{\rm KM}$ results in isotropic Dirac cones, thus mimicking the low-energy physics of bare graphene without SOC. The situation becomes richer when considering realistic systems with broken spatial symmetries as shown below. For example, Dirac fermions with isotropic behavior can be engineered by means of a pure Rashba SSOF, bypassing the need for a scalar periodic potential.

Realistic SSOFs and quantum geometry effects.—Now, we turn to the class of SSOFs that admix valley-Zeeman $(H_{\rm vz})$ and Rashba $(H_{\rm R})$ terms due to the breaking of spatial symmetries. Unlike the KM-type SOC in the example above, both $\lambda_{\rm R}$ and $\lambda_{\rm vz}$ can reach experimentally relevant energy scales, which is ideal for our proposal. We primarily focus on *pure Rashba SSOFs* [70], which can be realized via twist-angle engineering in graphene-ontransition metal dichalcogenides [43–46]. The idea is to tune the twist angle, so that the effective SOC of charge carriers on A and B sublattices coincide, yielding a vanishing valley-Zeeman effect, $\lambda_{vz} = (\lambda_A - \lambda_B)/2 = 0$. The resulting SOC is thus of Rashba type (allowed by the broken $z \to -z$ symmetry) [43, 44]. This intriguing possibility has been confirmed experimentally via quasiparticle interference imaging [46], showing that $\lambda_{vz} \approx 0$ and $\lambda_R \approx 15 \text{ meV}$ for 30° twist-angle graphene-on-WSe₂ systems. Armed with this important insight, we start by investigating the electronic structure induced by a squarewave Rashba SSOF. The energy dispersion of charge carriers in the three lowest-lying bands, above and below the charge neutrality point, is shown in Fig. 2(a). The calculated spectrum contains several genuine fingerprints of the SSOFs proposed in this work. Similar to the case above, the zero energy modes exhibit linear dispersion (i.e. the Dirac point degeneracy is protected). Furthermore, the behavior is isotropic. Thus, with regards to en-



FIG. 2. Mini-band dispersion and quantum geometry effects induced by a square-wave Rashba SSOF. (a) Energy dispersion along a cut with $k_x = 0$. (b) Berry curvature of bands near the Fermi level along the same **k**-path. Mini-bands are labelled by integers next to curves [positive (negative) *n* labels conduction (valence) bands]. Other parameters: $a_{\rm S} = 100$ nm and $\lambda_{\rm R} = 20$ meV.

ergy dispersion, this system emulates pristine graphene with a strongly renormalized Fermi velocity (see below). The massless nature of low-energy excitations is a robust feature of the 2D van der Waals metamaterials underpinning the SSOFs. In fact, only perturbations breaking the zero-average condition ($\langle \Phi \rangle = 0$) can gap out the massless Dirac states [69]. As such, the zero-energy modes can be mode as robust as desired in a realistic setup, by ensuring during that the fabrication method preserves the global average of the periodic perturbation. This confers protection against local SOC fluctuations that are unavoidable in realistic systems.

Next, we ask whether the SSOFs can endow 2D massless Dirac fermions with quantum geometric properties. We start by noting that the mini-bands due to a squarewave Rashba SSOF [see Fig. 2(a)] are two-fold spin degenerate, thus lacking a spin texture of their own. This is intriguing because the Rashba SOC breaks the spatial inversion symmetry and thus can lead to spin splittings. To explain this counter-intuitive result, we analytically compute the dispersion of the low-lying Dirac states using perturbation theory. While a standard second-order expansion in $\lambda_{\rm R}$ predicts a spin-degenerate spectrum, a cumbersome third-order calculation yields

$$\varepsilon_{\mathbf{k}s}^{(n=\pm1)} \approx \pm \left(\hbar v_{\rm ren} |\mathbf{k}| + s \frac{\tilde{\mu} \lambda_{\rm R}^3}{\hbar^2 v^2 G_1^4} |\mathbf{k}|^2 \right), \qquad (3)$$

where $s = \pm 1$ for spin-up (spin-down) low-energy branch, $G_1 = 2\pi/a_{\rm S}$, $v_{\rm ren} = v[1 - \mu(\lambda_{\rm R}/\hbar v G_1)^2]$ and $\tilde{\mu}$ is a geometric factor that equals zero for sine- and square-wave modulations, but is otherwise nonzero (e.g, for Kronig-Penney-type modulations, $|\tilde{\mu}|$ attains values close to 0.26 [69]). Hence, Rashba SSOFs with more general profiles can lift the spin degeneracy (as intuition would suggest), but only perturbatively. While the resulting spin splittings are typically small, a sizeable effect can be achieved by combining SSOFs with a periodic potential, providing a rich phenomenology for future exploration.

To examine the quantum geometry of SSOF-induced

mini-bands, we map out the momentum-space distribution of the spin Berry (SB) curvature

$$\Omega_n^z(\mathbf{k}) = -2\hbar^2 \operatorname{Im} \sum_{m \neq n} \frac{\langle m \mathbf{k} | v_x | n \mathbf{k} \rangle \langle n \mathbf{k} | v_y^z | m \mathbf{k} \rangle}{(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}})^2}, \quad (4)$$

where $v_i = v \sigma_x \otimes s_0$ and $v_i^z = v \sigma_i \otimes s_z$ (here, i = x, y) are the charge and spin velocity operators, respectively. This quantity governs the spin-Hall transport of electron wavepackets and therefore is the geometric analogue of the Berry curvature in the anomalous Hall effect [55, 71]. The SB curvature around the Dirac points is shown in Fig. 2(b). We see that the linearly dispersing zero energy modes (labelled $n = \pm 1$) are endowed with significant SB curvature, despite their massless nature. This is evidently at variance with 2D gapless Dirac systems, which have vanishing (charge) Berry curvature [10]. Thus, the emergent 2D Dirac cones reported here are not only robust against perturbations sharing the global average of the SSOFs but, remarkably, also display quantum geometric effects. Note that along the k_y -direction, the SB curvature of the massive Dirac mini-bands (|n| = 1, 2)resembles the Berry curvature of gapped 2D Dirac materials [10]. To explore this further, Figs. 3(a)-(b) show 3D plots of the SB curvature in the mini-Brillouin zone. Two features are of note: the central peaks in the SB curvature of massive Dirac mini-bands discussed earlier are identified as arising from hot spots of SB curvature [Fig. 3(b)]. On the other hand, the massless mini-bands attain a giant SB curvature at the edges of the mini-Brillouin zone $(k_x = \pm \pi/a_S)$ [Fig. 3(a)], about twice as large as the Dirac-point hot spot of the massive mini-bands. We attribute this feature to the emergence of large pseudogaps along the SSOF direction [69]. Finally, we note that the general behavior is highly anisotropic, except in the vicinity of the Dirac point.

The enhanced SB curvature of the SSOF-induced minibands indicates that the 2D van der Waals metamaterials proposed here support large spin-Hall responses. To confirm this, we compute the intrinsic spin Hall conductivity (σ_{ij}^z) from the flux of SB curvature using standard methods [69]. According to linear response theory, the z-polarized spin current density generated by an external electric field is $\mathbf{j}_s^z = \sum_{i,j=x,y} \sigma_{ij}^z E_j \mathbf{e}_j$, where E_j are the field components and \mathbf{e}_i is the unit vector along the *i*-axis. As shown in Fig. 3(c), the spin Hall response has a strong energy dependence and can reach sizeable values on the order of $e/4\pi$ for typical values of proximityinduced SOC at room temperature. This strong response is robust to design imperfections and weak disorder provided that the global average of the SSOFs is preserved $(\langle \Phi(x) \rangle = 0)$. We verified this with different types of proximity-induced SSOFs and spatial patterns $\Phi(x)$. At variance with 2D conductors subject to the usual uniform Rashba effect [49, 72], the spatial dependence of the Rashba SSOF protects our quantum geometry-driven



FIG. 3. (a) Momentum-space distribution of the spin Berry curvature of the massless Dirac mini-bands $(n = \pm 1)$. (b) Same as in (a) for the mini-bands $n = \pm 2$. SSOF parameters as in Fig. 2. (c) Room-temperature σ_{xy}^z as a function of the chemical potential for selected twisting-induced SOC modulations: pure Rashba SSOFs with amplitudes as indicated (solid lines) and admixed Rashba-valley-Zeeman SSOFs with $\lambda_{\rm vz} = \lambda_{\rm R}/2$ (dashed line) and $\lambda_{\rm vz} = \lambda_{\rm R}$ (dot-dashed line).

spin Hall effect from exact cancellations due to impurityscattering corrections. In fact, a SU(2)-covariant conservation law for the spin current can be derived in the vein of Ref. [49] yielding $\langle H_{\rm so}(x)v_i^z\rangle = 0$, with $\langle ... \rangle$ denoting a quantum and disorder average. For a uniform Rashba field, this relation (which holds in the presence of arbitrary non-magnetic impurity potentials) implies $\mathbf{j}_s^z = 0$. However, in our system this cancellation is circumvent due to the oscillatory nature of $H_{so}(x)$. The SSOFdriven SHE thus appears to be more robust than its counterpart in standard Rashba-coupled graphene. We now briefly address the case of 2D metamaterials with concurrent Rashba-type and valley-Zeeman SSOFs. Here, the condition $\langle \Phi(x) \rangle = 0$ could be achieved by alternating the relative rotation angle of consecutive TMD layers, exploiting the anti-periodicity of the valley-Zeeman effect, $\lambda_{vz}(\theta) = -\lambda_{vz}(\theta \pm \pi/3)$ [43, 44]. The ensuing SSOF in this case strongly renormalizes the group velocity of wavepackets that propagate parallel to the SSOF direction. The leading correction to Eq. (3) is given by $\delta \varepsilon_{\mathbf{ks}}^{(n=\pm 1)} = \pm \mu \Lambda_{vz} \cos^2 \theta_{\mathbf{k}}$, with $\Lambda_{vz} = \lambda_{vz}^2 / (\hbar v G_1)$, yielding an anisotropic energy dispersion and SB curvature. Interestingly, the valley-Zeeman SSOF leads to an overall decrease in the SB curvature magnitude, which is reflected in the spin Hall conductivity [Fig. (3)(c)]. This is also at odds with the expected behavior in (standard) proximitized graphene, where the spin-Hall conductivity has a non-monotonic behavior with λ_{yz} , with $\lambda_{yz} \neq 0$ [49] being essential to observe the SHE.

In closing, we have shown that the spatial patterning of symmetry-breaking spin-orbit fields gives rise to rich physics beyond that of conventional superlattices, most notably the emergence of 2D massless Dirac fermions with anomalous electrodynamic responses. The proposed periodic modulation of interface-induced SOC is within reach of current nano-fabrication methods, and is likely to have broad applications beyond those described in this work.

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SUPPLEMENTARY MATERIAL

PRELIMINARIES

Model and numerical approach

The low-energy Hamiltonian in the valley-isotropic form is

$$H_{\tau} = v\left(\boldsymbol{\sigma} \cdot \mathbf{p}\right) \otimes s_0 + U(x)\,\sigma_0 \otimes s_0 + H_{\mathrm{R}}(x) + H_{\mathrm{vz},\tau}(x) + H_{\mathrm{KM}}(x),\tag{5}$$

with $U(x) = u\Phi(x)$, $H_{\rm R}(x) = \lambda_R \Phi(x) (\sigma_x \otimes s_y - \sigma_y \otimes s_x)$, $H_{\rm vz,\tau}(x) = \tau \lambda_{\rm vz} \Phi(x) \sigma_0 \otimes s_z$, and $H_{\rm KM}(x) = \lambda_{\rm KM} \Phi(x) \sigma_z \otimes s_z$. The wavefunctions in valley $\tau = \pm 1$ are 4-component spinors of the form $\Psi_{\tau}(\mathbf{r}) = (\psi_{\tau\uparrow}^A(\mathbf{r}), \psi_{\tau\downarrow}^A(\mathbf{r}), \psi_{\tau\downarrow}^B(\mathbf{r}), \psi_{\tau\downarrow}^B(\mathbf{r}))^{\dagger}$. Moving to reciprocal space, the eigenproblem formally reduces to solving an infinite set of coupled equations for the plane-wave amplitudes $\{\psi_{\mathbf{k}s}^\sigma\}$:

$$\hbar v |\mathbf{k}| e^{-i\sigma\theta_{\mathbf{k}}} \psi_{\mathbf{k}s}^{-\sigma} + \sum_{p \in \mathbb{Z}} \left[\left(u + s\sigma\lambda_{\mathrm{KM}} + s\lambda_{\mathrm{vz}} \right) \Phi_{G_p} \psi_{\mathbf{k}-\mathbf{G}_p,s}^{\sigma} + i(s-\sigma)\lambda_{\mathrm{R}} \Phi_{G_p} \psi_{\mathbf{k}-\mathbf{G}_p,-s}^{-\sigma} \right] = E \psi_{\mathbf{k}s}^{\sigma} , \qquad (6)$$

where $s = \pm (\equiv \uparrow, \downarrow)$ and $\sigma = \pm (\equiv A, B)$ are the spin and pseudospin indices, respectively; the valley index is omitted for brevity. Furthermore, **k** is the Bloch wavevector from the Dirac point, $\theta_{\mathbf{k}} = \angle(\mathbf{k}, \hat{x})$, $\mathbf{G}_p = G_p \hat{x}$ with $G_p = 2\pi p/a_{\mathrm{S}}$ $(p \in \mathbb{Z})$, and Φ_{G_p} are the Fourier coefficients of the periodic modulation.

In our calculations, the summation over Fourier components in Eq. (6) is truncated to a finite, but large, number of terms ($|p| \leq N$). The resulting system of equations is solved numerically yielding d = 4(2N + 1) bands $\varepsilon_{n\mathbf{k}}$ and associated 4-component eigenvectors $\psi_{n\mathbf{k}}$.

The spin Berry curvature of each band n is calculated from [8]

$$\Omega_n^z(\mathbf{k}) = -2\hbar^2 v^2 \operatorname{Im} \sum_{m \neq n} \frac{\psi_{n\mathbf{k}}^{\dagger} \hat{\sigma}_y \otimes \hat{s}_z \,\psi_{m\mathbf{k}} \times \psi_{m\mathbf{k}}^{\dagger} \hat{\sigma}_x \otimes s_0 \,\psi_{n\mathbf{k}}}{(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}})^2}.$$
(7)

The linear-response intrinsic spin-Hall conductivity is $\sigma_{yx}^z = (e/2) \sum_{\mathbf{k}} \sum_n f(\varepsilon_{n\mathbf{k}}) \Omega_n^z(\mathbf{k})$, where $f(\varepsilon)$ is the Fermi-Dirac distribution function.

Spatial profile of the periodic perturbation

We consider Kronig-Penney (KP) and sinusoidal perturbations with zero spatial average. The KP profile is

$$\Phi(x) = 2\Phi \sum_{m=-\infty}^{\infty} \left(R(x + ma_{\rm S}) - r \right), \qquad 0 < r < 1,$$
(8)

where Φ is the amplitude and $R(x) = \Theta(x + \ell/2)\Theta(\ell/2 - x)$. Here, Θ is the Heaviside step function, $a_{\rm S}$ is the lattice width, ℓ is the barrier width ($\ell < a_{\rm S}$), and $r = \ell/a_{\rm S}$ (for a square wave r = 0.5). For pure sinusoidal modulations, we use $\Phi(x) = \Phi_c + \Phi \cos(G_1 x)$.

ELECTRONIC STRUCTURE

Numerics

Figure 4 shows the numerically calculated electronic structure of graphene subject to a *pure Rashba SSOF* for square-wave and KP modulations. We note that only positive-energy states are shown for clarity. Main findings are:

• spin-degenerate Dirac cones emerge at low energy (see remark below);

- the Dirac cones are isotropic around $\mathbf{k} = \mathbf{0}$ (see Fig. 6(a));
- the mini-bands at higher energy are separated by pseudo-gaps;
- spin splittings are visible for KP profiles with $r \neq 0$ (see panels (c) and (d)).



FIG. 4. Mini-band energy dispersion $\varepsilon(k_x, 0)$ (**a**,**c**) and $\varepsilon(0, k_y)$ (**b**,**d**) of graphene subject to a pure Rashba SSOF in the range $k_x \in [-\pi/a_{\rm S}, \pi/a_{\rm S}]$; only positive energy branches are shown. SSOF spatial profile: square wave in (**a**,**b**) and KP lattice with r = 0.3 in (**c**,**d**). The spin degeneracy of the bare system without SOC remains intact under square-wave SSOFs [(**a**,**b**)], while it is lifted in (**c**,**d**). Other parameters: $a_{\rm S} = 100$ nm and $\lambda_{\rm R} = 20$ meV. Bare energy dispersion is represented by dashed red lines as a guide to the eye.

The first point above is rigorously true for square-wave perturbations (i.e., r = 0.5). For KP profiles with $r \neq 0.5$, the spin degeneracy is perturbatively lifted (see Eq. (9)). We also verified that sine-wave SSOFs behave similarly to square-wave SSOFs but with less pronounced features. This is easily explained by comparing their Fourier coefficients. For a square wave profile, $\Phi_{\pm G_1}^{\text{square}} = (2/\pi)\Phi$, while for sine waves: $\Phi_{\pm G_1}^{\text{sine}} = (1/2)\Phi$.

The electronic structure for mixed *Rashba-valley-Zeeman SSOFs* is shown in Fig. 5. The main difference with respect to Fig. 4 is that the emergent Dirac cones become anisotropic irrespective of the SSOF's spatial profile.



FIG. 5. Mini-band energy dispersion $\varepsilon(k_x, 0)$ (**a**,**c**) and $\varepsilon(0, k_y)$ (**b**,**d**) for a mixed Rashba-valley-Zeeman SSOF. SSOFs spatial profile: square wave in (**a**,**b**) and KP lattice with r = 0.3 in (**c**,**d**). The valley-Zeeman strength is $\lambda_{vz} = 10$ meV. Other parameters as in Fig. 4.



FIG. 6. Low-energy dispersion for a pure Rashba SSOF (a) and a mixed Rashba-valley-Zeeman SSOF (b). Solid and dashed lines show $\varepsilon(k_x, 0)$ and $\varepsilon(0, k_y)$, respectively. The low-energy Dirac cones are isotropic in (a) and anisotropic in (b). Parameters: r = 0.5, $a_{\rm S} = 100$ nm, $\lambda_{\rm R} = 20$ meV (a,b) and $\lambda_{\rm vz} = 10$ meV (b).

Perturbation theory

We start with the class of 2×2 Dirac Hamiltonians subject to a periodic perturbation (period $a_{\rm S}$) with generic pseudospin structure of the type:

$$\hat{H} = \hbar v (\sigma_x \hat{k}_x + \sigma_y \hat{k}_y) + \hat{S}(x) + \hat{X}(x) + \hat{Y}(x) + \hat{Z}(x)$$

where $\hat{S}(x) = S\Phi(x)\sigma_0$ is the superlattice potential and $\hat{X}(x) = X\Phi(x)\sigma_x$, $\hat{Y}(x) = Y\Phi(x)\sigma_y$ and $\hat{Z}(x) = Z\Phi(x)\sigma_z$ are the SU(2)-pseudospin fields. We recall that the unperturbed eigenstates are the spinors $\psi_{\mathbf{k}}^{0\sigma}(\mathbf{r}) = \frac{1}{\sqrt{2}}(1, \sigma e^{i\theta_{\mathbf{k}}})^{\mathrm{t}}e^{i\mathbf{k}\cdot\mathbf{r}}$

corresponding to the eigenenergies $\varepsilon_{\mathbf{k}\sigma}^0 = \sigma \hbar v |\mathbf{k}|$. Using second order perturbation theory, we find that the correction to the lowest-lying energy states, $\delta \varepsilon_{\mathbf{k}\sigma}^{(2)} = \varepsilon_{\mathbf{k}\sigma}^{(2)} - \varepsilon_{\mathbf{k}\sigma}^0$ is

$$\delta \varepsilon_{\mathbf{k}\sigma}^{(2)} = \sigma \frac{1}{\hbar v} \sum_{n \neq 0} \left[\frac{2|\mathbf{k}| - |\mathbf{G}_n| \cos \theta_{\mathbf{k},\mathbf{G}_n}}{|\mathbf{k}|^2 - |\mathbf{k} - \mathbf{G}_n|^2} S_{G_n}^2 + \frac{|\mathbf{G}_n| \cos \theta_{\mathbf{k},\mathbf{G}_n}}{|\mathbf{k}|^2 - |\mathbf{k} - \mathbf{G}_n|^2} Z_{G_n}^2 \right]$$

$$+\frac{2|\mathbf{k}|\cos^2\theta_{\mathbf{k}}-|\mathbf{G}_n|\cos\theta_{\mathbf{k},\mathbf{G}_n}\cos\theta_{\mathbf{k}}}{|\mathbf{k}|^2-|\mathbf{k}-\mathbf{G}_n|^2}X_{G_n}^2+\frac{2|\mathbf{k}|\sin^2\theta_{\mathbf{k}}+|\mathbf{G}_n|\cos\theta_{\mathbf{k},\mathbf{G}_n}\cos\theta_{\mathbf{k}}}{|\mathbf{k}|^2-|\mathbf{k}-\mathbf{G}_n|^2}Y_{G_n}^2$$

$$+\frac{2|\mathbf{k}|\cos\theta_{\mathbf{k}}-|\mathbf{G}_{n}|\cos\theta_{\mathbf{k},\mathbf{G}_{n}}}{|\mathbf{k}|^{2}-|\mathbf{k}-\mathbf{G}_{n}|^{2}}S_{G_{n}}X_{G_{n}}+\frac{2|\mathbf{k}|\sin\theta_{\mathbf{k}}}{|\mathbf{k}|^{2}-|\mathbf{k}-\mathbf{G}_{n}|^{2}}S_{G_{n}}Y_{G_{n}}$$

+
$$\frac{4|\mathbf{k}|\cos\theta_{\mathbf{k}}\sin\theta_{\mathbf{k}}+2|\mathbf{G}_{n}|\cos\theta_{\mathbf{k},\mathbf{G}_{n}}\sin\theta_{\mathbf{k}}}{|\mathbf{k}|^{2}-|\mathbf{k}-\mathbf{G}_{n}|^{2}}X_{G_{n}}Y_{G_{n}}\Big|.$$

Expanding around the K point $(\mathbf{k} = \mathbf{0})$ up to first order in \mathbf{k} , we obtain

$$\varepsilon_{\mathbf{k}\sigma}^{(2)} \approx \sigma \hbar v \left[1 - \mu \frac{\sin^2 \theta_{\mathbf{k}} S^2 + \cos^2 \theta_{\mathbf{k}} Z^2 + Y^2 + \sin \theta_{\mathbf{k}} SY + 2\sin \theta_{\mathbf{k}} \cos \theta_{\mathbf{k}} XY}{\hbar^2 v^2 G_1^2} \right] |\mathbf{k}|$$

where μ is a geometric factor equal to 1 for a sine-wave modulation and $\sum_{n=1}^{\infty} (4r/n)^2 \operatorname{sinc}^2(n\pi r)$ for a KP profiles with zero spatial average. We note that the gapless nature of the spectrum has its origin in the chiral phase factors $e^{i\theta_k}$ of the unperturbed eigenstates as first discussed in Ref. [59] for pure scalar perturbations. Generalizing these

results to the 4×4 Dirac Hamiltonian in Eq. (5), containing the SSOFs, yields

$$\varepsilon_{\mathbf{k}s\sigma}^{(2)} \approx \sigma \hbar v \left[1 - \mu \frac{\sin^2 \theta_{\mathbf{k}} (u^2 + \lambda_{\mathrm{vz}}^2) + \cos^2 \theta_{\mathbf{k}} \lambda_{\mathrm{KM}}^2 + \lambda_{\mathrm{R}}^2 + 2s \sqrt{\sin^2 \theta_{\mathbf{k}} u^2 (\lambda_{\mathrm{vz}}^2 + \lambda_{\mathrm{R}}^2) + \cos^2 \theta_{\mathbf{k}} \lambda_{\mathrm{KM}}^2 \lambda_{\mathrm{R}}^2}}{\hbar^2 v^2 G_1^2} \right] |\mathbf{k}|. \tag{9}$$

Equation (9) provides the following insights:

- Symmetry protection: The Dirac point degeneracy is robust against all periodic perturbations with $\langle \Phi(x) \rangle = 0$, irrespective of the local spatial symmetries broken by the SSOF. A gap at $\mathbf{k} = 0$ can only be open by adding uniform SOC terms (i.e. for spatial profiles $\Phi(x)$ with non-zero spatial average).
- **Spin splitting**: Surprisingly, a particular type of SSOF *cannot* perturbatively lift the spin degeneracy of the low-lying states on its own. Only specific admixtures of periodic perturbations can lead to spin splitting of low-lying states (e.g., Rashba SSOF combined with a periodic potential).
- Emergent Dirac cones: Pure Rashba SSOFs generate *isotropic Dirac cones* around $\mathbf{k} = \mathbf{0}$. Because the spin degeneracy is intact in this case, the low-lying spectrum around the Dirac points mimic that of pristine graphene with a renormalized Fermi velocity.
- Anisotropic behavior: For SSOFs admixing Rashba and valley-Zeeman components, for example, or in the presence of a periodic potential, $u \neq 0$, the energy dispersion becomes anisotropic.

Third-order perturbation theory versus numerics

Our fully non-perturbative numerical calculations demonstrate that pure Rashba SSOFs lift the spin degeneracy of mini-bands for SSOFs with $r \neq 0.5$; see Fig. 7. This effect is significant away from the Dirac point. To capture this feature, one must turn to third-order perturbation theory. After tedious algebra, the energy dispersion to leading order in **k** and associated spin gap, $\Delta_{\text{spin}}(\mathbf{k})$, are obtained as

$$\varepsilon_{\mathbf{k}s\sigma}^{(3)} \approx \varepsilon_{\mathbf{k}\sigma}^{(0)} - \mu\sigma \frac{\lambda_{\mathrm{R}}^2}{\hbar v G_1^2} \left(|\mathbf{k}| - s\frac{\tilde{\mu}}{\mu} \frac{\lambda_{\mathrm{R}}}{\hbar v G_1^2} |\mathbf{k}|^2 \right), \qquad \Delta_{\mathrm{spin}}(\mathbf{k}) = 2\tilde{\mu} |\lambda_{\mathrm{R}}| \left(\frac{\lambda_{\mathrm{R}}}{\hbar v G_1^2} \right)^2 |\mathbf{k}|^2, \tag{10}$$

where $\tilde{\mu}$ is a geometric factor, $\tilde{\mu} = \sum_{n,m}' 4(2r)^3 \operatorname{sinc}(n\pi r) \operatorname{sinc}((n+m)\pi r)/[n^2(m+n)^2]$ (the primed summation is used to exclude the cases n = -m and n, m = 0). In accord with the numerics, we see that $\tilde{\mu} = 0$ for r = 0.5 (spin-degenerate states) and $\tilde{\mu} \neq 0$ for $r \neq 0.5$. The perturbative results reproduce well the numerics within their regime of validity, $|u|, |\lambda_{\text{KM}}|, |\lambda_{\text{R}}|, |\lambda_{\text{vz}}| \ll \pi \hbar v/a_{\text{S}} (\approx 20 \text{ meV}$ for $a_{\text{S}} = 100 \text{ nm}$).



FIG. 7. Perturbation theory versus numerics: Energy dispersion $\varepsilon(k_x, 0)$ of the lowest-lying electron band for a pure Rashba SSOF with r = 0.5 (a) [r = 0.3 (b)], obtained numerically (solid lines) and via Eq. (10) (dashed lines). Other parameters: $a_{\rm S} = 100$ nm and $\lambda_{\rm R} = 10$ meV.

Zero-energy solutions: analytical results

The spinor components can be cast as $\psi_s^{\sigma}(\mathbf{r}) = \phi_s^{\sigma}(x)e^{ik_y y}$, where k_y is the wavevector component perpendicular to the superlattice direction. The Dirac equation for zero-energy states ($\hbar \equiv 1$) yields

$$-i\hbar v \partial_x \phi_s^{-\sigma}(x) + \left(u + s\sigma\lambda_{\rm KM} + s\lambda_{\rm vz}\right) \Phi(x)\phi_s^{\sigma}(x) + i(s-\sigma)\lambda_{\rm R}(x)\phi_{-s}^{-\sigma}(x) = 0.$$
(11)

We write the solutions in terms of the function $\varphi_{\xi}(x) = \xi/v \int^x \Phi(x') dx'$. We denote by L the linear dimension of the system along x ($L \gg a_{\rm S}$). Equation (11) admits analytical solutions in a number of cases summarized below.

• Case 1: No Rashba field ($\lambda_{\rm R} = 0, \lambda_{\rm KM} \neq 0, \lambda_{\rm vz} \neq 0, u \neq 0$). In this case, up and down spin sectors decouple. The zero-energy eigenfunctions for $s = \uparrow, \downarrow$ may be written as

$$\phi_s^{\sigma}(x) = \frac{1}{\sqrt{L}} \begin{bmatrix} A\cos\varphi_{\gamma}(x) + iB\sin\varphi_{\gamma}(x) \\ -B\gamma/\Delta\gamma\cos\varphi_{\gamma}(x) - iA\gamma/\Delta\gamma\sin\varphi_{\gamma}(x) \end{bmatrix},$$
(12)

where $\gamma = ((u + \lambda_{vz})^2 - \lambda_{KM}^2)^{1/2}$, $\Delta \gamma = u + \lambda_{vz} - \lambda_{KM}$, and A and B are constants. There are two degenerate solutions for a each spin state. We present two examples. For $u \neq 0$ and all other potentials equal to zero, two orthogonal degenerate zero-energy eigenstates for $\mathbf{k} = 0$ corresponding to the two zero-energy modes (ZEMs) read

$$\phi_s^A(x) = \frac{1}{\sqrt{L}} \begin{bmatrix} \cos \varphi_u(x) \\ -i \sin \varphi_u(x) \end{bmatrix},\tag{13}$$

$$\phi_s^B(x) = \frac{1}{\sqrt{L}} \begin{bmatrix} -i\sin\varphi_u(x)\\ \cos\varphi_u(x) \end{bmatrix},\tag{14}$$

while for $\lambda_{\rm KM} \neq 0$ and all the other potentials zero, the ZEMs are

$$\phi_s^A(x) = \frac{1}{\sqrt{C_{\lambda_{\rm KM}}}} \begin{bmatrix} \cosh \varphi_{\lambda_{\rm KM}}(x) \\ -i \sinh \varphi_{\lambda_{\rm KM}}(x) \end{bmatrix},\tag{15}$$

$$\phi_s^B(x) = \frac{1}{\sqrt{C_{\lambda_{\rm KM}}}} \begin{bmatrix} i \sinh \varphi_{\lambda_{\rm KM}}(x) \\ \cosh \varphi_{\lambda_{\rm KM}}(x) \end{bmatrix},\tag{16}$$

where $C_{\lambda_{\text{KM}}} = \int_{-L/2}^{L/2} dx \cosh 2\varphi_{\lambda_{\text{KM}}}(x)$. Eq. (12) holds for $u + \lambda_{\text{vz}} \neq \lambda_{\text{KM}}$. When $u + \lambda_{\text{vz}} = \lambda_{\text{KM}} = \eta$, the ZEMs are

$$\phi_s^A(x) = \frac{1}{\sqrt{C_\eta}} \begin{bmatrix} 1\\ -2i\varphi_\eta(x) \end{bmatrix},\tag{17}$$

$$\phi_s^B(x) = \frac{1}{\sqrt{L}} \begin{bmatrix} 0\\1 \end{bmatrix},\tag{18}$$

where $C_{\eta} = \int_{-L/2}^{L/2} dx (1 + 4\varphi_{\eta}^2(x)).$

• Case 2: Pure Rashba field ($\lambda_{\rm R} \neq 0$, $\lambda_{\rm KM} = 0$, $\lambda_{\rm vz} = 0$, u = 0). In this case, four orthogonal degenerate zero-energy eigenstates for $\mathbf{k} = 0$ corresponding to the four ZEMs are found:

$$\phi_{\uparrow}^{A}(x) = \frac{1}{\sqrt{L}} \begin{bmatrix} 1\\0\\0\\0 \end{bmatrix}, \qquad (19)$$

$$\phi^B_{\uparrow}(x) = \frac{1}{\sqrt{C_{\lambda_{\rm R}}}} \begin{bmatrix} 0\\ 1\\ 0\\ -2\varphi_{\lambda_{\rm R}}(x) \end{bmatrix},\tag{20}$$

$$\phi_{\downarrow}^{A}(x) = \frac{1}{\sqrt{C_{\lambda_{\mathrm{R}}}}} \begin{bmatrix} 2\varphi_{\lambda_{\mathrm{R}}}(x) \\ 0 \\ 1 \\ 0 \end{bmatrix}, \qquad (21)$$

$$\phi_{\downarrow}^{B}(x) = \frac{1}{\sqrt{L}} \begin{bmatrix} 0\\0\\0\\1 \end{bmatrix}, \qquad (22)$$

where $C_{\lambda_{\mathrm{R}}} = \int_{-L/2}^{L/2} dx (1 + 4\varphi_{\lambda_{\mathrm{R}}}^2(x)).$

These analytical results highlight the robustness of the Dirac point degeneracy to SSOFs satisfying the zero spatialaverage condition, in accord with the exact numerical calculations.