Quantum Spin Hall Effect in Two-dimensional Crystals of Transition Metal Dichalcogenides

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We propose to engineer time-reversal-invariant topological insulators in two-dimensional (2D) crystals of transition metal dichalcogenides (TMDCs). We note that, at low doping, semiconducting TMDCs under shear strain will develop spin-polarized Landau levels residing in different valleys. We argue that gaps between Landau levels in the range of 10–100 Kelvin are within experimental reach. In addition, we point out that a superlattice arising from a Moiré pattern can lead to topologically non-trivial subbands. As a result, the edge transport becomes quantized, which can be probed in multi-terminal devices made using strained 2D crystals and/or heterostructures. The strong d character of valence and conduction bands may also allow for the investigation of the effects of electron correlations on the topological phases.

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There is currently much interest in two-dimensional (2D) crystals of transition metal dichalcogenides (TMDC) such as MoS2 or WSe2. Compared to Graphene, many of these materials are semiconductors with sizeable gaps (≈ 1 eV), which makes them good candidates for applications in conventional electronics such as the manufacture of transistors [2].

By contrast, the quantum spin Hall (QSH) effect has been postulated as the paradigm for future non-dissipative nano-electronics [4]. Indeed, provided that magnetic impurities (or other time-reversal symmetry-breaking perturbations) can be eliminated, electron transport through the edge of a QSH insulator becomes ballistic. This is because counter propagating channels of the same spin are spatially separated.

Nevertheless, the QSH effect has been observed in very few materials so far, making the search for new systems exhibiting this effect a major scientific endeavor. In the context of 2D crystals, Weeks and coworkers have recently proposed an approach to enhance the spin-orbit coupling in graphene by heavy ad-atom deposition [7], which could lead to a realization of the Kane-Mele model [8] and the QSH effect. The availability of 2D materials exhibiting this effect may allow for the construction of flexible electronic devices with low-power consumption.

In this work, we present a proposal for engineering the QSHE in strained 2D crystals and heterostructures made using TMDCs. Strain is known to induce pseudo-magnetic fields in 2D crystals [9, 11]. These fields have been predicted [9] and experimentally found [10] to produce Landau levels (LLs) in the electronic spectrum of 2D crystals such as graphene. As explained below, it is also possible to exploit these pseudo-magnetic fields to engineer time-reversal invariant topological phases in other 2D crystals such as the TMDCs. This approach has several attractive features. Using MoS2 as an example, we find that gaps between LLs scale as ℏωc/kB ≃ 2.7 B0[T] K, where B0[T] is the strength of the pseudo-magnetic field in Tesla. Fields B0[T] ~ 10 – 102 T have been experimentally demonstrated [9, 10], which in the case of TMDCs could lead to LL gaps of up to ≈ 100 K. By comparison, the gaps achievable by straining GaAs are in the range of tens of milli-Kelvin [12]. The much larger magnitude of the LLs gaps in the present proposal stems the strain coupling to the electron current, rather than the electron spin current as in Ref. [12]. These two coupling constants are, in general, vastly different in order of magnitude. However, in multi-valley systems like graphene, strain only leads to (spin) unpolarized LLs. What sets semiconducting TMDCs apart is the spin-orbit coupling (SOC) that produces a large spin splitting of the valence (and to a smaller extent, the conduction) band. For small doping, this leads to spin-polarized LLs in different valleys, which opens the possibility of realizing time-reversal invariant (TRI) topological phases. Furthermore, the valence and conduction band of semi-conducting TMDC have strong d character [13], which, along with the poor screening of the Coulomb interaction in 2D, means that electron interactions can have interesting effects on properties of the TRI topological phases realized in TMDCs.

Bulk TMDC are composed of X-M-X layers stacked on top of each other and coupled by weak Van der Waals forces. Therefore, like graphite, these materials can be exfoliated down to a single layer. The transition metal atoms (M) are arranged in a triangular lattice and each one is bonded to six chalcogen atoms (X) (see Fig. 1) for...
a top view of the lattice). The point group of the 2D crystal is $D_{3h}$. The Fermi level lies at the two inequivalent corners of the Brillouin zone, $K$ and $K'$ points, as in the case of graphene, but the spectrum is gapped.

The character of the conduction and valence bands is dominated by $d_{3z^2−r^2}$ and $d_{x^2−y^2} \pm id_{xy}$ orbitals from M atom, respectively, where the sign (+) holds for $K (K')$ point. Furthermore, both bands have a non-negligible hybridization with the bonding combination of $p_x \pm ip_y$ (in the conduction band) and $p_x \mp ip_y$ (in the valence band) orbitals from X atoms.

In the continuum limit, the system is well described by the following two-band Hamiltonian [2-13,15]:

$$H_0 = v(\tau^z \sigma^x p_x + \sigma^y p_y) + \Delta \sigma^z + \frac{\lambda_{SO}}{2} \tau^z s^z (1 − \sigma^z),$$

(1)

where $\mathbf{p} = (p_x, p_y)$ is the electron crystal momentum referred to the $K (K')$ point, for which we introduce $\tau^z = +1$ ($\tau^z = -1$); $\sigma^\alpha$ are Pauli matrices acting on the space span by conduction and valence band states; $\Delta$ is the band gap and $v = ta/\hbar$, where $a$ is the lattice parameter and $t$ is a phenomenological hybridization parameter; finally, $s^z$ is the spin projection along the $z$ axis perpendicular to the 2D crystal. The Hamiltonian [1] can be constructed phenomenologically by considering scalar invariants of $D_{3h}$ formed from operators $\sigma^\alpha$, $\mathbf{p}$ and spin $s^z$. The symmetry properties of these operators are listed in Table I. Besides the gap, another important difference with graphene is the spin splitting of the bands due to the strong spin-orbit interaction provided by M atoms.

Below, we focus on p-doped TMDCs, which allows us to neglect the smaller spin splitting of the conduction band. For the valence band, the latter is in the range of 100–400 meV depending on the material [16,15,13,19]. The Hamiltonian [1] can be also derived from a microscopic theory. From a simplified tight-binding model [17], we obtain $\Delta = 1.41$ eV and $t = 1.19$ eV.

In order to turn a TMDC into a TRI topological insulator, we need to consider the effect of strain on the band structure. Strain is described by a rank-2 tensor, $u_{\alpha\beta} = \frac{1}{2} (\partial_{\alpha} u_{\beta} + \partial_{\beta} u_{\alpha} + \frac{\partial v}{\partial x_{\alpha}} \frac{\partial v}{\partial x_{\beta}})$, where $u = (u_x, u_y)$ ($h$) is the in-plane (out-of-plane) displacement of the unit cell.

### Table I: Symmetry classification of the electronic operators and strain tensor components according to the irreducible representations (Irrep) of $D_{3h}$ and time reversal operation.

| Irrep | TR Even | TR Odd |
|-------|---------|--------|
| $A_1$ | $1, \sigma^z, \sum_\alpha u_{\alpha\alpha}$ | - |
| $A_2$ | - | $\tau^z, s^z$ |
| $E'$ | $(\sigma^x, \tau^z \sigma^y)$, $(u_{xx} - u_{yy}, -2u_{xy})$ | $\tau^z \sigma^x, \sigma^y$, $p = (p_x, p_y)$ |
| $E''$ | - | $(s^z, \sigma^y)$ |

Thus, the coupling with strain reads:

$$H_{\text{strain}} = \beta_0 \sum_\alpha u_{\alpha\alpha} + \beta_1 t \sum_\alpha u_{\alpha\alpha} \sigma^z + \beta_2 t \left[(u_{xx} - u_{yy}) \sigma^z - 2u_{xy} \tau^z \sigma^y\right].$$

(2)

Microscopically, the origin of these couplings is the change in the hybridization between $d$ orbitals from M atoms and $p$ orbitals from X atoms due to the distortion of the lattice. In our microscopic tight-binding model [17], the phenomenological constants $\beta_{0,1,2}$ are given by the Gr"uneisen parameters [11] associated to the hopping amplitudes considered in the calculation [17]. The trace of the strain tensor generates scalar potentials of different strength in the valence and conduction bands. In addition, strain can be introduced in Eq. (1) as a minimal coupling $p \rightarrow p - eA$ to a vector potential $eA = \frac{k_{SO}}{a} \tau^z (u_{yy} - u_{xx}, 2u_{xy})$. The presence of $\tau^z$ indicates that the pseudo-magnetic field has opposite sign on different valleys, which is necessary as strain does not violate TRI.

Henceforth, we assume that the system is doped with holes and therefore the Fermi level crosses the valence band. Integrating out the conduction band to leading order in $\Delta^{-1}$ yields:

$$H_v = -\frac{\Pi_+ (\tau^z) \Pi_- (\tau^z)}{2m^*} + U(\mathbf{r}) + \lambda_{SO} s^z \tau^z,$$

(3)

where $m^* = \Delta/2v^2 \approx 0.5$ [22], $U(\mathbf{r}) = g(u_{xx} + u_{yy})$ with $g = t (\beta_0 - \beta_1)$, and $\Pi_+ (\tau^z) = (\tau^z p^x \pm ip^y) - e(\tau^z A_x \pm iA_y)$, which obey the commutation relation $[\Pi_+ (\tau^z), \Pi_- (\tau^z)] = 2e\hbar r^z B(\mathbf{r})$, where $B(\mathbf{r}) = \partial_x A_y - \partial_y A_x$. Corrections of $O(\Delta^{-2})$ have been also obtained and can lead to mixing of the Landau levels, but they can be neglected as for typical parameters $\hbar \omega_c \lesssim 10^{-2} \Delta$.

In the absence of strain (i.e. $\mathbf{A} = U = 0$), Eq. (3) describes the Bloch states at the top of the valence band near $K, K'$. Owing to the spin-orbit coupling ($\propto \lambda_{SO}$), for small hole doping (i.e. $|eF| \ll \lambda_{SO}$), the spin and valley spin of the holes are locked to each other, i.e. only holes with either $(K, \uparrow)$ or $(K', \downarrow)$ can exist (cf. Fig. 2). Furthermore, the states at $K$ and $K'$ are Kramers pairs.
This yields a relation between the maximum pseudo-magnetic field (in Tesla) and the sample size \( L \) in \( \mu m \): 
\[ B_0[L] \approx \frac{8}{L[\mu m]} \]

Using \( \hbar \alpha /k_B = 2.7 B_0[T] \) and taking \( L \approx 1 \mu m \), we estimate \( \hbar \alpha /k_B \approx 20 \) K for MoS\(_2\).

For small strained 2D crystal flakes, it is necessary to take into account the effect of an inhomogeneous pseudo-magnetic field resulting from a non-uniform strain distribution. In this regard, we note that the lowest LL eigenfunctions are null eigenvectors of \( \Pi_-(\tau^z) \):

\[ \Pi_-(\tau^z)\psi(r) = 0, \]

Therefore, following Eq. 32, we write \( A(r) = \tau_z(\hat{z} \times \nabla \chi(r) + \nabla \phi(r)) \), which allows to solve for \( K[K'] \) and yields \( \psi(r) = f(z^*)e^{\frac{\pi}{20}(\chi(r) + i\phi(r))} \), where \( f(z^*) \) is a polynomial of \( z = (x + iy) \), \( z^* = (x - iy) \) of maximum degree \( N = |\Phi|\Phi_0 \), \( \Phi = \int d\mathbf{r} B_0(\mathbf{r}) \) being the total flux and \( \Phi_0 = h/e \) the flux quantum 33. Hence, the wave-function describing \( N_f = N_\uparrow \) (non-interacting) electrons in the lowest LL reads 32:

\[ \Phi_0(\{r_{i\alpha}\}) = e^{-F} \prod_{i<j}(z^*_i - z^*_j)(z_i - z_j), \]

where \( F(\{r_{i\alpha}\}) = \mathcal{F}_N \sum_{\alpha=\uparrow,\downarrow}^{\downarrow} |\chi(r_{i\alpha}) - i\alpha\phi(r_{i\alpha})| \).

Larger sample sizes can be achieved by other methods such in 2D crystal bubbles 9 10. A periodic array of such bubbles will lead to periodic modulation of strain and pseudo-magnetic field, which allows to create topologically non-trivial band structures 9 23. Alternatively, a superlattice can be used to create, within each valley, a band with non trivial topological properties. If we neglect trigonal warping, each valley has a spin splitting in each valley. Large enough periodicities can \( \chi \) be achieved by other methods such in 2D crystal bubbles 9 10. A periodic array of such bubbles will lead to periodic modulation of strain and pseudo-magnetic field, which allows to create topologically non-trivial band structures 9 23.

The strain configuration described above can be created by the methods described in Ref. 9. For a TMDC 2D crystal flake under trigonal strain 9 (cf. Fig. 2), one concern is the sample size. The latter is limited by the maximum tensile strength of the TMDCs, \( T_{\text{max}} \). For MoS\(_2\), the thermodynamic relation \( \sigma_{\alpha\beta} = 2\mu \alpha\beta \) (\( \sigma_{\alpha\beta} \) being the stress tensor and \( \mu \) is the shear modulus) allows us to estimate the maximum sample size \( L \approx \frac{2T_{\text{max}}}{\mu C} \). The values of \( \mu \approx 50.4 \) N/m and \( T_{\text{max}} \approx 16.5 \) N/m can be obtained from density-functional calculations 21.
quantized in units of $2e/4\pi$ \cite{3}. However, if the total $s^z$ is not a good quantum number (see discussion below), $\sigma_{xy}^{H}$ is not exactly quantized \cite{3}. Instead, charge transport through the (helical) edge channels provides a clearer signature of existence of a topological phase \cite{5,6}. Nevertheless, in the case of strained crystals in the absence of a superlattice potential, we must be careful in qualifying the strained 2D crystal as a topological insulator for arbitrary LL filling. This is because adatoms, a perpendicular electric field, out of plane deformations, etc. break the mirror symmetry about the 2D crystal plane, which induces a Rashba spin-orbit coupling. Rashba allows for spin flips and therefore can lead to backscattering between counter-propagating edge channels. For an odd number of occupied LLs, an odd number of Kramers’ pairs of edge modes cross the Fermi energy and, for weak to moderate electron-electron interactions, the integrity of at least one Kramers’ pair of edge modes against TRI perturbations that induce spin-flip scattering like Rashba spin-orbit coupling is always ensured \cite{34}. Thus, for $2n+1$ (with $n$ integer) occupied LLs, the system is TRI protected topological phase and a two-terminal measurement of the conductance will yield at least $2e^2/h$ and at most $2(2n+1)e^2/h$, depending of degree of edge disorder and other $s^z$ non-conserving perturbations.

On the other hand, if the number of occupied LLs is even ($= 2n$), there will an even number of pairs of edge modes crossing the Fermi level and this situation is no longer protected against e.g. Rashba-type disorder potential \cite{34} (although edge modes survive for strong enough electron-electron interactions \cite{34}). However, in sufficiently clean samples and provided interactions are weak, quantized conductance of $4ne^2/h$ may be observable. Furthermore, the existence of bulk LLs can be detected by means of scanning tunneling microscopy as in the case of graphene \cite{10}.

Finally, let us discuss the possible effect of interactions. The strong $d$ character of the valence and conduction bands means that electron correlations can have an important effect on the topological phases, especially on the edge states \cite{34,36}. Indeed, for MoS$_2$ the short-range part of the interaction (i.e. the Hubbard-$U$) has been estimated in Ref. \cite{35} to be $\sim 2$-10 eV. Thus, MoS$_2$ may present a scenario comparable to the Iridates \cite{36}. However, the QSH effect in the TMDCs may allow for a more complete understanding of the interplay between electron correlation and QSH physics, since correlation effects decrease as the metal atom $M$ is varied from the $4d$ series (as in MoS$_2$) to $5d$ series (as in WS$_2$).

In conclusion, we have presented a proposal to engineer time-reversal invariant topological phases in 2D crystals of transition metal dichalcogenides (TMDC) under strain and/or in heterostructures which induce superlattice potentials. We also note that the proposal can be extended to electron-doped TMDC. However, in this case, the separation between the Landau levels ($\hbar\omega_c/k_B \approx 2.2 B_0(T)$) and the strength of the superlattice potential are limited by the much smaller spin-orbit coupling ($\lambda_{SO} \sim 10$ meV $\sim 100$ K) \cite{16}, which also requires much lower temperatures. We hope that the feasibility of our proposal will stimulate further experimental work along these directions. We stress that compared to other QSH systems \cite{5,6}, strained 2D TMDCs allow for much larger tunability of material parameters as well as the strength of the Berry curvature responsible for the Landau levels. In this regard, the main obstacle for the observation of the QSH effect appears to be the reduced carrier mobility in currently available 2D crystals of TMDCs. However, given the notorious technological potential of these materials, we expect this obstacle will be overcome in the near future.

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SUPPLEMENTARY INFORMATION

Microscopic derivation of the two-bands Hamiltonian

Tight-binding model

We consider a simplified tight-binding Hamiltonian acting on the subspace span by the symmetry-adapted Bloch wave functions $|M_{3z^2-r^2}\rangle$, $|M_{x^2-y^2}\rangle$, $|X(b)\rangle p_y + i\tau p_x$, and $|X(b)\rangle p_y - i\tau p_x$. The model is strictly valid around $K_\tau$ points, where $\tau = \pm 1$ labels the two valleys $K$ ($\tau = +1$) and $K'$ ($\tau = -1$). The crystal field parameters are:

$$\langle M_{3z^2-r^2} | H_{TB} | M_{3z^2-r^2}\rangle = \Delta_0$$
$$\langle M_{x^2-y^2} + \tau id_{xy} | H_{TB} | M_{x^2-y^2} + \tau id_{xy}\rangle = \Delta_2$$
$$\langle X (b) p_y \pm \tau p_x | H_{TB} | X (b) p_y \pm \tau p_x\rangle = \Delta_p.$$  (7)

The hopping integrals sketched in Fig. 3 can be expressed in terms of the two-center Slater-Koster parameters $V_{pd\sigma}$, $V_{pd\pi}$ as follows:

$$t_x = \sqrt{3} \frac{2}{3} V_{pds} \cos \varphi$$
$$t_y = -V_{pds} \cos \varphi$$
$$t_z = \cos \varphi \left( \sin^2 \varphi - \frac{1}{2} \cos^2 \varphi \right) V_{pds} - \sqrt{3} \cos \varphi \sin^2 \varphi V_{pdz},$$  (8)

where the angle $\varphi$ is defined in the main text. The matrix elements between Bloch states of orbitals of M and X atoms at $\vec{q}$ read:

$$\langle M_{3z^2-r^2} | H_{TB} | X (b) p_y \pm i\tau p_x\rangle = \sum_\delta e^{-i\vec{q} \cdot \hat{\delta}} t_z \left( \hat{y} \pm i\hat{x} \right) \cdot \hat{\delta}$$

$$\langle M_{x^2-y^2} + \tau id_{xy} | H_{TB} | X (b) p_y \pm \tau p_x\rangle = \sum_\delta e^{-i\vec{q} \cdot \hat{\delta}} \left[ \hat{x} \cdot \hat{\delta} \right] \left[ 2 \left( \hat{x} \cdot \hat{\delta} \right)^2 - 2i\tau \left( \hat{y} \cdot \hat{\delta} \right)^2 + i\tau - 1 \right] +$$

$$+ \sum_\delta e^{-i\vec{q} \cdot \hat{\delta}} \left( \hat{y} \pm i\tau \hat{x} \right) \cdot \hat{\delta}_\perp \times \left[ 2 \left( \hat{\delta} \cdot \hat{x} \right) \left( \hat{\delta}_\perp \cdot \hat{x} \right) - 2i\tau \left( \hat{\delta} \cdot \hat{xy} \right) \left( \hat{\delta}_\perp \cdot \hat{y} \right) \right]$$  (9)

where the unit vectors are defined as:

$$\hat{x} = (1, 0)$$
$$\hat{y} = (0, 1)$$
$$\hat{xy} = \frac{1}{\sqrt{2}} (1, 1)$$

and $\hat{\delta}_\perp = (\delta_y, -\delta_x)$

(10)

and $\hat{\delta} = (\delta_x, \delta_y)$ are the three unit vectors connecting nearest-neighbors in the honeycomb lattice:

$$\hat{\delta} = \left\{ \hat{y}, \left( \frac{\sqrt{3}}{2}, \frac{1}{2} \right), \left( -\frac{\sqrt{3}}{2}, -\frac{1}{2} \right) \right\}$$  (11)

This model for the case of MoS$_2$ leads to the electronic bands shown in Fig. 4.
\[
\begin{align*}
-+ &= t_x \\
+- &= t_y \\
+- &= t_z \\
\end{align*}
\]

FIG. 3: Hopping integrals considered in the tight-binding model.

| Tight-binding parameter | Value (eV) |
|-------------------------|------------|
| \(\Delta_0\)           | -1.512     |
| \(\Delta_2\)           | -3.025     |
| \(\Delta_p\)           | -1.276     |
| \(V_{pd\sigma}\)       | -2.619     |
| \(V_{pd\pi}\)          | -1.396     |

TABLE II: Tight-binding parameters considered in the calculation. The values for MoS\(_2\) are taken from Ref. 2.

\[\mathbf{k} \cdot \mathbf{p} \text{ theory}\]

At \(\mathbf{K}_\tau\) points the Hamiltonian in first quantization reads as the matrix:

\[
\begin{pmatrix}
\Delta_0 & 0 & 3t_z & 0 \\
0 & \Delta_2 & 0 & -3(t_x + t_y) \\
3t_z & 0 & \Delta_p & 0 \\
0 & -3(t_x + t_y) & 0 & \Delta_p \\
\end{pmatrix}
\]

(12)

FIG. 4: Bands calculated within the tight-binding model described in the text. The model is only valid around \(\mathbf{K}_\tau\) points (highlighted in the figure). We take the values summarized in Table II for MoS\(_2\).
By diagonalizing this Hamiltonian we obtain the eigenvectors of the Bloch states maximally localized at $d_{3z^2-r^2}$ and $d_{x^2-y^2} + i\tau d_{xy}$ respectively, which define the conduction and band states respectively:

$$|\psi_c\rangle = \frac{1}{\sqrt{1 + |c|^2}} \begin{pmatrix} 1 \\ 0 \\ c \\ 0 \end{pmatrix}$$

$$|\psi_v\rangle = \frac{1}{\sqrt{1 + |v|^2}} \begin{pmatrix} 0 \\ 1 \\ 0 \\ v \end{pmatrix}$$

(13)

where:

$$c = -\frac{6t_z}{\sqrt{36t_z^2 + (\Delta_p - \Delta_0)^2 + \Delta_p - \Delta_0}}$$

$$v = \frac{6 (t_x + t_y)}{\sqrt{36 (t_x + t_y)^2 + (\Delta_p - \Delta_2)^2 + \Delta_p - \Delta_2}}$$

(14)

Then, the $k \cdot p$ Hamiltonian is just:

$$\mathcal{H}_{k \cdot p} = \begin{pmatrix} \langle \psi_c | \mathcal{H}_{TB} | \psi_c \rangle & \langle \psi_c | \mathcal{H}_{TB} | \psi_v \rangle \\ \langle \psi_v | \mathcal{H}_{TB} | \psi_c \rangle & \langle \psi_v | \mathcal{H}_{TB} | \psi_v \rangle \end{pmatrix}$$

(15)

If we write $\vec{q} = \mathbf{K}_r + \vec{k}$ and expand in powers of $\vec{k}$ up to first order we get the Hamiltonian of Eq. (1) of the main text with:

$$\Delta = \frac{1}{2} \left( \Delta_0 - \Delta_2 - \sqrt{36t_z^2 + (\Delta_0 - \Delta_p)^2} - \sqrt{36 (t_x + t_y)^2 + (\Delta_2 - \Delta_p)^2} \right) = 1.41 \text{ eV}$$

$$t = \frac{\sqrt{3} [c(t_x - t_y) + vt_z]}{2\sqrt{1 + |c|^2}\sqrt{1 + |v|^2}} = 1.19 \text{ eV}$$

(16)

**Coupling with strain**

We repeat this calculation by considering the change in the hopping integrals $t_{x,y,z}$ due to the displacement of the atoms. For the hopping integral between atoms at sites $\alpha, \beta$ we have:

$$t_{\alpha\beta} \rightarrow t_{\alpha\beta} + \frac{\partial t_{\alpha\beta}}{\partial \mathbf{r}} (\mathbf{u}_\alpha - \mathbf{u}_\beta)$$

(17)

where $\mathbf{u}_\alpha(\beta)$ is the displacement of the atom at site $\alpha (\beta)$. For small displacements we can approximate:

$$\frac{\partial t_{\alpha\beta}}{\partial \mathbf{r}} \approx \frac{\sqrt{3}}{a} t_{\alpha\beta} \beta_{\alpha\beta} \delta_{\alpha\beta}$$

$$\mathbf{u}_\alpha - \mathbf{u}_\beta \approx \frac{a}{\sqrt{3}} \beta_{\alpha\beta} \cdot \mathbf{\delta u}$$

(18)

where $\beta_{\alpha\beta} = -\partial \ln t_{\alpha\beta}/\partial \ln a$ is the Grüneisen parameter associated to $t_{\alpha\beta}$. Therefore, in the the previous matrix elements we have to consider now:

$$t_{x,y,z} \rightarrow t_{x,y,z} (1 + \beta_{x,y,z} \delta_{ij} u_{ij})$$

(19)
where \( u_{ij} \) are the components of the strain tensor. By repeating the previous calculation at \( \mathbf{K}_r \) we obtain the Hamiltonian of Eq. (2) of the main text with:

\[
\begin{align*}
t_\beta_0 &= \frac{3}{2} \left( \frac{c_\beta x t_x - v (\beta_x t_x + \beta_y t_y)}{1 + |c|^2} \right) \\
t_\beta_1 &= \frac{3}{2} \left( \frac{c_\beta x t_x + v (\beta_x t_x + \beta_y t_y)}{1 + |v|^2} \right) \\
t_\beta_2 &= \frac{3 (c_\beta x t_x - c_\beta y t_y - v \beta_z t_z)}{4 \sqrt{1 + |c|^2} \sqrt{1 + |v|^2}} \quad (20)
\end{align*}
\]

Gaps induced by superlattice potentials and Haldane-Kane-Mele phase

We next provide the details of how a superlattice can be used to induce the subbands conduction and valence bands of a doped TMDCs. We approximate the bands of the homogeneous system by the two-band continuum-limit Hamiltonian introduced above, whose eigenvalues and eigenfunctions read:

\[
\begin{align*}
\epsilon_\mathbf{k} &= \pm \sqrt{\Delta^2 + (v |\mathbf{k}|)^2} \\
|\mathbf{\tilde{k}}\rangle &= \begin{pmatrix} \cos \left( \frac{\theta_\mathbf{k}}{2} \right) \\ \sin \left( \frac{\theta_\mathbf{k}}{2} \right) \end{pmatrix} e^{i\phi_\mathbf{k}} \quad (21)
\end{align*}
\]

where \( \theta_\mathbf{k} = \arctan(|vF| \mathbf{k}|)/\Delta \) and \( \phi_\mathbf{k} = \arctan(k_y/k_x) \).

A superlattice potential hybridizes states \( |\mathbf{k}\rangle \) and \( |\mathbf{k} + \mathbf{G}\rangle \) where the vectors \( \mathbf{G} \) define the superlattice. We consider the six lowest vectors \( \mathbf{G} \), with \( |\mathbf{G}| = (4\pi)/\sqrt{3L} \), where \( L = Na \) is the lattice constant of the \( N \times N \) superlattice. We assume that \( v|\mathbf{G}| \ll \Delta \) and that the superlattice potential, \( V_\mathbf{G} \), is such that \( V_\mathbf{G} \ll (v|\mathbf{G}|)^2/(2\Delta) \), so that perturbation theory in \( V_\mathbf{G} \) applies. We also assume that the lattice potential is sufficiently smooth, \( |\mathbf{G}| \ll |\mathbf{K}_+ - \mathbf{K}_-| \), where \( \mathbf{K}_\pm \) are the corners of the Brillouin Zone of the TMDC lattice, and neglect intervalley scattering.

Using first order perturbation theory, each set of three points at corners of the Brillouin Zone connected by superlattice reciprocal vectors leads to a \( 3 \times 3 \) matrix:

\[
\mathcal{H}_{\kappa,\kappa'} = \begin{pmatrix}
\epsilon_{\kappa,\kappa'} \pm \bar{v} k_x & V_{\kappa,\kappa'} & V_{\kappa,\kappa'}^* \\
V_{\kappa,\kappa'}^* & \epsilon_{\kappa,\kappa'} \pm \bar{v} \left( -\frac{k_y}{2} + \frac{\sqrt{3} k_y}{2} \right) & V_{\kappa,\kappa'} \\
V_{\kappa,\kappa'} & V_{\kappa,\kappa'}^* & \epsilon_{\kappa,\kappa'} \pm \bar{v} \left( -\frac{k_y}{2} - \frac{\sqrt{3} k_y}{2} \right)
\end{pmatrix} \quad (22)
\]

where \( \epsilon_{\kappa,\kappa'} = \epsilon_0 + (v|\mathbf{K}|)^2/(2\Delta) \), \( \bar{v} \approx (v^2|\mathbf{K}|)/\Delta \), and the two signs correspond to the \( \kappa \) and \( \kappa' \) points. For \( V_{\kappa,\kappa'} = |V_{\kappa,\kappa'}| e^{i\phi_{\kappa,\kappa'}} \), the the energies and eigenfunctions at the \( \kappa \) and \( \kappa' \) points, in the basis used to write eq.(22) are:

\[
\begin{align*}
\epsilon_a &= \epsilon_0 + 2 |V_{\kappa,\kappa'}| \cos (\phi_{\kappa,\kappa'}) \\
\epsilon_b &= \epsilon_0 + 2 |V_{\kappa,\kappa'}| \cos \left( \frac{2\pi}{3} + \phi_{\kappa,\kappa'} \right) \\
\epsilon_c &= \epsilon_0 + 2 |V_{\kappa,\kappa'}| \cos \left( \frac{4\pi}{3} + \phi_{\kappa,\kappa'} \right)
\end{align*}
\]

\[
\begin{align*}
|a\rangle &= \frac{1}{\sqrt{3}} \left( |1\rangle + |2\rangle + |3\rangle \right) \\
|b\rangle &= \frac{1}{\sqrt{3}} \left( |1\rangle + e^{2\pi i/3} |2\rangle + e^{-2\pi i/3} |3\rangle \right) \\
|c\rangle &= \frac{1}{\sqrt{3}} \left( |1\rangle + e^{-2\pi i/3} |2\rangle + e^{2\pi i/3} |3\rangle \right) \quad (23)
\end{align*}
\]

In the case of \( \phi_{\kappa,\kappa'} = 0, \pi \), then \( V_{\kappa,\kappa'} \) real, an expansion in powers of \( |\mathbf{K}| \) shows that states \( |b\rangle \) and \( |c\rangle \) define an effective \( 2 \times 2 \) Dirac Hamiltonian with velocity \( \bar{v}/2 \). For \( \phi_{\kappa,\kappa'} = 0 \) this Dirac point gives the lowest edge of the highest valence subband, and for \( \phi_{\kappa,\kappa'} = \pi \) the upper edge of the lowest conduction band. The degeneracy of these Dirac points is lifted for complex values of \( V_{\kappa,\kappa'} \). The problem is equivalent to a gapped Dirac equation with gap \( \Delta_{\kappa,\kappa'} = 2\sqrt{3}|V_{\kappa,\kappa'}| \sin (\phi_{\kappa,\kappa'}) \). If \( \phi_{\kappa'} \) and \( \phi_{\kappa''} \) have different signs, the two gaps also have opposite signs, leading to a lowest subband with a Chern number equal to one. This is a realization of Haldane’s model [3].
Ref. 4, we define the functions: divided into scalar, mass and vector components, which, in turn, can be even or odd under spatial inversion. Following potential.

FIG. 5: (Color online). Sketch of the effect of the Brillouin Zone in a superlattice, and states mixed by the superlattice potential.

The superlattice potential is a $2 \times 2$ matrix in the space span by conduction and valence band states, and can be divided into scalar, mass and vector components, which, in turn, can be even or odd under spatial inversion. Following Ref. 4, we define the functions:

$$f_1 (r) = \sum_{m=0...5} e^{iG_m \cdot r}$$

$$f_2 (r) = i \sum_{m=0...5} (-1)^m e^{iG_m \cdot r}$$

(24)

Then, we can construct the inversion-symmetric superlattice potentials as:

$$V_s = v |G| \Delta_s f_1 (r)$$

$$V_m = v |G| \Delta_m f_1 (r) \sigma_z$$

$$V_g = v \Delta_g (\sigma_x, \sigma_y) \cdot (\hat{z} \times \nabla) f_2 (r)$$

(25)

The coefficients $\Delta_{s,m,g}$ in these expressions are dimensionless phenomenological constants with the energy scale set by $v |G| = \frac{4\pi}{\sqrt{N}}$.

The scalar potential has matrix elements:

$$\langle k + G_m | V_s (G_m) | k \rangle = v |G| \Delta_s \left[ \cos \left( \frac{\theta_k + G_m}{2} \right) \cos \left( \frac{\theta_k}{2} \right) + \sin \left( \frac{\theta_k + G_m}{2} \right) \sin \left( \frac{\theta_k}{2} \right) e^{i(\phi_k - \phi_{k+G_m})} \right]$$

(26)

Equivalently for the mass potential:

$$\langle k + G_m | V_m (G_m) | k \rangle = v |G| \Delta_m \left[ \cos \left( \frac{\theta_k + G_m}{2} \right) \cos \left( \frac{\theta_k}{2} \right) - \sin \left( \frac{\theta_k + G_m}{2} \right) \sin \left( \frac{\theta_k}{2} \right) e^{i(\phi_k - \phi_{k+G_m})} \right]$$

(27)

The edges of the first subband are determined by the shifts in the energies of the corners of the superlattice Brillouin Zone. We assume that $|k| = |k + G_m| = \kappa = (4\pi)/(3Na)$. Then:

$$\langle k + G_m | V_{s,m} (G_m) | k \rangle \approx v |G| \Delta_{s,m} \left[ 1 - \frac{v^2 \kappa^2}{4\Delta^2} \left( 1 \mp e^{i(\phi_k - \phi_{k+G_m})} \right) \right]$$

(28)

For the gauge potential we have:

$$\langle k + G_m | V_g (G_m) | k \rangle \approx (-1)^m \frac{v \kappa}{\Delta} |G| \Delta_g e^{i(\phi_k - \phi_{k+G_m})} \cos \left( \frac{m\pi}{3} - \frac{\phi_k + \phi_{k+G_m}}{2} \right)$$

(29)
The same can be done with the inversion-asymmetric superlattice potentials, defined as:

\[ \tilde{V}_s = v |G| \tilde{\Delta}_s f_2 (r) \]
\[ \tilde{V}_m = v |G| \tilde{\Delta}_m f_2 (r) \sigma_z \]
\[ \tilde{V}_g = v \tilde{\Delta}_g (\sigma_x, \tau_z \sigma_y) \cdot (\hat{z} \times \nabla) f_1 (r) \]

(30)

By repeating the same calculation we obtain:

\[ \langle \mathbf{k} + G_m | \tilde{V}_{s,m} (G_m) | \mathbf{k} \rangle \approx i (-1)^m v |G| \tilde{\Delta}_{s,m} \left[ 1 - \frac{v^2 \kappa^2}{4 \Delta^2} \left( 1 \mp e^{i(\phi_k - \phi_{k+G_m})} \right) \right] \]
\[ \langle \mathbf{k} + G_m | \tilde{V}_g (G_m) | \mathbf{k} \rangle \approx -i \frac{v \kappa}{\Delta} v |G| \tilde{\Delta}_g e^{i \frac{2 \kappa - \phi_k + G_m}{2} \cos \left( \frac{m \pi}{3} - \frac{\phi_k + \phi_{k+G_m}}{2} \right) } \]

(31)

From this analysis it is clear that inversion-asymmetric potentials are needed in order to induce a topological subband structure. To the leading order in \( v \kappa / \Delta \), considering scalar potentials only, we have:

\[ V_\kappa = \langle \kappa_1 = \kappa_2 + G_4 | V_s (G_4) + \tilde{V}_s (G_4) | \kappa_2 \rangle = v |G| \left( \Delta_s + i \tilde{\Delta}_s \right) \]
\[ V_{\kappa'} = \langle \kappa'_1 = \kappa'_2 + G_1 | V_s (G_1) + \tilde{V}_s (G_1) | \kappa'_2 \rangle = v |G| \left( \Delta_s - i \tilde{\Delta}_s \right) \]

(32)

So \( V_{\kappa,\kappa'} = v |G| \sqrt{\Delta_s^2 + \tilde{\Delta}_s^2} \times e^{\pm i \arctan \left( \frac{\Delta_s}{\tilde{\Delta}_s} \right) } \). Hence, the gap is \( \Delta_{\kappa,\kappa'} = \pm 2 \sqrt{3} v |G| \tilde{\Delta}_s \). Either the lowest conduction or valence subbands derived from the bands at a given spin polarized valley in the band structure of the TMDC have a Chern number equal to one. This Chern number is compensated by the opposite value from the other valley due to time-reversal symmetry. Therefore, this system is effectively a realization of the Kane-Mele model [5].

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