Three-Dimensional Fractional Topological Insulators in Coupled Rashba Layers

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(Dated: April 18, 2018)

We propose a model of three-dimensional topological insulators consisting of weakly coupled electron- and hole-gas layers with Rashba spin-orbit interaction stacked along a given axis. We show that in the presence of strong electron-electron interactions the system realizes a fractional strong topological insulator, where the rotational symmetry and condensation energy arguments still allow us to treat the problem as quasi-one-dimensional with bosonization techniques. We also show that if Rashba and Dresselhaus spin-orbit interaction terms are equally strong, by doping the system with magnetic impurities, one can bring it into the Weyl semimetal phase.

I. INTRODUCTION

In recent years, the study of topological phases of matter has become one of the prominent subjects in condensed matter research. Soon after the theoretical prediction and experimental confirmation of topological band insulators (TI) in two (2D)1-5 and three dimensions (3D)6-9, it was theoretically shown that the class of topologically non-trivial matter is much larger and the corresponding phases even more exotic once interacting systems are considered that can allow phases hosting gapless excitations with fractional charges or spin quantum numbers10-12. The realization of such unconventional phases in Nature is not only of fundamental interest, but also promising for applications such as topological quantum computation, where Fibonacci anyons can serve as qubits which allow for universal quantum computation13. However, the basic ingredients for obtaining a Fibonacci phase are parafermions, also called fractional Majorana fermions, which emerge only in the presence of electron-electron interactions. Many proposal for experimental realizations of parafermions rely on a combination of superconductivity and fractional TIs14-19. So far, fractional TIs still lack experimental realization and it is thus of great importance searching for models possibly realizable in future experiments.

It is the purpose of this Letter to introduce a model which shows how, in principle, a 3D fractional TI can be engineered. We generalize the approach of weakly coupled wires20 to 3D by considering a stack of weakly coupled 2DEG layers. Although the coupled wires approach is a very successful method for theoretically constructing 2D12,20-22 and 3D32-34 topological systems, the coupled layers approach24 is simpler to handle and is physically more transparent when describing 3D systems. We consider a stack of 2D layers with Rashba spin-orbit interaction (SOI) weakly tunnel coupled to each other. Such a system could be realized in a semiconductor superlattice where the 2DEGs form at heterojunctions and the SOI can be controlled with electrical gates25-27. Alternatively, one could realize our setup in a van der Waals heterostructure, by stacking a carefully chosen sequence of different atomically thin layers on top of each other28-30.

The paper is organized as follows. In Section II we introduce the system composed of weakly coupled layers. In Section III we study its properties in the non-interacting regime. We derive the bulk spectrum, discuss the computation of the topological invariant, and show the existence of gapless surface states using analytical and numerical methods. We conclude that the non-interacting model realizes a 3D TI. This sets the stage for the main part of the work presented in Section IV—the fractional topological phase. We identify the regime where the interacting system forms a fractional strong 3D TIs32-34 in the regime of strong electron-electron interactions. The main idea of the analysis is to search for solutions minimizing the energy of the system, which translates into maximizing the size of the gap opened by backscattering-assisted tunneling processes and should stabilize the system, similar to nesting conditions discussed before in various systems34-47. Importantly, the condensation energy gain is maximum for processes that do not break the rotational and translation symmetries of the system34,48. This helps us to reduce the problem effectively to one dimension where we can then use bosonization and Luttinger liquid techniques to show the existence of fractionally charged surface states with a non-degenerate helical Dirac cone spectrum in the topological phase. Additionally, in Section V we discuss how an equal combination of Rashba and Dresselhaus SOI leads to a Weyl semimetal phase in non-interacting systems. We summarize our results in Section VI.
dimensional electron gas (2DEG) layers stacked along the 
respectively [see Eqs. (12) and (13)]

Each layer has a SOI of Rashba type. The strength of 
consists of four layers, two of which have an electron-like 
indices to label the layers:

ternates its sign from layer to layer. We introduce two 
sisted by backscattering dominate resulting in the bulk gap .

The orange and black arrows represent terms in 
In the presence of strong interactions, tunneling processe s as-

servation laws. (b) The chemical potential is tuned to 

\( \eta_\tau \sigma \sigma_\sigma \) are tuned 
to the SOI energy 
\( E_{\text{so}} \)

to the unit cell but al-

\( \eta_\tau \sigma \sigma_\sigma \)

\( \eta, \tau, \sigma, \theta \) = \( (1, -i \eta \tau \sigma e^{i \theta})^T / \sqrt{2} \),

where the \( \theta \) is the angle between the 2D momentum vector 
and the \( k_z \) axis.

In the following, we consider spin-conserving tunneling 
between layers. For a tunneling process of amplitude 
\( t_1, t_2 \) between layers of the same (opposite) mass the Hamiltonian is given by

\[
H_{t_2} = t_2 \sum_{n \sigma} \int dx dy \left( \Psi_{n11}^\dagger \Psi_{(n-1)11} + \Psi_{n11}^\dagger \Psi_{n11} + \text{H.c.} \right),
\]

\[
H_{t_1} = t_1 \sum_{n \sigma \eta} \int dx dy \left( \Psi_{n11}^\dagger \Psi_{n11}^\eta + \text{H.c.} \right).
\] (3)

Without loss of generality, we assume that 
\( t_1, t_2 \geq 0 \).

**III. THREE DIMENSIONAL STRONG TOPOLOGICAL INSULATOR**

**A. Bulk Spectrum and Symmetry Class**

To begin with, we show that there is a bulk gap at \( \mu = 0 \) 
and the symmetry class the Hamiltonian falls into is AII.

In order to do so, we first consider an infinite system and introduce momenta \((k, k_z)\). The total Hamiltonian is given by 

\[
H = H_0 + H_{t_1} + H_{t_2} \quad \text{[see Eqs. (11)–(3) and (6)]}
\]

with the exact bulk spectrum

\[
E_{\pm}(k, k_z) = \epsilon^2 + (\alpha k)^2 + (t_1^2 + t_2^2)
\]

\[
\pm 2{\sqrt{(\alpha k)^2 \epsilon^2 + t_1^2 \epsilon^2 + t_2^2 \epsilon^2}} \cos^2(k_z a_z / 2),
\] (4)

where \( \epsilon(k) = \hbar^2 k_z^2 / 2m \).

If \( t_1 \neq t_2 \) and \( t_2 > 0 \), the bulk is fully gapped.

If \( t_1 = t_2 > 0 \), the bulk gap closes at 
\( (k, k_z) = (0, 0) \).

The system can be tuned into topological 
\((t_1 > t_2)\) and trivial \((t_2 > t_1)\) phase, as shown below.

In order to discuss the symmetry class of the Hamiltonian we rewrite the total Hamiltonian in terms of Pauli matrices \( \sigma_i \), \( \eta_i \), and \( \tau_i \) acting in spin and layer space, respectively. As a result, we obtain

\[
H = \int dkd\bar{z} \Psi^\dagger(k, k_z) h(k, k_z) \Psi(k, k_z),
\] (5)

\[
h(k, k_z) = \left[ \frac{\hbar^2 (k_x^2 + k_y^2)}{2m} - \mu \right] \eta_3 + \alpha \tau_3 (\sigma_1 k_y - \sigma_2 k_x) + t_1 \tau_1
\]

\[
+ t_2 \left[ \cos^2(k_z a_z / 2) \eta_1 \tau_1 + \sin^2(k_z a_z / 2) \eta_2 \tau_2 + \sin(k_z a_z) (\eta_1 \tau_2 + \eta_2 \tau_1) / 2 \right].
\] (6)
The Hamiltonian is invariant under time reversal operation $\Theta = i\sigma_y \mathcal{K}$, where $\mathcal{K}$ is the complex conjugation operator. In the Altland-Zirnbauer classification, there are three symmetry classes with $\Theta^2 = -1$, two of which have additional particle-hole symmetry. Under particle-hole transformation $C$ the Bloch Hamiltonian has to satisfy $C \mathcal{H}^\dagger C^{-1} = -\mathcal{H}(k, k)$, No such operator could be found for $h(k, k)$ [see Eq. (5)] and it therefore belongs to the AII symmetry class. In three dimensions, the system is classified by a $\mathbb{Z}_2$ invariant and can be a strong topological insulator hosting single helical Dirac cones at each surface.

We end this subsection by computing the topological invariant explicitly following Ref. 52. We derive an effective Hamiltonian by identifying the low-energy bands that close at the phase transition and the level crossing wave vector and then expand the Hamiltonian around these points. From our analysis we know that the topological phase transition takes place at $t_1 = t_2$, and the gap closes at $(k, k_x) = (0, 0)$. Expanding Eq. (6) around this momentum point and performing a unitary transformation, the Hamiltonian can be brought into a form consisting of two decoupled $4 \times 4$ blocks containing the low-energy and high-energy bands. The low-energy bands undergo the topological phase transition at $t_1 = t_2$. Projecting onto the subspace containing these low-energy bands that close at the critical point, one obtains the effective Hamiltonian given by

$$h_{\text{eff}}(k, k_x) = \alpha k_x \sigma_2 - \alpha k_y \sigma_3 + \frac{\alpha_2}{2} k_x n_2 \sigma_3 + M n_1 \sigma_3, \quad (7)$$

where we introduced the mass $M = t_1 - t_2$. Using this simplified Hamiltonian, one can calculate the $\mathbb{Z}_2$ invariant $\nu_0$ explicitly. We find that $\nu_0 = 1$ ($\nu_0 = 0$) if $M > 0$ ($M < 0$). We note that the same Hamiltonian was studied before in Ref. 52, where it was shown that $h_{\text{eff}}(k, k_x)$ [Eq. (7)] corresponds to a 3D strong TI.

B. Existence of Surface States

The presence of one helical Dirac cone at any surface is a central feature of a strong TI. In this subsection, we show the existence of these surface states in the topological regime $t_1 > t_2$ using analytical and numerical methods. First, we prove the existence of surface states on the top and bottom surface of the stack, i.e. at the boundaries orthogonal to the stacking direction. To this end, we restrict the discussion to the low-energy regime and perform a linearization of the Hamiltonian by assuming $t_1, t_2 \ll E_{\text{so}}$. We represent the momentum in polar coordinates to exploit the rotational symmetry of the layers. Being functions of good quantum numbers, the modulus $k$ and the polar angle $\theta$ are constants for $k_x$ and $k_y$ fixed. The spectrum of each layer is isotropic and, therefore, independent of $\theta$, which means that there are only fluctuations in $k$ direction. States with different $\theta$ are decoupled from each other and we can treat the problem as effectively one-dimensional in direction of propagation $r^z$.

We linearize the spectrum and represent the field operators around the Fermi surface (FS) in terms of slowly varying fermionic field operators $S^\alpha_\beta(n)\dagger$. We first take into account the fields that are uncoupled to each other and we can treat the problem decoupled from each other and we can treat the problem.

$$\Psi_{\alpha_\beta n \eta \tau}(x, y) = \sum_{\delta} \alpha_{\delta_\beta n \eta \tau} c^{\delta_\beta n \eta \tau} e^{i(\delta_\beta n \eta \tau \bar{k}_F x \cos \theta + y \sin \theta)}, \quad (8)$$

where $\delta = e, i$ labels the exterior ($\theta \equiv 1$) and interior ($\theta \equiv 0$) FS, with corresponding Fermi momenta $k_F^e = 2m_\alpha / \hbar^2$ and $k_F^i = 0$. Here, $\beta, \tau \equiv 0, 1$ refers to ‘right’ (1) and ‘left’ (0) movers propagating in opposite $r$-directions. In this representation the polar angle $\theta$ is restricted to $[0, \pi]$. The spin overlap amplitude is given by $\alpha_{\delta_\beta n \eta \tau} = \langle \sigma | n, \tau, \delta, \theta + \pi - \eta \beta \rangle / 2$. The linearized kinetic term [see Eq. (1)] becomes $H_0 = \int dr \bar{\mathcal{H}}_0(r) \mathcal{H}_0(r)$ with $v_F = \alpha / \hbar$ is the Fermi velocity.

We next employ a two-step perturbation approach by considering the regime $t_1 \gg t_2$. We first take into account the $t_1$ tunnelings and obtain after linearization,

$$\bar{\mathcal{H}}_{t_1} = t_1 \sum_{n=1}^N \sum_{\theta_0} \left( S^\alpha_{n \eta_0 1} \right) \left( S^\beta_{n \eta_0 1} \right) \left( \bar{\mathcal{H}}_{n \eta_0 1} + \text{H.c.} \right). \quad (10)$$

Important, $\bar{\mathcal{H}}_{t_1}$ couples fields of opposite velocities at $k = 0$ resulting in a partial gap (see also Fig. 2b). In a next step, we take into account the fields that are unaffected by the $t_1$-term and neglect the already gapped fields. Analogously, one obtains

$$\bar{\mathcal{H}}_{t_2} = t_2 \sum_{\theta_0} \left( \sum_{n=1}^N \left( S^\alpha_{n \eta_0 1} \right) \left( S^\beta_{n \eta_0 1} \right) + \sum_{n=1}^N \left( S^\alpha_{n \eta_0 1} \right) \left( S^\beta_{n \eta_0 1} \right) + \text{H.c.} \right). \quad (11)$$

These terms gap out the remaining fields in the bulk but do not affect the two fields at the top, $S^e_{N_{\eta_0 1}}$ and at the bottom, $S^i_{N_{\eta_0 1} 1}$, of the stack, since they do not appear in Eq. (11). These surface states are gapless, have a linear dispersion and the spin of each state is locked to be orthogonal to its momentum, in other words, they form a single helical Dirac cone at each of the two surfaces. We remark that starting the perturbative analysis in the opposite regime $t_2 \gg t_1$ all fields at the top and bottom surfaces are gapped and the system is in the trivial insulating state. The result obtained in the perturbative regimes smoothly connects to the region of the phase diagram where $t_1 > t_2$, and due to their topological nature the gapless surface states persist over the whole parameter range, see Fig. 3.

To access the spectrum of the, say, $xz$ surface at $y = 0$, we employ numerical diagonalization (see Appendix for more details) and consider the system finite in $y$-direction with $N_x$ lattice sites. The spectrum of the tight-binding Hamiltonian [see Eq. (22)] in the topological phase is
shown in Fig. 3. It can be seen that the bulk states are separated by an energy gap and that there exist states with a Dirac spectrum. In Fig. 4 we show the modulus squared of the wavefunction of a state on the Dirac cone on the first hundred lattice sites. One can observe that, indeed, the state is localized at the surface of the system and therefore conclude that the Dirac cone is represented by an anisotropic Dirac cone. The inset shows the helical spin structure in the layer $\eta = \tau = 1$ at $y/a_y = 1$ for $E/t = 0.02$ (dashed line), confirming the presence of a single helical Dirac cone at the $xz$-surface.

emphasize that the gapless surface states were obtained in a non-perturbative regime which proves that their existence does not rely on the perturbative approach considered above, underlining their topological nature.

For completeness we also show the spectrum in the region $t_1 < t_2$ which is separated by the gap closing line $t_1 = t_2$ from the region where we found the Dirac cone. As can be seen in Fig. 5 the spectrum is fully gapped and there are no surface states. The system is a trivial insulator in the whole region where $t_1 < t_2$. This analysis confirms that for $t_1 > t_2$ ($t_1 < t_2$), the strong topological $Z_2$ invariant $\nu_0$ is given by $\nu_0 = 1$ ($\nu_0 = 0$), which is consistent with our analysis above.

To emphasize the topological origin of surface states, we show their stability against non-magnetic disorder. In order to do so, we modified our tight-binding model to implement detuning of the chemical potential in the $(\eta, \tau)$-layer at lattice site $i$ by $\delta \mu_{i\eta\tau}$. The perturbations were randomly generated from a normal distribution centered at $\langle \delta \mu \rangle = 0$ and the variance characterizing the disorder strength was chosen such that $\sqrt{\langle \delta \mu^2 \rangle} < t_2$. As can be seen from Fig. 5 the surface states remain intact in the presence of non-magnetic disorder. There is no gap opening. Moreover, this analysis also confirms that our initial assumption of the rotational and translational symmetries is not crucial for the existence of the topological phase.

IV. FRACTIONAL TOPOLOGICAL INSULATOR

Next, our goal is to identify the regime in which the system is a fractional strong 3D TI. For this, we detune the chemical potential in $H_0$ [see Eq. (2)] to $\mu_{i\eta\tau} = E_{\eta\tau}/9$. This particular choice of $\mu$ fixes the ratio between the radii of the interior and exterior FS to $2k_F^i = k_F^e = 4ma/3h^2$. We, again, restrict the discus-
sion to the regime $t_1 \gg t_2$ and treat the $t_1$-terms first. The direct tunneling ($t_1$) between layers of the same mass is forbidden by spin/momentum conservation and do not result in a gap. Repulsive electron-electron interactions, however, open the channel for backscattering assisted tunneling which has a chance to open a gap. These processes consist of a tunneling with non-zero momentum transfer which is accompanied by two backscattering events (in leading order) ensuring overall momentum conservation. If the tunneling occurs between two states where the spins are misaligned, the tunneling amplitude gets suppressed by a factor of the spin overlap (see Fig. 7). Thus, we only take into account events where the tunneling amplitude and correspondingly the size of the bulk gap becomes maximal, which corresponds to processes preserving the rotational and translational symmetries of the system and do not mix states characterized by different values of $\ell$, see Fig. 2). Such processes similar to nesting conditions on Fermi surfaces allow us to maximize the condensation energy gain (also known as Peierls-type energy gain) and stabilize the topological phase (44–47).

The Hamiltonian density describing tunneling between layers of the same mass becomes (see also Fig. 2)

$$\mathcal{O}_{t_1} = g_{11} \sum_{n_i \eta \ell} \left[ \left( S_{n_i \eta \ell}^1 \right)^\dagger S_{n_i \eta \ell}^1 \left( S_{n_i \eta \ell}^1 \right)^\dagger S_{n_i \eta \ell}^1 \right] + \text{H.c.},$$

with $g_{11} = t_1 g_B^2$ and $g_B$ being the strength of the backscattering term due to interactions. For the $t_2$ processes we distinguish the cases where tunneling occurs between the interior (exterior) FS. The operator that commutes with the one in Eq. (12) is given in leading order by

$$\mathcal{O}_{t_2} = g_{22} \sum_{\ell \in \{1, 2\}} \left[ \left( S_{n_\ell}^{\dagger, \ell} \right)^\dagger S_{n_\ell}^{\dagger, \ell} \left( S_{n_\ell}^{\dagger, \ell} \right)^\dagger S_{n_\ell}^{\dagger, \ell} \right] + \text{H.c.},$$

with $g_{22} = t_2 g_B^2$ and where tunneling occurs between the exterior FSs. For brevity we use the index-dependent unit cell labels $n_i = n - (1 - l)/2$ and $n_\ell = n - (1 + l)/2$.

For completeness we give the expression for the second operator describing $t_2$ tunneling processes between the interior FS of layers with opposite mass

$$\mathcal{O}_{t_2} = g_{22} \sum_{\ell \in \{1, 2\}} \left[ \left( S_{n_\ell}^{\dagger, \ell} \right)^\dagger S_{n_\ell}^{\dagger, \ell} \left( S_{n_\ell}^{\dagger, \ell} \right)^\dagger S_{n_\ell}^{\dagger, \ell} \right] + \text{H.c.},$$

with $n_i$ and $n_\ell$ as above. While $\mathcal{O}_{t_1}$ and $\mathcal{O}_{t_2}$ commute, $\mathcal{O}_{t_2}$ does not commute with $\mathcal{O}_{t_1}$ and therefore these operators can not be diagonalized simultaneously. Thus, they leave the system gapless and, consequentially, do not result in an energy gain. Such terms can therefore be dropped.

The terms $\mathcal{O}_{t_1}$ and $\mathcal{O}_{t_2}$ open a gap in the bulk spectrum but in order to access the nature of the gapless surface states we employ the bosonization procedure for 1D systems. This is justified since in the limit of dominant tunneling, fields with different angles $\theta$ are not coupled.
Dresselhaus SOI by gate tuning\textsuperscript{55,62}, such that the spin gets coupled only to the momentum in one particular direction\textsuperscript{55,63}, a Weyl semimetal phase (WSM) can be realized in the same setup. The modified SOI term reads

$$\hat{H}_{\text{SOI}} = -i\alpha \sum_{n\eta\tau} \int dxdy \bar{\Psi}_{n\eta\tau}^\dagger (\sigma_1)_{\alpha\alpha'} \partial_y \Psi_{n\eta\tau'}. \quad (16)$$

As a result, the Hamiltonian density for each $\eta\tau$ layer is given by

$$\hat{H}_0(x,y) = \sum_{n\eta\tau} \bar{\Psi}_{n\eta\tau}^\dagger \left( \frac{\hbar^2}{2m} \nabla^2 - \mu \right) - i\tau \alpha \sigma_1 \partial_y \Psi_{n\eta\tau}. \quad (17)$$

In Refs.\textsuperscript{55-61} it was shown that combining Rashba and Dresselhaus SOI in a 2DEG can lead to a partial compensation of the two. The above term arises when Rashba and Dresselhaus SOI are of equal strength. The tunneling part of the total Hamiltonian $H_t$ + $H_\text{SOI}$ remains the same. From the above equation it is evident, that spin projection along the $x$-axis is a good quantum number $\sigma = \pm 1$. The total 8 × 8 Bloch Hamiltonian is block diagonal and can be written in terms of Pauli matrices as

$$\hat{h}(k) = \frac{\hbar^2}{2m} \eta_3 - \alpha k_y \sigma_1 \tau_3 + t_1 \tau_1$$

$$+ t_2 \left[ \cos^2(k_z a_z/2) \eta_1 \tau_1 + \sin^2(k_z a_z/2) \eta_2 \tau_2 \cos(k_z a_z) (\eta_1 \tau_2 + \eta_2 \tau_1)/2 \right]. \quad (18)$$

From now on $k$ denotes the 3D momentum and $k_0$ the in-plane momentum. The energy spectrum of this Hamiltonian is found to be

$$E_z^2 = \epsilon_\parallel^2 + t_1^2 + t_2^2 + (\alpha k_y)^2$$

$$\pm 2 \sqrt{\epsilon_\parallel^2 t_1^2 + (\alpha k_y)^2} t_2 \cos^2(k_z a_z/2), \quad (19)$$

with $\epsilon_\parallel = \hbar^2 k_0^2/2m$. If $t_1 < t_2$, the spectrum degenerates to a bulk gap. For $t_1 > t_2$ there are two doubly degenerate gapless bulk states at $\pm k_D$ with $k_D = (k_{z0}^*, 0, 0)$ and $k_{z0}^* = \sqrt{2m/\hbar^2} (t_2 - t_1^2)^{1/4}$. These are Dirac nodes hosting two Weyl nodes of opposite chirality at the same point. The two Weyl nodes are not coupled in the absence of disorder and, therefore, do not annihilate each other. Such Dirac nodes can, however, be stable only if additional crystal symmetries are present that stabilize these nodes\textsuperscript{55,66}. Next, we would like to eliminate the twofold degeneracy of the Dirac node by splitting it into two Weyl nodes. This can be achieved if the time-reversal symmetry is broken, for example, via magnetic impurities which order ferromagnetically (FM) along a direction orthogonal to the SOI direction, let say, in the $y$ direction\textsuperscript{63-66}. The exchange interaction between the electron spins and the magnetic impurities reads,

$$H_J = -J \sum_{n\eta\tau} \sum_{\alpha\alpha'} \int dx \bar{\Psi}_{n\eta\tau}(\sigma_2)_{\alpha\alpha'} \Psi_{n\eta\tau'}. \quad (20)$$

![FIG. 8: The Weyl semimetal spectrum for the parameters $t_1/E_{\text{so}} = 0.3$, $t_2/E_{\text{so}} = 0.19$, and $k_z = 0$. Left: Four Weyl nodes exist for weak exchange interaction ($J/E_{\text{so}} = 0.08$). Right: In the regime $|J - t_1| < t_2$, only two Weyl outer nodes remain ($J/E_{\text{so}} = 0.17$).](image)

V. WEYL SEMIMETAL PHASE

Remarkably, if the SOI is no longer of pure Rashba type but given by an equal combination of Rashba and

[\text{interaction terms become balanced and all other commutators vanish. In a more convenient basis defined as $\eta_\alpha = 2\phi_\alpha - \phi_{\alpha'}$, the above interaction terms become}]

$$\mathcal{O}_{t_2} = g_2 \sum_{n\eta\tau} \left[ \sum_{l=1}^N \cos(\eta_n^\dagger - \eta_n^\dagger l) + \sum_{n=2}^{N} \cos(\eta_n^\dagger - \eta_n^\dagger l) \right],$$

$$\mathcal{O}_{t_1} = g_1 \sum_{n\eta\tau} \cos(\eta_n^\dagger - \eta_n^\dagger l). \quad (15)$$

We work in the limit where $g_i$ are large compared to the quadratic part of the Hamiltonian and the fields get pinned to one of the minima of the cosine\textsuperscript{25,58}. Using Eqs.\textsuperscript{15}, we infer that all the fields in the bulk get pinned pairwise and, therefore, the bulk spectrum is fully gapped. However, as in the previous section, two fields at the top surface and two fields at the bottom surface do not appear in the tunneling terms, namely $\eta_{11111}$, $\eta_{11111}$, $\eta_{11111}$, and $\eta_{11111}$. These fields do not get pinned and stay gapless\textsuperscript{24}. We conclude that the interacting system hosts gapless surface states that have their spin locked orthogonal to their momentum. The quasi-particle excitations on the surface are directly given by the exponential of the gapless bosonic fields listed above. These excitations have been shown to carry fractional charge $q = e/2n$. This procedure can be generalized to other odd integers $n > 3$ to obtain fractional TIs with $q = e/n$. 

V. WEYL SEMIMETAL PHASE

Remarkably, if the SOI is no longer of pure Rashba type but given by an equal combination of Rashba and
with $J > 0$. Gapless states only exist in the $k_z = 0$ plane where the spectrum is given by
\[
\tilde{E}_{k_x,k_y,0} = \epsilon_0^2 + (J \pm t_1)^2 + t_2^2 + (\alpha k_y)^2 \\
\pm 2\sqrt{(\epsilon_0^2 + t_2^2)(J \pm t_1)^2 + \epsilon_0^2(\alpha k_y)^2}. \tag{21}
\]
If $|J - t_1| > t_2$ the bulk spectrum has four gapless states at $\pm k_a$ with $k_a = (k_{a,x}, 0, 0)$ and 
\[
k_{a,x} = \sqrt{\frac{2m}{\hbar^2}} (J \mp t_1)^2 - t_2^2 \]
This means that the initial twofold degeneracy gets lifted and we end up with four distinct nodes (see Fig. 8). The nodes at $k_a$ and $-k_a$ have opposite chirality (see Fig. 3). If the exchange interaction strength is tuned to $J = t_1 - t_2$, the two inner nodes meet and annihilate. As long as $|J - t_1| < t_2$, only the nodes at $\pm k_a$ exist, while at $J = t_1 + t_2$ the two inner nodes reappear and separate when $J$ is increased further.

In the Appendix B, we find explicitly spectrum and wavefunctions of surface states in the WSM phase. Here, we present the numerical spectrum obtained from a tight-binding model defined in Appendix A with polarized magnetic impurities in the regime $J < t_1 - t_2$, see Fig. 10. We confirm the existence of gapless bulk states and of surface states that are dispersionless in $x$ direction. The surface states have a linear dispersion in the $z$ direction as expected. In order to check the chirality of the Weyl nodes, we also access the spin structure of the states on the Weyl cones, see Fig. 4. Indeed, the overall chirality of four Weyl cones is zero. We note that the Weyl phase is defined strictly at the absence of disorder. Any finite disorder will scatter between Weyl cones as discussed in literature.

VI. CONCLUSIONS

We considered a layered system that realizes a 3D fractional strong TI. We constructed a simple model that solely consists of weakly coupled 2D layers with Rashba SOI. We also show that if Dresselhaus and Rashba SOI term are of the same strength, the system can be brought into the Weyl semimetal phase. The motivation for such setups is given by the vast progress in fabricating superlattices and van der Waals heterostructures. We believe that these engineered materials provide a promising route towards realizing 3D (fractional) TIs and Weyl semimetals as proposed in this work.

ACKNOWLEDGEMENTS

We acknowledge support from the Swiss National Science Foundation and NCCR QSIT, and the Marie Sklodowska-Curie Innovative Training Network (ITN-ETN) Spin-NANO.

APPENDIX A: TIGHT-BINDING MODELS

In Sect. III we address the question of whether a helical Dirac cone exists at any boundary numerically by implementing a tight-binding model for a system with $N_y$ lattice sites. We impose a hard wall boundary at $y = 0$ and consider the system to be infinitely extended along the $x$ and $z$ directions such that we can introduce momenta $k_x$ and $k_z$. The tight-binding Hamiltonian $H = \sum_{k_x,k_z} H_{k_x,k_z}$ for this setup reads

![Figure 9: Spin structure of the states on the Weyl cones at an energy of $E/t = 0.02$ at $y/a_y = 260$ ($N_y = 400$). For clarity we projected the spin onto the $k_x,k_z$ plane. The parameters used for the numerics are $t_1/t = 0.2$, $t_2/t = 0.1$, $\alpha/t = 0.4$, and $J/t = 0.07$.](image)

![Figure 10: Spectrum in the Weyl semimetal phase in half of the BZ as a function of momenta ($k_x, k_z$). The spectrum of semi-infinite system ($y > 0$) was obtained numerically [cf. Eq. 20] for $N_y = 800$, $\tilde{a}/t = 0.45$, $t_1/t = 0.3$, $t_2/t = 0.19$, and $J/t = 0.08$, i.e. in the regime $J < t_1 - t_2$ where we expect four Weyl nodes from the analytical analysis. The bulk (surface) states are colored in blue (green). The spectrum is cut in half along the line connecting the gap closing points. The spectrum indeed features two (since we show only one half) gapless points as well as the Fermi arcs. The gap is not closed exactly due to finite size effects.](image)
Here, \( c_{\eta \tau n \sigma} \equiv c_{\eta \tau n \sigma}c_{x}k_{y}k_{z} \) is the annihilation operator for an electron with spin \( \sigma \) in the layer \((\eta \tau)\) with momentum \((k_{x}, k_{y})\) at position \( y = na_{y} \), where \( a_{y} \) is the lattice constant along the \( y \) direction. The spin-flip hopping amplitude is related to the SOI parameter by \( \tilde{\alpha} = \alpha / 2a_{y} \) (we take the lattice constants \( a_{x} = a_{y} \)).

To describe the Weyl phase in Sect. V, we use the same Hamiltonian as in Eq. (22) besides adding exchange interaction term and modifying the SOI term, such as

\[
\tilde{H}_{1k_{x}k_{y}z} = t_{1} \sum_{n \sigma} \left[ c_{11n \sigma}^{\dagger}c_{11n \sigma} + c_{11n \sigma}^{\dagger}c_{11n \sigma} + \text{H.c.} \right],
\]

(24)

\[
H_{2k_{x}k_{y}z} = t_{2} \sum_{n \sigma} \left[ e^{-ik_{z}a_{z}}c_{11n \sigma}^{\dagger}c_{11n \sigma} + c_{11n \sigma}^{\dagger}c_{11n \sigma} + \text{H.c.} \right].
\]

(25)

with the magnetic impurities of the strength \( J \) polarized along \( y \) direction.

**APPENDIX B: Analytical Calculation of Surface States in Weyl Semimetal phase**

In this Appendix we explicitly show the analytical calculation of the surface states that appear in the WSM phase. We restrict the discussion to the regime where \( t_{1} - t_{2} < J < t_{1} + t_{2} \) with \( t_{1} > t_{2} \). Without loss of generality all three parameters are considered to be positive. In this range of the exchange interaction strength there exist two Weyl nodes at \( \pm \mathbf{k}_{z} \) (see above) and the associated Fermi arcs are located on the \( xz \) and \( xy \) surface BZ. For simplicity we calculate the surface states on the \( xz \) surface for \( y = 0 \). In order to perform the linearization of the Hamiltonian [see Eq. (15)] we again assume \( t_{1}, t_{2} \ll E_{so} \) (see also text above). The chemical potential is tuned to the Weyl nodes.

We start with the full 3D bulk Hamiltonian \( \tilde{h}(k_{x}, k_{y}, k_{z}) \). Since the Fermi arc is the line connecting the projections of the Weyl nodes on the corresponding surface BZ, it is clear that the surface states occur with \((k_{x}, 0)\) in the \( k_{x}k_{z} \) plane. Before linearization the Hamiltonian reads

\[
\tilde{h}(k_{x}, k_{y}, 0) = \frac{\hbar}{2m} (k_{x}^{2} + k_{y}^{2})\gamma_{3} - \alpha k_{y} \tau_{3} \sigma_{3} + t_{1} \tau_{1} + t_{2} \tau_{3} \gamma_{1} + J \sigma_{2}.
\]

(27)

For a clean surface \((k_{x}, k_{z})\) are good quantum numbers and we can solve Eq. (27) for fixed \( k_{x}, k_{z} \), i.e. the problem reduces to a one-dimensional problem solving for the zero-energy eigenstates of \( \tilde{h}_{k_{x}}(k_{y} \rightarrow -i \partial_{y}) \) \((k_{z} \text{ is fixed to zero})\). Since \( k_{z} \) is fixed in Eq. (27) we treat the term containing \( k_{x} \) as a detuning of the chemical potential from the spin-orbit energy. This procedure is justified since \( k_{x}^{2} \in [0, \frac{\hbar}{2m} \sqrt{(J + t_{1})^{2} - t_{2}^{2}}]\) and therefore \( k_{x}^{2} \) is bounded from above by \( k_{x}^{2} < \frac{4\hbar^{2}}{m^{2}} t_{2} \). This yields \( \delta \mu_{k_{x}} = \frac{\hbar^{2}k_{x}^{2}}{2m} < 4\sqrt{2} t_{1} \ll E_{so} \) in the perturbative regime \( t_{1}, t_{2} \ll E_{so} \).

Linearizing the Hamiltonian in Eq. (27) gives

\[
\tilde{h} = v_{F} \tilde{k} \gamma_{3} + t_{1} (\tau_{1} \gamma_{1} - \tau_{2} \gamma_{2}) / 2 + t_{2} \tau_{1} \gamma_{1} + J (\sigma_{2} \gamma_{1} + \sigma_{1} \tau_{2}) / 2 + \delta \mu_{k_{x}} \eta_{1},
\]

(28)

with \( \tilde{k} = -i \partial_{y} \) the momentum operator around the Fermi points and \( \gamma_{i} \) acts in left/right mover space. The effect of spin-orbit coupling enters in two ways, firstly it determines the Fermi velocity (since \( v_{F} = \alpha / \hbar \)) and secondly it prevents the exchange interaction term from being diagonal in spin space, which would otherwise just lead to an

\[
H_{k_{x}k_{z}} = \sum_{\eta \tau} H_{0k_{x}k_{z}\eta \tau} + \sum_{i=1,2} H_{i k_{x}k_{z}},
\]

\[
H_{0k_{x}k_{z}\eta \tau} = - \sum_{n \sigma} \left[ \eta (t \cos(k_{x}a_{x}) - \mu / 2) c_{\eta \tau n \sigma}^{\dagger}c_{\eta \tau n \sigma} + \eta \alpha \tau_{3} c_{\eta \tau n \sigma}^{\dagger}c_{\eta \tau n \sigma} + \eta t c_{\eta \tau n \sigma}^{\dagger}c_{\eta \tau(n+1)\sigma} \right]
\]

\[
+ \tau \tilde{\alpha} \sum_{n} \left[ i (c_{\eta \tau(n+1)\sigma}^{\dagger}c_{\eta \tau n \sigma} - c_{\eta \tau(n-1)\sigma}^{\dagger}c_{\eta \tau n \sigma} + 2i \sin(k_{x}a_{x}) c_{\eta \tau n \sigma}^{\dagger}c_{\eta \tau n \sigma}) + \text{H.c.} \right]
\]

\[
H_{1k_{x}k_{z}} = t_{1} \sum_{n \sigma} \left[ c_{11n \sigma}^{\dagger}c_{11n \sigma} + c_{11n \sigma}^{\dagger}c_{11n \sigma} + \text{H.c.} \right],
\]

\[
H_{2k_{x}k_{z}} = t_{2} \sum_{n \sigma} \left[ e^{-ik_{x}a_{x}}c_{11n \sigma}^{\dagger}c_{11n \sigma} + c_{11n \sigma}^{\dagger}c_{11n \sigma} + \text{H.c.} \right].
\]
energy shift of the two spin subbands and not produce any interesting effects. For the eigenstate we make the Ansatz \( \psi_s(x, y, z) = e^{i k_x x} \varphi(y) = e^{i k_x x} e^{i \lambda y} \phi_\lambda \), where \( \phi_\lambda \) is a 16-component vector. Acting with the Hamiltonian \( \rho, \kappa \)

\[
\text{Ansatz}
\]

\[
(\text{suppressing the normalization factors}) \text{ are given by}
\]

The surface states are the zero-energy eigenstates which decay for \( y > 0 \) (this translates into the criterion \( \text{Re}(i \lambda) < 0 \)). The zero-energy states can simply be found by solving \( \text{Det}(\hat{h}(k_x, i \lambda)) = 0 \). In the regime \( t_1 - t_2 < J < t_1 + t_2 \) we find the following decaying solutions characterized by

\[
\lambda_{1,s} = \frac{it_2 \pm \delta \mu_{k_s}}{\hbar v_F},
\]

\[
\lambda_{2,\rho, \kappa} = \rho^{1-\rho} \frac{v_F}{\hbar} \sqrt{(J + \rho t_1)^2 - \delta \mu_{k_s}^2} + \kappa t_2,
\]

where \( \rho, \kappa \in \{-1, 1\} \) and the corresponding eigenvectors (suppressing the normalization factors) are given by

\[
\phi_1 = (0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0),
\phi_2 = (0, 0, i, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0),
\phi_3 = (0, 0, 0, 0, 0, 0, 0, 0, 0, -i, 1, 0, 0, 0, 0),
\phi_4 = (0, -i, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0),
\phi_5 = (i g^*, 0, 0, i, -1, 0, 0, g^*, 0, -i, -i g^*, 0, 0, -g^*, 1, 0),
\phi_6 = (i g^*, 0, 0, i, -1, 0, 0, g^*, 0, -i, -i g^*, 0, 0, -g^*, 1, 0),
\phi_7 = (-i g^*, 0, 0, i, 1, 0, 0, g^*, 0, i, -i g^*, 0, g^*, 0, 1, 0),
\phi_8 = (i g^*, 0, 0, -i, 1, 0, 0, g^*, 0, -i, i g^*, 0, 0, g^*, 1, 0),
\]

with \( g_s = \frac{\delta \mu_{k_s} - i\sqrt{(J + t_1)^2 - \delta \mu_{k_s}^2}}{J + t_1} \). Some of these solutions seem to be ill-defined at \( J = t_1 \), but they actually have a finite limit once they are normalized. However, the expressions are too lengthy to be displayed here.

We write the general solution as linear combination in the basis \( (\Psi_{11}, \Psi_{1\bar{1}}, \Psi_{11}, \Psi_{1\bar{1}}, \Psi_{11}, \Psi_{1\bar{1}}, \Psi_{11}) \) and impose a hard-wall boundary condition at \( y = 0 \). Dropping rapidly oscillating terms, we write

\[
\psi(y) = \frac{1}{\sqrt{N}} \sum_{j=1}^{8} c_j e^{i \lambda_j y} \phi_{j},
\]

with \( N \) as a normalization constant and \( \phi \) an 8 component vector. We find a non-trivial zero energy solution characterized by coefficients \( (c_5 = c_6 = c_8 = 0) \),

\[
c_2/c_1 = -c_2/c_4 = 1, \ c_3/c_1 = c_4/c_1 = g_s.
\]
