Exotic surface states in hybrid structures of topological insulators and Weyl semimetals

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The study of topological properties in a semiconductor environment has become a strong and flourishing field in condensed matter physics. Topological insulators (TIs) and Weyl semimetals (WSMs) are two realizations of topological matter usually appearing separately in nature. However, they are directly related to each other via a topological phase transition. In this paper, we investigate the question whether these two topological phases can exist together at the same time, with a combined, hybrid surface state at the joint boundaries. We analyze effective models of a 3D TI and an inversion symmetric WSM and couple them in a way that certain symmetries, like inversion, are preserved. A tunnel coupling approach enables us to obtain the hybrid surface state Hamiltonian analytically. This offers the possibility of a detailed study of its dispersion relation depending on the investigated couplings. For spin-symmetric coupling, we find that two Dirac nodes can emerge out of the combination of a single Dirac node and a Fermi arc. For spin-asymmetric coupling, the dispersion relation is gapped and the former Dirac node gets spin-polarized. We propose different experimental realization of the hybrid system, including compressively strained HgTe as well as heterostructures of TI and WSM materials.

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I. INTRODUCTION

The study of topological properties in a semiconductor environment has become a strong and flourishing field in condensed matter physics. Topological insulators (TIs) and Weyl semimetals (WSMs) are two realizations of topological matter usually appearing separately in nature. However, they are directly related to each other via a topological phase transition. In this paper, we investigate the question whether these two topological phases can exist together at the same time, with a combined, hybrid surface state at the joint boundaries. We analyze effective models of a 3D TI and an inversion symmetric WSM and couple them in a way that certain symmetries, like inversion, are preserved. A tunnel coupling approach enables us to obtain the hybrid surface state Hamiltonian analytically. This offers the possibility of a detailed study of its dispersion relation depending on the investigated couplings. For spin-symmetric coupling, we find that two Dirac nodes can emerge out of the combination of a single Dirac node and a Fermi arc. For spin-asymmetric coupling, the dispersion relation is gapped and the former Dirac node gets spin-polarized. We propose different experimental realization of the hybrid system, including compressively strained HgTe as well as heterostructures of TI and WSM materials.

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models for the separate phases of TIs and WSMs\cite{40,41,42} and discuss their symmetry properties and surface states in Sec. IV. The coupling of the Hamiltonians and the analytic form of the surface state is discussed in Sec. III. Sec. V focuses on the different ways to influence and tune the combined surface dispersion relation. Possible experimental realizations are proposed in Sec. VI.

II. SEPARATE MODELS

The model of the TI phase we will use was originally derived for the Bi$_2$Se$_3$ family of materials in Refs. 40, 41. It contains four bands and serves as a minimal, but general, TI model. The Weyl Hamiltonian considered in the following originates from Refs. 42, 43. It contains two bands and models an inversion symmetric type I or II WSM with two Weyl points. We simplify the models as far as possible without losing too much versatility. It is important to retain terms quadratic in momentum for the introduction of the surface in the z direction. This is done via hardwall boundary conditions on a half space $z \leq 0$ or $z \geq 0$.

A. Topological Insulator

The effective Hamiltonian for a 3D TI is given by the 4x4 matrix\cite{10,11}

$$H_{TI} = \begin{pmatrix} M(k)\tau_3 + Bk_+\tau_2 + C\tau_0 & iAk_-\tau_1 \\ -iA^*k_+\tau_1 & M(k)\tau_3 + Bk_+\tau_2 + C\tau_0 \end{pmatrix} ,$$

(2.1)

with $M(k) = M_0 + M_1\left(k_\parallel^2 + k_\perp^2\right)$, $k_\parallel^2 = k_x^2 + k_y^2$ and $k_\perp = k_z \pm ik_y = k_y e^{\pm ik_y}$. In the original derivation for Bi$_2$Se$_3$ the Pauli matrices $\tau$ describe an orbital degree of freedom. $H_{TI}$ is written in a spin-up/down basis, represented by the Pauli matrices $\sigma$. The coupling $A = |A|e^{i\phi_A}$ can in principle be complex. The model is in the strong TI phase for $M_0M_1 < 0$.

We define the inversion operator $P_{TI} = \sigma_0 \otimes \tau_3$ and time-reversal operator $T_{TI} = i\sigma_2 \otimes \tau_0K$ with $K$ the complex conjugation operator. $H_{TI}$ is symmetric under both operations, fulfilling

$$P_{TI}^\dagger H_{TI} (-k) P_{TI} = H_{TI} (k),$$

$$T_{TI}^\dagger H_{TI} (-k) T_{TI} = H_{TI} (k).$$

(2.2)

The bulk dispersion relation is double degenerate and given by

$$E_{TI} = C \pm \sqrt{|A|^2 k_\parallel^2 + B^2k_\perp^2 + M(k)^2}.$$

(2.3)

Based on the method described in App. A the surface states can be calculated analytically. We assume opposite surfaces to be well separated, which offers the possibility to treat them individually. Thus in the calculation we only consider one of them via hardwall boundary conditions at $z = 0$. The surface wave function is then given by

$$\Psi(z) = \frac{1}{\sqrt{2}} \left( e^{ik_zz} - e^{ik_zz} \right) \left( \frac{\pm i\eta k_z}{\sqrt{\eta^2 + \left| A \right|^2}} \right) \psi_\eta$$

(2.4)

with $\psi_\eta = \frac{1}{\sqrt{2}} \left( \frac{1}{\eta} \right)$ and the inverse localization length $ik_z \frac{1}{2} = \frac{1}{2M_1} \left[ -\eta B \pm \sqrt{4M_1 \left( M_0 + M_1k_\parallel^2 \right) + B^2} \right]$. The sign $\eta = \pm$ depends on the surface, $\eta = -\text{sgn} \left( \frac{B}{M_1} \right)$ (upper surface) or $\eta = \text{sgn} \left( \frac{B}{M_1} \right)$ (lower surface).

The existence condition for the surface state, see App. A, is

$$M_1 \left( M_0 + M_1k_\parallel^2 \right) < 0$$

(2.5)

stressing the importance of being in the inverted regime.

The surface Hamiltonian (dispersion relation) is obtained from $H_{TI}$ by projecting out the orbital (orbital & spin) degrees of freedom with the help of $\psi_\eta (\Psi(z))$. We find the usual Dirac form

$$H_{TI}^{\text{sur}} = \begin{pmatrix} C & i\eta A^*k_- \\ -i\eta A^*k_+ & C \end{pmatrix} ; \quad E_{TI}^{\text{sur}} = C \pm |A| k_\parallel,$$

(2.6)

experiencing spin-momentum locking, with the angle $\phi_A + \frac{\eta\pi}{2}$ between the spin projection and momentum vector in the $x$-$y$ plane. The combined dispersion relations of the bulk and surface of the TI are shown in Fig. 1.
B. Inversion symmetric Weyl Semimetal

A WSM exists in different flavors. On the one hand, one distinguishes type I and type II depending on preserved or broken Lorentz invariance at the Weyl points \[^{11,12,16}\]. Secondly, either time-reversal or inversion symmetry has to be broken to get from a Dirac to a Weyl semimetal. For all these phases minimal models have been proposed in the literature\[^{38,42,43,47}\].

For simplicity, we focus on the model with broken time-reversal and preserved inversion symmetry, as it has the minimal number of one pair of Weyl points. The Hamiltonian is

\[
H_W = t(k)\tau_3 + v_z k_z \tau_2 + v_y k_y \tau_1 + \gamma t \left( k_x^2 - k_y^2 \right) \tau_0
\]

(2.7)

with \( t(k) = t \left( k_0^2 + k_z^2 - k_W^2 \right) \). The degree of freedom described by the Pauli matrices \( \tau \) can be orbital, spin or a combination of the two, depending on the specific material realization. For the concrete form of the symmetry operations considered in the following we assume a spinless system\[^{13}\]. The two Weyl points are specified by \( k_x = \pm k_W \). The parameter \( \gamma \) leads to a tilting of the dispersion relation at the Weyl points. For \( |\gamma| < 1 \) one has a type I, otherwise a type II WSM. Expanding \( H_W \) around \( k_x = \pm k_W \) yields a Hamiltonian with linearized Weyl form

\[
H_W^{lin} = v_y k_y \tau_1 + v_z k_z \tau_2 \pm 2tk_W k_x (\tau_3 + \gamma \tau_0).
\]

(2.8)

The Hamiltonian \( H_W \) fulfills the symmetry conditions

\[
P_W H_W (-k) P_W = H_W (k),
\]

\[
T_W H_W (-k) T_W \neq H_W (k)
\]

(2.9)

with the inversion operator \( P_W = \tau_3 \) and time-reversal operator \( T_W = \tau_0 K \) with \( K \) the complex conjugation operator. Hence, parity is preserved and time-reversal symmetry broken.

The bulk dispersion relation is then given by

\[
E_W = \gamma t \left( k_x^2 - k_W^2 \right) \pm \sqrt{v_y^2 k_y^2 + v_z^2 k_z^2 + t(k)^2}. \tag{2.10}
\]

The surface states can be calculated analytically based on the method discussed in the App. A. Their wave function is given by

\[
\psi(z) = \left( e^{ik_z z} - e^{-ik_z z} \right) \psi_\eta \tag{2.11}
\]

with \( \psi_\eta = \frac{1}{\sqrt{2}} \left( \begin{array}{c} 1 \\ \eta \end{array} \right) \) and inverse localization length

\[
\frac{i}{k_z^{\perp}} = \frac{1}{2t} \left[ -\eta v_z \pm \sqrt{4t^2 \left( k_0^2 - k_W^2 \right) + v_z^2} \right]. \tag{2.12}
\]

The sign \( \eta = \pm \) depends on the surface; \( \eta = -\text{sgn} \left( \frac{v_x}{v_y} \right) \) (upper surface) or \( \eta = \text{sgn} \left( \frac{v_x}{v_y} \right) \) (lower surface).

The existence condition for the surface state is

\[
k_0^2 < k_W^2 \tag{2.12}
\]

such that Fermi arcs can only exist between the Weyl points.

Hence, the surface dispersion relation yields the known Fermi arc spectrum

\[
E_{\text{Fermi arc}} = \gamma t \left( k_x^2 - k_W^2 \right) + \eta v_y k_y. \tag{2.13}
\]

The combined dispersion relations of the bulk and surface of the WSM are shown in Fig. 2.

![Graph showing bulk and upper surface dispersion relations](image)

**FIG. 2**: Bulk and upper surface dispersion relations, Eqs. (2.10) and (2.13), of the Weyl model. The surface band is plotted in red. Parameters: \( \gamma = \frac{1}{t}, k_W = 1, t = 1, v_y = 1, v_z = 1, k_z = 0 \).

III. COUPLED SYSTEM

The Hamiltonians and surface wave functions of the TI and WSM phases discussed in Sec. II are very similar. Thus, we conjecture that also the combined system may have surface states which can be calculated by the simplified method described in App. A. This will allow us to discuss the surface physics analytically.

In this section, we define the combined Hamiltonian and discuss the couplings allowed by symmetry under the assumptions that certain symmetries are preserved. The surface state Hamiltonian and wave function are derived and the limitations due to the approximated calculation method are discussed.

The combined Hamiltonian of the TI and WSM phases is defined by

\[
H_{WTI} = \begin{pmatrix} H_{TI} & H_C \\ H_C^\dagger & H_W \end{pmatrix} \tag{3.1}
\]

with the coupling \( H_C \). Such a coupling can be regarded as a tunneling Hamiltonian approach where \( H_C \) (weakly)
couples the two entities $H_{TI}$ and $H_W$. A similar approach has been considered in Ref. 48 to combine topological systems of different kinds with each other and study their emerging physics. The combined symmetry operator for inversion symmetry is now given by

$$ P_{WTI} = \begin{pmatrix} P_{TI} & 0 \\ 0 & P_W \end{pmatrix}. $$

As time-reversal symmetry is already broken in the sub-system of the WSM, it will also be absent in the combined system. The study of the effect on the TI of such a breaking of time-reversal symmetry via coupling, applicable e.g. in the setup of spatially separate Weyl and TI phases as depicted in Fig. 8 (b), is one of the goals of this paper. The stability of gapless edge states to time-reversal symmetry breaking via coupling, applicable in a time-reversal breaking environment. Close to the Weyl points or the TI bulk band edge where the surface states delocalize a $k_z$ dependent coupling should be taken into account.

The ansatz we will consider is

$$ \Psi(z) = (e^{ik_z z} - e^{ik_z z^2}) \begin{pmatrix} L_1(k_\parallel \psi_{\eta TI} \\ L_2(k_\parallel \psi_{\eta TI} \\ L_3(k_\parallel \psi_{\eta W}) \end{pmatrix} $$

with $\psi_\eta = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \eta \end{pmatrix}$. This is a special case of the general form of the surface wave function $\Psi_g(z) = \sum_j a_j e^{ik_z z^2} \psi(k_\parallel j, k_{z,j}), j \in \{1, ..., 6\}$. Its choice is motivated by the ability to obtain analytical solutions for the surface states. Physically it means that we only consider solutions were the TI and WSM surface states have the same exponential localization with the same localization length. This implies that phase transitions of the subsystems, such as normal insulator (NI) to TI or NI to WSM, can not be discussed separately in this treatment. However, for a system deep in the TI and WSM phase, the simplification should not alter the essential physics. We have checked numerically that small differences in the localization lengths of the subsystems do not alter the surface dispersion relations in a qualitative way, see App. 13.

Projecting the Hamiltonian Eq. (3.1) on the surface, this separates the eigenvalue equation into simpler problems

$$ H^\text{sur}_{WTI}(L_1 L_2 L_3) = E^\text{sur}_{WTI}(L_1 L_2 L_3), $$

$$ H^k_{WTI}(L_1 L_2 L_3) = 0 $$

with the Hamiltonians from the overlap of the wave functions of the different materials. As an example, this is done in Ref. 51 for a bilayer HgTe quantum well system by fitting a $k \cdot p$ model to experimentally obtained band structures. In general, all symmetry allowed couplings can be relevant for the following discussion. In this paper however, coupling terms proportional to $k_z$ are not considered, for simplicity. This is a physically reasonable assumption at least for the surface states if one assumes them to be 2D, perfectly localized in the $z$-direction. Close to the Weyl points or the TI bulk band edge where the surface states delocalize a $k_z$ dependent coupling should be taken into account.
for \( \eta = \eta_{TI} = \eta_{W} \). In Eq. (3.9), we partially diagonalize the Hamiltonian and define \( \phi^{a}_{k} = \phi_{k} - \eta_{\xi} A - \eta_{\pi} t_{w} \), \( H_{c} = a(k_{\parallel}) + \eta b_{1} k_{z} \), and \( H_{s} = \tilde{a} (k_{\parallel}) + \eta b_{1} k_{z} \). This will help in the interpretation of the surface dispersion relation in terms of coupled Dirac cone and Fermi arc. In the case of \( \eta = \eta_{TI} = -\eta_{W} \), one has to replace in Eqs. (3.8) - (3.10) \( a(k_{\parallel}) \leftrightarrow d(k_{\parallel}), b_{1} \leftrightarrow i c_{1}, v_{y} \rightarrow -v_{y} \), and \( v_{z} \rightarrow -v_{z} \).

We will focus in the following on the former, \( \eta_{TI} = \eta_{W} \), case. Taking \((L1 \ L2 \ L3)^{T}\) as the same eigenvector in Eqs. (3.6) and (3.7), the latter can only be fulfilled by further restrictions on the parameters. We choose a locking between some of the TI and the WSM parameters, i.e. \( t(k) = \nu M(k) \) and \( v_{z} = \nu B \) with \( \nu \) a constant (set to 1 in the following). This ensures the same localization length for the two subsystems. Additionally, the couplings \( c_{1} \) and \( c_{2} \) are set to be 0 for simplicity. Therefore the total coupling does not change the original orbital character of the TI and WSM surface states, being eigenstates of the \( \tau_{1} \) matrix with fixed eigenvalue + or -.

With regard to these restrictions, we have checked that the neglected couplings can be considered numerically with only quantitative changes to the surface dispersion relations, see App. B.

In total, this leads to the same quadratic equation for \( k_{z} \) as in the pure TI case, \( i k_{z} = \frac{1}{2 M_{1}} \left[ -\eta B \pm \sqrt{4 M_{1} \left( M_{0} + M_{1} k_{z}^{2} \right) + B^{2}} \right] \). The existence condition is again

\[
M_{1} \left( M_{0} + M_{1} k_{z}^{2} \right) < 0 \tag{3.11}
\]

and the (unnormalized) eigenvectors are given by

\[
\begin{pmatrix}
L1 \\
L2 \\
L3
\end{pmatrix} = \begin{pmatrix}
(E_{W_{TI}}^{\text{sur}} - C) H_{c} + i \eta A k_{-} \tilde{H}_{c} \\
(E_{W_{TI}}^{\text{sur}} - C) H_{c} - i \eta A k_{+} H_{c} \\
(E_{W_{TI}}^{\text{sur}} - C)^{2} - |A|^{2} k_{\parallel}^{2}
\end{pmatrix} \tag{3.12}
\]

The eigenenergies \( E_{W_{TI}}^{\text{sur}} \) are too lengthy to state them here, but can also be derived analytically.

The obtained solution leads to the possibility to tune bulk and surface dispersion relations rather independently. Parameters \( M_{1} \) and \( B \) influence the surface dispersion relation only indirectly via the existence condition and finite \( \gamma \) parameter, while they strongly influence the bulk band structure as will be shown in the next section. Tuning the coupling constants \( v_{y}, A, a \( (k_{\parallel}) \), \( b_{1} \) and their relative phase will still provide a rich parameter space to be explored below.

**IV. SURFACE DISPERSION RELATION**

In this section, we discuss the influence of the different coupling parameters on the combined surface states of TIs and WSMs. Depending on the choice of symmetries of the coupling, observed phenomena are the generation of additional Dirac points in the dispersion relation or the spin polarization of certain surface bands.

**A. Uncoupled scenario**

Beginning with the uncoupled case, \( H_{C,1S} = 0 \), the dispersion relations of the surface and bulk states are shown in Fig. 3. The black lines denote the bulk dispersion relation, cyan (from blue (green) for spin up (down)) and red stand for the TI and WSM surface states, respectively. The two black dots give the position of the bulk Weyl points. We note that the surface states originate at the bulk states, but cross them unaffectedly. Together with the fact that one can tune the bulk gap \( M_{0} \) without changing the surface dispersion relation (aside from the existence condition), we find the possibility to discuss the bulk and surface dispersion relations rather separately from each other. It will always be possible to increase the bulk gap and the distance between the two Weyl points such that the interesting surface physics happens in regions of the Brillouin zone where no bulk state is located. Therefore, we will focus in the following on tuning of the surface dispersion relation only. In numerical calculations, see App. B purely exponentially decaying surface states do not coexist with bulk states at the same energy and momenta. This is due to finite hybridization between the bulk and surface states.
FIG. 3: (a) and (b) Bulk and upper surface dispersion relations of the uncoupled TI and WSM models. Color code: Black lines for the bulk states, red for WSM character and cyan for the TI character of the surface states. (c) 3D plot of the surface dispersion relation. The two black dots denote the position of the bulk Weyl points.

Parameters: \( C = \frac{1}{2}, M_0 = -1, M_1 = 1, B = 1, k_z = 0, \gamma = -\frac{1}{4}, A = 1, v_y = 1, a(k_{||}) = b_1 = 0, H_c = \tilde{H}_c. \)

B. Real, spin-symmetric coupling: Creation of additional Dirac points

A straightforward way to couple TI and WSM is a real and spin-symmetric coupling via \( a(k_{||}) > 0 \) or \( b_1 > 0 \) with \( H_c = \tilde{H}_c. \) This kind of coupling leads generally to two Dirac points in the combined surface dispersion relation, as plotted in Fig. 4. One Dirac point is just shifted by the coupling to the Weyl surface state. The other one is created out of the Weyl and Dirac states along a momentum direction where there is no coupling between these two bands. Under the assumption that both spin species couple equally strong to the WSM, \( |\tilde{H}_c| = |H_c|, \) there is always such a momentum direction \( \phi_k \) where one part (hole or electron) of the Dirac cone is not coupled to the WSM surface state, while the other part is maximally coupled, see Eq. (3.9) above. For the lower, hole-like cone, using the parameters in Fig. 4, this direction is \( \phi_k = -\frac{\pi}{2}, \) thus the negative \( k_y \) axis with \( k_x = 0. \) The dispersion relation is then \( E = C + Ak_y \) corresponding to the cyan line in Fig. 4(a) which crosses the other two straight lines.

Considering finite couplings \( a_0 \neq 0 \) or \( b_1 \neq 0 \) gives only quantitative differences in the dispersion relations (not shown). The Dirac point generation is unaffected.
Evidently, a difference in the absolute values of the couplings between the Weyl system and the different spin species of the TI system will open a gap. In the limit of spin degeneracy, where $H_c = H_e$, we insert the coupling from Eq. (3.4), expand Eq. (4.1) for small momenta and find

$$H_D^1 = \begin{pmatrix} C & i\eta A k_- \\ -i\eta A^* k_+ & C \end{pmatrix} + \frac{1}{C - \gamma(M_0 + M_1 k_z^2) - \eta v_0 k_y} \begin{pmatrix} |H_c|^2 & H_e \bar{H}_c^* \\ \bar{H}_e H_c^* & |\bar{H}_c|^2 \end{pmatrix}.$$  

(4.2)

corresponding to a Dirac cone shifted in energy and momentum by the coupling. For real $A$ the shift occurs in the $k_y$ direction as shown in Fig. [3].

The creation of the second Dirac point can be understood from a similar calculation. The perturbative Hamiltonian for this Dirac point is given by

$$H_D^2 = \begin{pmatrix} C - |A| k_0 \\ \frac{1}{\sqrt{2}} H_c^* \left(1 - e^{-i\phi_k^0}\right) \gamma(M_0 + M_1 k_z^2) + \eta v_0 k_y - |H_c|^2 \end{pmatrix}.$$  

(4.3)

C. Spin-asymmetric coupling: Creation of gaps & spin polarization

The spin-up and spin-down TI bands do not need to have the same coupling to the WSM. If the absolute values are different, $|H_c| \neq |H_e|$, the Dirac points in the surface dispersion relation are gapped out, see Eq. (4.1) and Fig. [6]. The bulk Weyl points are, however, unaffected. The resulting bands are partly spin polarized as shown in Fig. [6]. The weaker coupled spin up electrons form a band with the Weyl surface state at intermediate energies, while the stronger coupled spin down electrons are pushed into the upper and lower bands. Considering a finite $b_1 \neq 0$ instead of a $a_0$ coupling, only the lower Dirac point will split. As the upper one is located at $k_x = k_y = 0$ for a pure momentum dependent coupling, the effective coupling between the WSM and TI surface states is zero here.

D. Phase-shifted coupling: Moving Dirac points, tilting dispersion relation

Including complex coupling constants, this offers additional ways to alter the bulk and surface spectrum. In general, the dispersion relation will look much less symmetric compared to the previous, real couplings.

Assuming $H_c = H_e$, one can directly conclude from the Hamiltonian in Eq. (3.9) that a complex coupling $A = i$ will lead to two Dirac points lying on the $k_x$, rather than...
FIG. 5: (a) Bulk and upper surface dispersion relations of the TI and WSM models with a coupling that changes sign. Color code: Black lines for the bulk states, red for WSM character and cyan for the TI character of the surface states. (b) 3D plot of the surface dispersion relation. Four Dirac points are visible.

Parameters: \( C = \frac{1}{2}, M_0 = -1, M_1 = 1, B = 1, k_z = 0, \gamma = -\frac{1}{4}, A = 1, v_y = 1, a_0 = \frac{1}{2}, a_2 = -\frac{1}{2}, b_1 = 0, H_c = \tilde{H}_c. \)

on the \( k_y \) axis as discussed in Sec. [IVB]. This is confirmed in Fig. [7]. One also sees that the bulk Weyl points lie not on the \( k_x \) axis, but are rotated by the complex coupling. Yet the rotation is much smaller than the \( \pi/2 \) rotation of the surface Dirac points.

The same effect is obtained by a complex phase difference between the couplings \( H_c \) and \( \tilde{H}_c \). It can even undo the rotation induced by \( A = i \). Note also that in the spin-symmetric case, already for real and finite \( a(k_\parallel) \) and \( b_1 \) the Weyl points are rotated away from the \( k_x \) axis. Here the effective coupling is complex, with a phase changing with \( k_\perp \). Supplementing this with a complex \( a(k_\parallel) \), this can again lead to points where the effective coupling is zero, resulting in additional Dirac points like in Sec. [IVB].

FIG. 6: (a) Bulk and upper surface dispersion relations of the TI and WSM model with a spin-asymmetric coupling. Color code: Black lines for the bulk states, red for WSM character and blue (green) for the TI spin up (down) character of the surface states. (b) Character of the three surface bands, shifted for clarity. (c) 3D plot of the surface dispersion relation. All Dirac points are gapped.

Parameters: \( C = \frac{1}{2}, M_0 = -1, M_1 = 1, B = 1, k_z = 0, \gamma = -\frac{1}{4}, A = 1, v_y = 1, a(k_\parallel) = \frac{1}{4}, \tilde{a}(k_\parallel) = \frac{2}{4}, b_1 = \tilde{b}_1 = 0. \)
FIG. 7: (a) and (b) Bulk and upper surface dispersion relations of the TI and WSM model with a complex coupling. Color code: Black lines for the bulk states, red for WSM character and cyan for the TI character of the surface states. (c) 3D plot of the surface dispersion relation. Two Dirac points on the $k_x$ axis are visible. Parameters: $C = \frac{1}{2}$, $M_0 = -1$, $M_1 = 1$, $B = 1$, $k_z = 0$, $\gamma = -\frac{1}{4}$, $A = i$, $v_y = 1$, $a(k_\parallel) = \frac{1}{4}$, $b_1 = 0$, $H_c = \tilde{H}_c$.

V. EXPERIMENTAL REALIZATION

We propose two ways to realize the physics of hybrid TI and WSM phases in an experimental setup. First, a material that naturally is in this combined phase will have corresponding surface states, as depicted in Fig. 8 (a). Compressively strained HgTe is a candidate material for this phase: the compressive strain pushes the $\Gamma_8$ bands against each other creating Weyl points in addition to the prevailing topological band inversion between the $\Gamma_8$ and $\Gamma_6$ bands. A difference to our calculation is the preserved time-reversal symmetry, leading to eight Weyl points in HgTe instead of two. However, if HgTe is doped with Mn the number of Weyl points could be reduced by a (partial) magnetic ordering.

The second realization consists of a WSM in contact with a 3D TI, possibly separated by a thin buffer layer as depicted in Fig. 8 (b). This should lead to a hybrid surface state at the joint boundary. The finite coupling $H_C$ could be provided by tunneling or Coulomb interaction. While this surface state is not exactly of the form of the ansatz in Eq. (3.5), the surface Hamiltonian, Eq. (3.8), should still be valid with the modification $\eta = \eta_{TI} = -\eta_W$. As several proposals of TRS-broken WSM with two Weyl points are based on magnetically doped 3D TI materials, the fabrication of the described hybrid system should be technically feasible.
VI. CONCLUSION & OUTLOOK

We have analyzed a hybrid system composed of a 3D TI coupled to an inversion symmetric, TRS-broken WSM. In the spirit of a tunnel coupling between the two topological phases, the use of a simplified ansatz made it possible to find an analytical solution for the surface states. The resulting surface Hamiltonian, Eq. (3.8), is a major result of this paper. The dispersion relation of the hybrid system shows different phenomena depending on the assumed coupling between WSM and TI. Preserved spin symmetry e.g. leads to the creation of additional Dirac points in the surface dispersion relation.

Breaking of spin symmetry on the other hand, this opens gaps and induces spin polarization in the former Dirac surface cone. As an experimental realization we have presented both strained HgTe, which might naturally be in the discussed hybrid phase, and a heterostructure of TI and WSM. In the latter case, the joint boundary would harbor the interesting hybrid surface state.

There are several directions how to proceed with this research. Looking for measurable consequences, e.g. in transport or spectroscopy, of the new hybrid surface states should be the most immediate one. We expect, for example, a measurable consequence in the discussed hybrid phase, and a heterostructure of TI and WSM. In the spirit of a tunnel coupling approach between WSM and TI. In the latter case, the joint boundary would harbor the interesting hybrid surface state.

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The general ansatz for the eigenstate is

$$\Psi_{g}(z) = \sum_{j=\{1,2\}} a_{j} e^{i k_{\pm, z} z} \psi(k_{\pm}, k_{\pm, j})$$  \hspace{1cm} (A2)

which could be used to solve for the surface states of Eq. (A1) in the usual manner. Due to the specific structure of our Hamiltonian, we can choose a simplified version of the ansatz, given by

$$\Psi(z) = (e^{i k_{\pm, z} z} - e^{i k_{\mp, z} z}) \psi(k_{\pm})$$ \hspace{1cm} (A3)

The relative sign ensures that the wave function vanishes at $z = 0$. The ansatz offers the possibility to separate Eq. (A1) into two parts

$$[h_{1} (k_{\pm} + \tau_{1} + h_{0} \tau_{0}) \Psi(z) = E_{\tau_{0}} \Psi(z) \hspace{1cm} (A4)$$

Eq. (A4) is independent of $k_{z}$ and can be solved for the surface dispersion relation $E_{\tau_{0}}$, while the solution of Eq. (A5) defines the two quantized values of $k_{z}$ needed for the surface eigenstate.

Following this procedure, $\psi(k_{\pm}) = f(k_{\pm}) \psi_{\pm}$ is taken to be proportional to the eigenstate of the $\tau_{1}$ Pauli matrix, $\tau_{1} \psi_{\pm} = \pm \psi_{\pm}$ and

$$\psi_{\pm} = \frac{1}{\sqrt{2}} \left( \begin{array}{c} 1 \\ \pm 1 \end{array} \right)$$ \hspace{1cm} (A6)

with $f(k_{\pm}) = 1$. Using $\tau_{2} \psi_{\pm} = \mp i \psi_{\mp}$ and $\tau_{3} \psi_{\pm} = \psi_{\mp}$, Eq. (A4) reduces to the quadratic equation

$$h_{4} k_{\mp} + h_{3} - \eta h_{2} k_{2} = 0 \hspace{1cm} (A7)$$

with $\eta = \pm$ the sign inherited from $\psi_{\pm}$. Solving for $k_{z}$, we find the two solutions

$$ik_{z} = \frac{1}{2h_{4}} \left[ -\eta h_{2} \pm \sqrt{4h_{4} \left( h_{3} + h_{4} k_{\mp}^{2} \right) + h_{5}^{2}} \right].$$ \hspace{1cm} (A8)

In order to obtain a wave function, exponentially decaying of the form of Eq. (A3), both $k_{z}$ need a real part of the same sign. For real $h_{j}$, this gives us the existence condition

$$h_{4} \left( h_{3} + h_{4} k_{\mp}^{2} \right) < 0.$$ \hspace{1cm} (A9)

Depending on the sign of $h_{3}/h_{4}$ and the direction in which the wave function should decay, $z \to +\infty$ or $z \to -\infty$, one chooses the corresponding eigenstate $\psi_{\pm}$, fixing $\eta = -\text{sgn} \left( \frac{h_{2}}{h_{4}} \right)$, top; $\eta = \text{sgn} \left( \frac{h_{2}}{h_{4}} \right)$, bottom. \hspace{1cm} (A10)

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Appendix A: Hardwall boundary condition 2x2

In this section, we recap a simple method for calculating exponentially localized boundary states of a 2x2 Hamiltonian following Ref.\cite{141} and references therein. We introduce hardwall boundary conditions on a half space $z \leq 0$ or $z \geq 0$. Thus, the surface state is localized at $z = 0$ and decays either in direction $z \to -\infty$ (upper surface) or $z \to +\infty$ (lower surface). The state should fulfill the eigenvalue equation

$$H \Psi(z) = E \Psi(z)$$ \hspace{1cm} (A1)
The surface dispersion relations and wave functions are then given by

\[ E^{surf} = h_0 + \eta h_1 (k_z) ; \quad \Psi(z) = (e^{ik_+ z} - e^{ik_- z}) \psi_0. \tag{A11} \]

The localization length is \( l_c = \max \left\{ \left| \frac{1}{\Re \left( i k_{\pm} \right)} \right| \right\}. \)

The surface solution described in this section fulfills the eigenvalue Eq. \( (A1) \) and is thus a valid, non-perturbative eigenstate of the Hamiltonian. Calculating the surface state with the general ansatz \( \text{(A2)} \), this gives the same dispersion relation as for the simplified ansatz \( \text{(A3)} \) for the TI model in Sec. \( \text{II.A} \).

Appendix B: Numerical validation of approximate solution method

In this article we use an analytical method to calculate the localized boundary states, described in App. \( \text{A} \). It requires certain restrictions on the parameters of the coupled TI-Weyl Hamiltonian, such as the same localization length for both TI and Weyl phase and half of the symmetry allowed couplings to be zero, see Sec. \( \text{III} \).

These constraints might seem quite restrictive. In order to proof the general applicability of our results, we have checked numerically that the neglected couplings have no qualitative effect on the surface band structure if kept reasonably small. The same is true for variations that alter the localization lengths of the subsystems. The numerical method is similar to the analytical approach: We solve for exponentially localized surface wave functions on the half space \( z \leq 0 \) or \( z \geq 0 \) with hard-wall boundary condition at \( z = 0 \). The differences to the approximate solution is the use of the full ansatz for the wave function, i.e.

\[ \Psi_g(z) = \sum_{j \in \{1,...,6\}} a_j e^{ik_z,j z} \psi(k_{\pm}, k_{\pm j}). \tag{B1} \]

As an example, we take the case of the generation of the second Dirac point, discussed in Sec. \( \text{IV.B} \) and depicted in Fig. 4. Besides the finite \( a_0 = \frac{1}{4} \), we add an additional coupling \( a_0 = \frac{1}{4} \) or change the localization length of the Weyl Hamiltonian by setting \( v_z = \frac{3}{4} \neq B = 1 \) and \( t = \frac{3}{4} \neq M_1 = 1 \). The latter choice leads then to differing localization lengths of the separate systems of

\[ ik_{z, TI} = \frac{1}{2} \left[ \frac{B}{M_1} \pm \sqrt{4 \left( k_{\parallel}^2 - 1 \right) + \left( \frac{B}{M_1} \right)^2} \right], \tag{B2} \]

\[ ik_{z, WSM} = \frac{1}{2} \left[ \frac{v_z}{t} \pm \sqrt{4 \left( k_{\parallel}^2 - 1 \right) + \left( \frac{v_z}{t} \right)^2} \right]. \tag{B3} \]

The resultant dispersion relations are shown in Fig. 9 depicted by blue dots. The analytical solution for the \( a_0 = \frac{1}{4} \) coupling alone is displayed as a continuous surface.

**FIG. 9** Dispersion of the upper surface of the combined TI and WSM models. The continuous surface is the analytical solution from Fig. 4, the blue dots represent the full numerical solution. In (a) the additional coupling \( a_0 = \frac{1}{4} \) was considered in the numerical solution, in (b) the altered parameters \( v_z = \frac{3}{4} \neq B = 1 \) and \( t = \frac{3}{4} \neq M_1 = 1 \). The large black dots denote the position of the Weyl notes of the analytical solution.

First we notice that the numerical and analytical solution agree very well and show no qualitative difference. The added coupling \( a_0 = \frac{1}{4} \) in Fig. 9 (a) has almost no effect, the same was found for a finite \( c_1 = \frac{1}{8} \). The changed localization length in Fig. 9 (b) shifts a bit the lower Dirac point, but does not open a gap. The major difference between the analytical and numerical solutions is the restriction of the surface solution to energies and momenta where no bulk state exists. This becomes especially clear for the upper and lower parts of the Dirac cone in Fig. 9 and is due to hybridization between the bulk and surface states. It prevents the existence of purely exponentially localized surface wave functions in this parameter range.

We conclude that the physical results and conclusions of this paper are valid beyond the restrictions on allowed couplings and localization lengths which are necessary to
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