Nodal-line semimetals from Weyl superlattices

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The existence and topological classification of lower-dimensional Fermi surfaces is often tied to the crystal symmetries of the underlying lattice systems. Artificially engineered lattices, such as heterostructures and other superlattices, provide promising avenues to realize desired crystal symmetries that protect lower-dimensional Fermi surface, such as nodal lines. In this work, we investigate a Weyl semimetal subjected to spatially periodic onsite potential, giving rise to several phases, including a nodal-line semimetal phase. In contrast to proposals that purely focus on lattice symmetries, the emergence of the nodal line in this setup does not require small spin-orbit coupling, but rather relies on it. We show that the stability of the nodal line is understood from reflection symmetry and a combination of a fractional lattice translation and charge-conjugation symmetry. Depending on the choice of parameters, this model exhibits drumhead surface states that are exponentially localized at the surface, or weakly localized surface states that decay into the bulk at all energies.

I. INTRODUCTION

Symmetries play a crucial role in the realization of lower-dimensional Fermi surfaces: while Dirac semimetals with degenerate Fermi points require time-reversal in combination with crystal symmetries, such as reflection or rotational invariance, Weyl semimetals are stable even in absence of these. However, Weyl nodes may be gapped by coupling two nodes of opposite chirality. Although isolated Weyl nodes are generally stable towards small disorder, scattering between different Weyl nodes couples them and may open up a gap in the spectrum by annihilating the Weyl nodes. Alternatively, we demonstrate that Weyl nodes can couple such that a new phase arises: a nodal-line semimetal with a one-dimensional Fermi surface.

Nodal-line semimetals exhibit surface bands at a limited range of momenta. These bands may serve as a basis for correlated physics in the presence of interactions. In the bulk, the implications of the nodal line include a sharply peaked magnetic susceptibility at zero energy, three-dimensional integer quantum Hall effect, and intriguing transport and density response properties. However, nodal-line phases generically do not survive the inclusion of spin-orbit coupling, which lifts the nodal degeneracy leading to isolated Weyl points. It is thus desirable to conceive realizations of nodal-line semimetals that do not rely on a small or vanishing spin-orbit coupling, as already suggested in previous proposals that require time-reversal and inversion symmetry, or nonsymmorphic symmetries.

In this work, we show that a Weyl semimetal subjected to a spatially periodic modulation of the onsite potential can undergo a transition to various phases, including a nodal-line semimetal. Since spin-orbit coupling is usually a requirement to have a Weyl phase, the nodal-line semimetal also relies on it, contrary to other proposals that require small spin-orbit coupling. We present the topological classification of the nodal line, showing that its stability relies on reflection symmetry and a combination of a fractional lattice translation and charge-conjugation symmetry.

The nodal-line semimetal phase that we predict exhibits surface states that are not pinned to zero energy, similar to previously studied models with drumhead surface states. The extra charge accumulation due to states at the surface is tied to the intercellular Zak phase. This implies that realizations without surface states exponentially localized to the boundary are possible. Nodal-line semimetals without surface states at low energies enable the direct study of the bulk properties of the nodal line.

Periodic superlattices can be implemented both in solid-state and synthetic systems. Heterostructures can effectively realize superlattices for Weyl fermions in crystalline solids. A Weyl phase realized on an optical lattice can be complemented with a superlattice to obtain the nodal-line semimetal phase proposed here. Since Weyl fermions are realized in photonic crystals, and superlattice structures have been engineered to observe Brillouin zone folding effects, these systems may also serve as a natural platform for the phenomena we study.

The paper is organized as follows. After introducing the superlattice model in Sec. II, we diagonalize the full Hamiltonian to obtain its band structure, revealing a nodal-line semimetal. The emergence of the nodal line is understood from the derivation of a low-energy effective theory that we discuss in Sec. III. To predict the stability of the nodal line we supplement the low-energy theory with a symmetry classification based on reflection symmetry and a combination of a fractional lattice translation and charge-conjugation symmetry in Sec. IV.

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The circumstances under which the model exhibits drum-head surface states are understood via the intercellular Zak phase and explained in Sec. V. The existence of the nodal line is in all cases protected by at least one symmetry, and therefore a wave-vector mismatch between the superlattice and the Weyl semimetal does not immediately open a gap, as shown in Sec. VI. Our results do not hinge on a specific lattice model of a Weyl semimetal; in Sec. VII we demonstrate that a nodal line also arises in a superlattice of a time-reversal invariant Weyl semimetal.

II. MODEL: WEYL SEMIMETAL ON A SUPERLATTICE

We start from the time-reversal-breaking two-band lattice Hamiltonian\(^5\)

\[ \mathcal{H}_0(k) = v \left( \sin k_x \sigma_x + \sin k_y \sigma_y \right) + M_k \sigma_z, \]

where \( M_k = t \left( 2 - \cos k_x - \cos k_y \right) + v \left( \cos k_z - m \right) \) and the lattice constant is set to \( a = 1 \). For certain values of \( m \), e.g., \(-1 < m < 5\) at \( v = t \), the model describes a Weyl semimetal\(^5\). The Hamiltonian obeys a charge conjugation symmetry, which may be broken in higher-energy bands in more realistic systems. In the course of this work, we consider this symmetry to be fulfilled. Here, we focus on \( 0 < m < 1 \), when there is one pair of Weyl nodes at \((0,0, \pm \text{arccos} m)\). This Hamiltonian is perturbed by the periodic potential

\[ U(\mathbf{r}) = 2 \sum_{\mu=0,z} u_\mu \cos(\mathbf{r} \cdot \mathbf{K} - \theta_\mu) \sigma_\mu, \]

where \( \sigma_\mu = (\sigma_0, \sigma) \), \( \sigma_0 \) is the \( 2 \times 2 \) identity matrix, \( \sigma \) is the vector of Pauli matrices, and \( \mu = 0, x, y, z \). Depending on the physical realization of this low-energy Hamiltonian, \( \sigma_\mu \) may act in spin or orbital space, or, when realized on an optical lattice, in sublattice space\(^5\). The angles \( \theta_\mu \) denote a shift of each component of the periodic potential towards the original lattice.

In the interest of clarity, we make two provisional simplifying assumptions: first, we assume that \( \mathbf{K} \) is commensurate with a reciprocal-lattice vector in the \( z \)-direction, which sets \( \mathbf{K} = (2\pi/n) \mathbf{e}_z \) for a folding degree \( n \in \mathbb{N} \) and the unit vector \( \mathbf{e}_z \). Second, the vector \( \mathbf{K} \) is chosen to match the wave vector connecting the two Weyl nodes, \( \mathbf{K} = 2 \text{arcos} m \mathbf{e}_z \), thereby restricting our discussion to the specific values of \( m = \cos \pi/n \). We postpone discussing the consequences of relaxing these two assumptions to Sec. VI.

Such choice of \( \mathbf{K} \) enlarges the unit cell by the folding degree \( n \) in the \( z \)-direction, as shown in Fig. 1 (a). The full Hamiltonian can be written in a form representing the larger unit cell

\[ \mathcal{H}_{n,k} = \begin{pmatrix} h_k + U_0 & h_k + U_1 & \cdots & h_k + U_{n-1} \\ \frac{1}{2} \sigma_z & h_k + U_1 & \cdots & \frac{1}{2} \sigma_z \\ \cdots & \cdots & \cdots & \cdots \\ \frac{1}{2} e^{-i n k_z} \sigma_z & \frac{1}{2} \sigma_z & \cdots & h_k + U_{n-1} \end{pmatrix}, \]

There is a gauge freedom in choosing the phases of the basis functions for the sites that constitute the superlattice. Our gauge choice ensures that the Hamiltonian is invariant under a shift by a reciprocal-lattice vector. The \( j \)-th diagonal element of the Hamiltonian is \( h_k + U_j \) with

\[ h_k = \mathcal{H}_0(k) - v \cos k_z \sigma_z, \quad U_j = U \left( \mathbf{r} = j \mathbf{e}_z \right). \]

To gain further intuition of the nature of the perturbation, one can express Eq. (3) as \( n \) copies of a Weyl Hamiltonian at different momenta, coupled by the superlattice perturbation (2). To this end, we rotate the Hamiltonian using the unitary transformation \( V = V_0 \otimes \sigma_0 \) with elements

\[ (V_0)_{jk} = \frac{1}{\sqrt{n}} \exp \left[-i \theta_n \left( k_z + \frac{2 \pi j}{n} \right) \right], \]

with the Weyl Hamiltonian \( \mathcal{H}_0(k) \) and the perturbation \( U_k = \sum_{\mu} u_\mu e^{i \theta_\mu} \sigma_\mu \). Thus, the periodic perturbation couples Weyl Hamiltonians evaluated at momenta that differ by \( 2 \pi/n \mathbf{e}_z \).

To begin understanding the physics of the Hamiltonian (6), we diagonalize it to obtain the band structure shown in Fig. 1. Anticipating the key differences between even and odd \( n \), and the central role played by the presence or absence of reflection symmetry along \( z \), we show the band structure along the path through momentum space defined in panel (b) for representatives of the four possible cases in panels (c) to (f). We find that in all but the reflection-symmetry broken case with odd \( n \), the low-energy band structure has a nodal line. All realizations have low-energy surface states that are degenerate in the presence of reflection symmetry. To obtain a deeper understanding of these observations, in the next two sections we derive an effective low-energy theory and then provide a symmetry classification of the emergent nodal line.

For our later symmetry analysis, it is important to note that there are \( n \) equivalent definitions of the bulk unit cell [an example is shown in Fig. 2 (a)]. It will therefore prove useful to define the translation operator

\[ T_{n,m} = \left( \mathbb{1}_{n-m} \otimes \mathbb{1}_m \right) \otimes \sigma_0, \]

where \( \mathbb{1}_m \) is the an identity matrix of size \( m \). The operator \( T_{n,m} \) translates the Hamiltonian’s unit cell by \( m \) sites and satisfies \( T_{n,m} T_{n,n-m} = e^{i \theta_m} \mathbb{1}_{n-m} \). The transformation

\[ T_{n,m} \mathcal{H}_{n,k} T_{n,m}^\dagger \rightarrow \mathcal{H}_{n,k} \]

is equivalent to changing all angles of the perturbation (2) as \( \theta_n \rightarrow \theta_n + 2 \pi m/n \). All bulk properties stay invariant upon such a transformation.
III. EMERGENT NODAL PHASES

To understand the emergence of a nodal line, we introduce a low-energy approximation developed by projecting the full Hamiltonian to bands close to the Weyl nodes. As described above, the system may be seen as \( n \) copies of the Hamiltonian that realize the Weyl phase, Eq. (1), coupled at different momenta, Eq. (6). For a folding degree of \( n = 2 \), this especially means that the full Hamiltonian equals two copies of the Weyl Hamiltonian that are coupled at opposite chirality,

\[
\tilde{H}_{n=2, k} = \begin{pmatrix} \mathcal{H}_0(k - \pi \mathbf{e}_z) & U_+ + U_- \\ U_+ + U_- & \mathcal{H}_0(k + \pi \mathbf{e}_z) \end{pmatrix}.
\]

This relatively simple \( 4 \times 4 \) Hamiltonian allows a detailed investigation of the model’s properties in this special case of \( n = 2 \), including an extensive phase diagram. This is discussed in the appendix.

For \( n > 2 \), the full Hamiltonian can be expanded around the Weyl nodes at \((0, 0, \pm \pi/n)\) and projected down to the lowest bands, giving a form similar to Eq. 9, i.e., two Weyl nodes of opposite chirality that are coupled by the potential \( U_{\pm} \). Up to linear order in momentum and first order in \( U \), the low-energy Hamiltonian has the form

\[
\mathcal{H}^\text{low}_k = v (k_x \sigma_x + k_y \sigma_y) + v \sqrt{1 - m^2} q_z \sigma_z + U_+ \tau_x + U_- \tau_z,
\]

where \( q_z \) is the momentum along \( z \) measured from the Weyl point. The matrices \( \tau_\mu \) act in the space of the different Weyl nodes that are coupled by \( U_{\pm} \). We introduce the Euclidean Dirac matrices

\[
\gamma_1 = \sigma_x, \quad \gamma_2 = \sigma_y, \quad \gamma_3 = \sigma_z \tau_z, \quad \gamma_4 = e^{i \theta_x} \tau_x \tau_z \sigma_z,
\]

and \( \gamma_5 = \gamma_1 \gamma_2 \gamma_3 \gamma_4 = -e^{-i \theta_x} \tau_y \sigma_y \) plus the identity and the commutators \( \gamma_{ij} = -\frac{i}{2} [\gamma_i, \gamma_j] \) to rewrite Eq. (10) in terms of perturbed Dirac fermions. It reads, upon rescaling of momenta

\[
\mathcal{H}^\text{low}_k = \sum_{i=1}^{3} k_i \gamma_i + u z \gamma_4 + v \cdot b' + w \cdot p,
\]

with the definitions

\[
p = (\gamma_{14}, \gamma_{24}, \gamma_{34}), \quad b' = (\gamma_{15}, \gamma_{25}, \gamma_{35}),
\]

\[
w = \begin{pmatrix} -u_y \cos(\theta_y - \theta_z) \\ u_x \cos(\theta_x - \theta_z) \\ -u_0 \sin(\theta_0 - \theta_z) \end{pmatrix}, \quad v = \begin{pmatrix} -u_y \sin(\theta_y - \theta_z) \\ u_x \sin(\theta_x - \theta_z) \\ u_0 \cos(\theta_0 - \theta_z) \end{pmatrix}.
\]

As discussed in Ref. 4, a perturbation \( u_z \) introduces a mass to the Dirac Hamiltonian and all other terms can lead to Weyl or nodal-line semimetal phases. However, as shown before in Fig. 1 (f), the nodal line that forms is not necessarily stable: it may gap out when taking into account higher orders in momentum and \( U \). In Sec. IV, the stability of the nodal line is investigated beyond the low-energy approximation.

Let us focus on a case where the emergence of a nodal line in the spectrum simply follows from the low-energy perspective. For a perturbation \( U_{\pm} = u_0 e^{\pm i \theta_0} \sigma_0 \), we may rotate the low-energy Hamiltonian, Eq. (10) by a unitary transformation

\[
U = \frac{1}{\sqrt{2}} (\sigma_x + \sigma_z) e^{i \phi/2 \sigma_z},
\]
with $\phi$ being the polar angle in the $k_x$-$k_y$ plane. This transformation gives

$$\mathcal{U} H_{k}^{\text{low}} \mathcal{U}^\dagger = v q \sigma_z + v \sqrt{1 - m^2} q_z \sigma_x \tau_z + u_0 e^{i \theta_0} \tau_x \tau_z,$$

(15)

with $q = \sqrt{k_x^2 + k_y^2}$. After applying the canonical transformation

$$\sigma_\pm \rightarrow \sigma_\pm \tau_z, \quad \tau_\pm \rightarrow \tau_\pm \sigma_z,$$

(16)

the Hamiltonian takes the simple form

$$\tilde{H}_k = \Delta_\pm \sigma_z - v \sqrt{1 - m^2} q_z \sigma_x,$$

(17)

where we replaced the operator $\Delta = v q + u_0 e^{i \theta_0} \tau_z \tau_x$ by its eigenvalues $\Delta_\pm = v q \pm u_0$. The nodal line therefore emerges at $q_z = 0, v q = u_0$.

### IV. Symmetry Classification of the Nodal Line

Generally, there are two different ways to obtain a protected nodal line in the model (3): by fulfilling reflection symmetry or a combination of a fractional lattice translation and charge-conjugation symmetry—we explain this in the current section. The symmetry classification of the nodal line depends on the folding degree of the unit cell $n$. In its most general form, the full Hamiltonian, Eq. (3), does not possess any commuting anti-unitary or anticommuting unitary symmetries, i.e., it is in symmetry class A. The system is reflection symmetric along $z$ if the operator

$$\mathcal{R} = \begin{pmatrix}
\sigma_0 & \cdots \\
\cdots & \sigma_0
\end{pmatrix}$$

commutes with $H_{n,k}$ or with any shifted Hamiltonian $T_{n,m} H_{n,k} T_{n,m}^\dagger$ at momenta that are invariant under reflection along $z$, i.e., $k_z = 0$ and $k_z = \pi/n$, where we choose $\mathcal{R}$ such that $\mathcal{R}^2 = +1$, using the convention by Ref. 42. This is the case when all angles $\theta_i$ are the same and equal $\theta_i = m \pi/n$ for all $i$ with the integer $m$ at $k_z = 0$ and $k_z = \pi/n$, the eigenstates of the Hamiltonian are simultaneously eigenstates of $\mathcal{R}$, $\mathcal{R}|\psi\rangle = r |\psi\rangle$ with eigenvalues $r = \pm 1$ (the bands are either even or odd under reflection). Bands with different eigenvalues $r$ cannot mix, which is the mechanism that protects the nodal line, cf. Fig. 3 (a). The invariant characterizing this protection is the mirror Chern number $42$, the difference in the number of occupied bands that are even under reflection within and outside the nodal line.

For odd folding degree $n$, reflection symmetry is the only symmetry that protects the nodal line. In absence of reflection symmetry, the nodal line gaps out, giving rise to two Weyl nodes. This can be achieved in two ways. One relies on setting at least one angle to be $\theta_i \neq m \pi/n$, which opens up a gap along the nodal line, cf. Fig. 1 (f) for $n = 3$. A second option is to break mirror symmetry by adding a term $\gamma \sin k_z \sigma_0$ to the Weyl Hamiltonian, Eq. (1). A nonzero $\gamma$ shifts the Weyl nodes to different energies, breaking mirror symmetry and opening up a gap in the nodal line, cf. Fig. 4.

For even $n$, the system is partitioned into two sublattices A and B, cf. Fig. 2 (b), where the superpotential has opposite sign. The system can be understood as a sublattice potential has opposite sign. The system can be understood as a sublattice potential has opposite sign. The system can be understood as a sublattice potential has opposite sign.

![Sublattice A Sublattice B](image)

**FIG. 2.** Unit cell in the superlattice. (a) Illustration of the equivalent definitions of the bulk unit cell for a folding degree of $n = 3$. All bulk properties stay invariant when the definition of the unit cell is changed between the three different options A,B and C. (b) For an even folding degree $n$, each unit cell can be split up into two sublattices A and B where the superlattice potential has opposite sign.
rewritten in terms of Majorana modes as a skew symmetric matrix $X^T = -X$, which can be diagonalized by an orthogonal matrix $O$, i.e., $W(k, \pi/n) = \pm 1$. The value of $\det W(k, \pi/n) = \pm 1$, which is the reflection-symmetry-breaking term $\gamma \sin k x \sigma_0$, with $v = t$, $u_0 = 0.2 t$, and $u_{x,y,z} = 0$, evaluated at $k_y = 0.05$, $k_x = \pi$. (a) For odd folding degree $n$, the reflection-symmetry-breaking term $\gamma$ immediately opens a gap in the spectrum. (b) For even folding degree, the gap is stable due to the combination of a fractional lattice translation and charge-conjugation symmetry.

V. SURFACE STATES

In the model investigated here, surface states play a crucial role: it is possible to have realizations of a stable nodal-line phase with drumhead surface states as well as surface states that are not exponentially localized at the boundary. The emergence of surface states close to zero energy is discussed in this section.

In Fig. 5 (a), the energy dispersion of a finite system with folding degree $n = 4$ that respects reflection symmetry is plotted, along with the location of the states encoded by a color scale. The system exhibits drumhead surface states at small energies that are exponentially localized at the surface. However, not all realizations of a stable nodal line share this feature: an example without drumhead surface states is given in Fig. 5 (b), where the dispersion for a finite system with folding degree $n = 2$ is shown. It is not possible to find a surface termination that respects the reflection symmetry of the bulk system. This results in states that are not exponentially localized at the surfaces of the system. To explain the properties of the surface states, we introduce and compute the Zak phase.

In the modern theory of polarization, the Zak phase is associated with the surface charge. Here, we employ the intercellular Zak phase that reflects the choice of a bulk unit cell to relate the extra charge accumulation at the surface with bulk properties of the system. The intercellular Zak phase and extra charge accumulation are proportional when the finite system is commensurate with the unit cell used to compute the intercellular Zak phase. While the Zak phase is generally given by $\gamma_j(k_x, k_y) = \int_0^{2\pi/n} dk_z |u_{j k}|^2$, we can use the Zak phase to characterize the system.
with the lattice-periodic part of the wave function $u_{j\mathbf{K}}(\mathbf{r}) = e^{-i\mathbf{K}\mathbf{r}}\psi_{j\mathbf{K}}(\mathbf{r})$, we rather focus on

$$\gamma_{j}^{\text{inter}}(k_x, k_y) = \int_{0}^{2\pi/n} dk_z \langle \psi_{j\mathbf{K}} | \partial_{k_z} | \psi_{j\mathbf{K}} \rangle,$$  \hspace{1cm} (25)

neglecting the "classical" contribution to the surface charge, coming from the polarization within a unit cell. The functions $|\psi_{j\mathbf{K}}\rangle$ are chosen such that all sites in one unit cell carry the same Bloch phase$^{43}$. This quantity can be numerically evaluated efficiently by calculating the corresponding Wilson loop$^{63}$.

The intercellular Zak phase is only quantized to 0, $\pi$ for a reflection-symmetric unit cell, when it equals the total Zak phase, otherwise it can take an arbitrary value. Extra charge accumulation $Q_{\text{acc}}^{L(R)}$ and intercellular Zak phase are related via

$$Q_{\text{acc}}^{L(R)} = +(-)\frac{e}{2\pi} \sum_{j\in\text{occ.}}\gamma_{j}^{\text{inter}} \mod 2 \hspace{1cm} (26)$$

where $L(R)$ stands for the left (right) surface region commensurate with the bulk unit cell used for the calculation of the intercellular Zak phase. Furthermore, Eq. (26) does not allow us to make a statement about the energy of the extra-charge accumulation. It has been shown that the above relation leads to the $\mathbb{Z}_2$ bulk-boundary correspondence for the reflection symmetric insulators: we have $\gamma_{\text{inter}} \mod 2$ in-gap surface modes, with $\gamma_{\text{inter}} = \sum_{j\in\text{occ.}}\gamma_{j}^{\text{inter}}$, if the finite system (i) respects the reflection symmetry and (ii) is commensurate with the bulk unit cell$^{43}$.

As shown in Fig. 5 (a), the intercellular Zak phase for a reflection symmetric system with folding degree $n = 4$ is quantized to 0, $\pi$, correctly predicting the number of in-gap surface modes. However, the $n = 2$ case violates the condition (i) for the bulk-boundary correspondence, and surface modes are not guaranteed to exist although the total Zak phase is quantized. Instead, the intercellular Zak phase explains the extra charge accumulations for both surfaces correctly as plotted in Fig. 5 (b).

VI. STABILITY AGAINST WAVE VECTOR MISMATCH

In the previous discussion, the focus was on a perfect match of the superlattice’s wave vector and the node separation of the underlying Weyl semimetal. In any realistic system, such a perfect agreement may be hard to realize. There are two possibilities for a vector mismatch: we can change the superlattice’s wave vector $\mathbf{K} = (2\pi/n + \delta\mathbf{k}) e_z$ or we can change the node separation by changing $m \rightarrow \eta/v + \cos \pi/n$.

When the wave vector $\mathbf{K}$ is changed, it generally fits neither the node separation nor the lattice. In such a case, translational invariance is lost, as investigated in Ref. 51. Here, we are interested in the fate of the nodal line in presence of a wave vector that does not match the node separation, i.e., we choose a vector $\mathbf{K}$ that is commensurate with periodic boundary conditions. In Fig. 6, the radius of the nodal line is shown for several lattices with periodic boundary conditions that allow certain $\mathbf{K}$. The diameter of the nodal line shrinks with increasing $\delta\mathbf{k}$ until it vanishes at a critical value that depends on $u_0$ and the folding degree $n$.

By changing $m \rightarrow \eta/v + \cos \pi/n$, the position of the Weyl nodes in the original unperturbed system are modified. The position of the nodal line can be obtained from modifying Eq. (17). This gives the condition for the po-
The outer matrix structure is described for nonzero $\eta = u_0$, with $v = t$ and $u_{x,y,z} = 0$. (a) The superlattice is varied $K \rightarrow (2\pi/n + \delta k) e_z$ so that it does not match the node separation. (b) The mass parameter is varied $m \rightarrow \cos \pi/n + \eta/v$ so that the node separation does not match the superlattices. Solid lines and crosses show the results using the full Hamiltonian, and the dashed line shows the lowest order prediction.

VII. TIME-REVERSAL SYMMETRIC WEYL SEMIMETAL

The previous findings can be extended to a model that is closer to currently available materials that respect time-reversal symmetry. Two copies of the Weyl Hamiltonian

$$H_0^{(\pm)}(k) = v (\pm \sin k_x \sigma_x + \sin k_y \sigma_y) + M_k \sigma_z$$

with $M_k$ from Eq. (1) give rise to several phases, including Dirac semimetals, Weyl semimetals with four Weyl nodes and strong topological insulators, all described by\textsuperscript{64}

$$H_k = \begin{pmatrix} H_0^{(+)}(k - k_1) & B_1 e^{i\phi} \sin(k_z) \sigma_x \\ B_1 e^{-i\phi} \sin(k_z) \sigma_x & H_0^{(-)}(k + k_1) \end{pmatrix}.$$  \hfill (29)

The vector $k_1$ lies in the $k_x$-$k_y$-plane and it breaks inversion symmetry. The outer matrix structure is described by the Pauli matrices $s_\mu$ acting in spin space. This Hamiltonian is time-reversal symmetric with $\Theta = i s_y K$ and has reflection symmetry along $z$ with $R = s_z$. When $k_1 = 0$ and $B_1 = 0$, the system has a $C_4$ rotational symmetry in the $k_x$-$k_y$-plane. Then, there are two degenerate Dirac nodes at $(0,0,\pm \arccos m)$. In absence of inversion and rotational symmetry, the Dirac nodes either split up into four Weyl nodes for $|k_1| > B_1$ or gap out when $|k_1| < B_1$.

A periodic perturbation with a wave vector $K = 2 \arccos m e_z$ can lead to protected line nodes. The most general perturbation

$$U(r) = \sum_{\mu,\nu} u_{\mu\nu} \cos (r \cdot K - \theta_{\mu\nu}) \sigma_\mu s_\nu$$  \hfill (30)

may give rise to a plethora of different phases. For simplicity, we just discuss the simplest case of a onsite potential, i.e., just $u_{00}$ is nonzero (see Fig. 7). In the Dirac phase, such a perturbation can give rise to a fourfold-degenerate nodal line. In presence of reflection symmetry, the symmetry class is AI with $R_-$, i.e., $R$ and $\Theta$ anti-commute\textsuperscript{32}. Although this symmetry class only allows a $Z_2$ classification that does not protect the nodal line, the $M Z$ classification inherited from $\Theta$ remains\textsuperscript{60}.

Breaking inversion and $C_4$ symmetry by $k_1$ and $B_1$ splits up the fourfold-degenerate nodal line into two twofold-degenerate nodal lines. The protection mechanism of these nodal lines is analogous to the previously considered time-reversal-breaking case, since the additional time-reversal symmetry does not change the clas-
sification. The operator
\[ \tilde{C}_k = \left( \begin{array}{c} e^{-i n k_z} \\ \sin \phi s_0 - i \cos \phi s_z \end{array} \right) \sigma_y K \]
anti-commutes with the Hamiltonian and squares to
\[ C_k C_{-k} = -e^{-i n k_z}, \] giving a \( Z_2 \) invariant defined in the \( k_z = \pi/n \) plane, analogous to the classification for the time-reversal breaking case in Sec. IV.

VIII. SUMMARY AND CONCLUSION

We showed that a Weyl semimetal subjected to a periodic modulation of the onsite potential can give rise to a nodal-line semimetal that is not gapped out by spin-orbit coupling. Since the nodal line is protected by mirror symmetry and/or the combination of a fractional lattice translation and charge-conjugation symmetry, its presence does not rely on details of the Hamiltonian. Although this work focused, because of its simplicity, on a Weyl semimetal with two Weyl nodes as a starting point, we further show that nodal lines also arise in periodically perturbed Weyl semimetals that respect time-reversal symmetry, by using a model that has four Weyl nodes without the perturbation.

An unusual feature of this proposal are the surface states that are not necessarily exponentially localized at the surface close to zero energy; this may open possibilities for experimental investigations of bulk properties that are not disturbed by any low-energy surface states. Similarly, quasiparticle interference \(^{65} \) is a promising tool for probing the nodal line at the Fermi level.

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Appendix A: Exact Hamiltonian and Phases for a Commensurate Perturbation with Folding Degree \( n = 2 \)

When the unit cell contains two sites \((n = 2)\), we can solve the Hamiltonian,
\[ \mathcal{H}_{n=2,k} = \begin{pmatrix} \tilde{h}_k + U_0 & v e^{-i k_z} \cos k_z \sigma_z \\ v e^{i k_z} \cos k_z \sigma_z & \tilde{h}_k - U_0 \end{pmatrix} \]
fully analytically, and obtain a complete phase diagram as shown in Fig. 8(a). From Fig. 8(b) to (j), we exhibit various evolutions of nodal lines and show how one can achieve the phase transitions between different nodal-line phases through the singular nodes.

When \( U(r) = 2 u_0 \cos (\pi z) \sigma_0 \), the four eigenvalues of Eq. (A1) are given by
\[ E_k^{q_1,q_2} = \eta \left[ (M_k - a_k)^2 + 4u_0^2 + a_k^2 + v_k^2 \right]^{1/2} + 2n \eta \left[ (M_k - a_k)^2 + 4u_0^2 + a_k^2 + v_k^2 \right]^{1/2} \]
where \( a_k = v \cos k_z, \eta_k = v (\sin^2 k_x + \sin^2 k_y)^{1/2}, \) and \( \eta = \pm \). We assume, without loss of generality, that \( v \) is positive.

Because \((M_k - a_k)^2 + 4u_0^2 + a_k^2 + v_k^2 \) is positive, nodal points can be found from the zeros of \( E_k^{\pi,n} \), which are given by
\[ a_k^2 = (M_k - a_k)^2 - v_k^2 - 4u_0^2 \pm 2v_k \sqrt{4u_0^2 - (M_k - a_k)^2}. \]

In the limit of the small external potential \((u_0 \ll 1)\), this equation reduces to \( 8u_0^2/(t^2 + 2v^2) = k_x^2 + k_y^2 \) which is a nodal ring enclosing the origin \((\Gamma \) point\). This is consistent with the phase diagram Fig. 8(a).

Figure 8(a) shows the full phase diagram of 15 nodal semimetal phases as a function of the parameters \( v/t \) and \( u_0/t \) obtained from (A4). There are six nodal-line semimetal phases denoted by \( \Gamma_1, X_1, \Gamma_1 X_2, \Gamma_1 M_2, \Gamma_1 M_2 X_1, \) and \( X_2, \) and \( X_4 \). They consist of closed curves as Fermi surfaces, where each of them encloses a certain high symmetry point, or a point on the straight line connecting two high symmetry points. The name of each nodal-line phase in the above is composed of those high symmetry points.

One can see that the Fermi surfaces of the intermediate singular nodal phases drawn by red dashed curves and red dots always have singular points.
FIG. 8. (a) Phase diagram for various nodal semimetal phases as a function of $v/t$ and $u_0/t$. There are six nodal-line phases which are distinguished by different colors. We classify them based on how many nodal rings are in the Brillouin zone, and where the centers of nodal rings are located. Those properties of each nodal-line phase are reflected in its name where the capital letters denotes the positions of the centers of nodal rings, and their subscript represent the number of nodal rings centered on them. As an example, in the phase $\Gamma_M^{2}X^{1}$, we have one nodal ring around the $\Gamma$ point, two around two M points, and one around an X point as shown in panel (h) by black solid curves. On the other hand, in the phase $\Gamma X^{4}$, there are four nodal rings around four points on four high symmetry lines $\Gamma X$, as plotted in panel (j) by black solid curves. At boundaries between those six nodal-line phases, we have intermediate phases which contain singular nodes in addition to nodal lines. In panels (b) to (j), we plot nodal Fermi surface structures corresponding to the phases marked by black and red dots in panel (a). On top of each panel, we specify the tight-binding parameters $(v/t, u_0/t)$ for the black solid and red dashed curves. For example, the band structure for the black dot at $(v/t, u_0/t) = (4, 0.5)$ in panel (a) is drawn by the black solid curve in panel (c) whereas the band structure for the red dot at $(4, 1)$ in panel (a) is plotted by the red dashed curve and red dots in panel (c).

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Orders of $O(U^2)$ appear on the diagonal of this matrix. They are additionally suppressed by the eigenvalues of $H_{k\pm k_0}$, i.e., they do not play a role close to the nodal line.

The exponential phase dependence in $\gamma_4$ and $\gamma_5$ is equivalent to a rotation of the Hamiltonian.