A. SYMMETRY CRITERIA FOR THE APPEARANCE OF NON-SYMMORPHIC NODAL LOOPS AND NODAL CHAINS

Here we provide a derivation of the criteria for the appearance of the non-symmorphic nodal loops (NSNLs) and nodal chains presented in the main text. We also discuss the appearance of NSNLs formed by valence or conduction bands, providing real materials where such a situation occurs. Finally, we discuss the NSNLs in antiferromagnetic systems.

1. Non-symmorphic nodal loops

We first recall a few definitions. Reciprocal lattice vectors $G$ fulfill

$$G \cdot R = 0 \mod 2\pi$$

for every Bravais vector $R$. Two momenta are called equivalent if they differ by a reciprocal lattice vector $G$. Time-reversal invariant momenta (TRIMs) $\Gamma$ are equivalent to their time-reversed images, $\Gamma = -\Gamma + G$. Combining this relation with equation (1), we obtain

$$\Gamma \cdot R = 0 \mod \pi.$$  (2)

Similarly, in a mirror-symmetric crystal, a mirror-invariant momentum $k$ is equivalent to its mirror image $\sigma_n k$ if

$$2n (k \cdot n) = 0 \mod G,$$  (3)

where $n$ is the normal vector of the mirror plane.

A mirror invariant plane contains four inequivalent TRIMs. To see this, pick up two arbitrary reciprocal lattice vectors $G_{1,2}$ such that they both have non-zero in-plane components ($G_{1,2} \parallel G_{1,2}$). By symmetry, the mirror images $\sigma_n G_i$ are also reciprocal lattice vectors, and hence $2G_{1,2} = G_{1,2} + \sigma_n G_i$ are in-plane reciprocal lattice vectors.

Let $G_i$ be the shortest reciprocal lattice vector in the direction $G_{i,2}$. Then, by taking all linear combinations $n_1 G_1 + n_2 G_2, n_1,2 \in \mathbb{Z}$, we construct all in-plane reciprocal lattice vectors. These vectors form a grid of equivalent $k$-points. The midpoints of these vectors form a four-times denser mesh of all the in-plane TRIMs. Thus, there are four inequivalent in-plane TRIMs.

We now consider a spin-orbit coupled (SOC) system with only two symmetries: Time-reversal $\Theta$ and a glide plane $g = \{\{\sigma_n \parallel t\}$, i.e. a mirror symmetry $\sigma_n$ with respect to normal vector $n$ followed by a translation by $t$. Such a system supports only one-dimensional irreducible representations (IRs) everywhere apart from TRIMs. The square of the glide plane is $g^2 = \{E\}2t_{||}$ where $t_{||} = \frac{1}{2}(t + \sigma_n t)$ is the in-plane component of the translation vector, and $E$ is a $2\pi$-rotation, represented by $-\parallel$ in SOC systems.

It can be seen that $g^2$ corresponds to a pure translation, and hence $2t_{||}$ must be a Bravais vector. Consequently, $g^2$ is represented at $k$ by $-e^{-i \mathbf{k} \cdot 2t_{||}}$ from which we conclude that the possible glide eigenvalues are [1]

$$\eta_{\pm} (k) = \pm ie^{-i \mathbf{k} \cdot t_{||}}.$$  (4)

Since $2t_{||}$ is a Bravais vector, we find from (2) that

$$\Gamma \cdot t_{||} = 0 \mod \frac{\pi}{2}.$$  (5)
This leads to two possibilities. Either \( \mathbf{\Gamma} \cdot \mathbf{t} = 0 \pmod{\pi} \) at all four mirror-invariant TRIMs, in which case the glide eigenvalues (4) are imaginary at all TRIMs and no band crossings are enforced. The second possibility is

\[
\mathbf{\Gamma}_1 \cdot \mathbf{t} = 0 \pmod{\pi} \quad \text{and} \quad \mathbf{\Gamma}_2 \cdot \mathbf{t} = \frac{\pi}{2} \pmod{\pi}
\]

(6)

for \( \mathbf{\Gamma}_{1,2} \) within the mirror-invariant plane. We argue that in such a case \( \mathbf{\Gamma}_1 \) and \( \mathbf{\Gamma}_2 \) have to be separated by a nodal line (NL) located within the mirror-invariant plane.

Consider any in-plane path \( \mathbf{p} \) that connects \( \mathbf{\Gamma}_1 \) to \( \mathbf{\Gamma}_2 \). The Kramer’s theorem forces the bands to doubly degenerate at \( \mathbf{\Gamma}_{1,2} \), and the trivial commutator \( [\mathbf{g}, \Theta] = 0 \) makes the glide eigenvalues of a Kramer’s doublet complex conjugate. According to equations (4) and (6), the glide eigenvalues of a Kramer’s doublet at \( \mathbf{k} = \mathbf{\Gamma}_1 \) are \((+i, -i)\). As one moves along \( \mathbf{p} \), the phase of the eigenvalues has to change by

\[
(\mathbf{\Gamma}_1 - \mathbf{\Gamma}_2) \cdot \mathbf{t} = \frac{\pi}{2} \pmod{\pi},
\]

(7)

so they evolve into \((+1, -1)\) at \( \mathbf{\Gamma}_2 \). However, these are not complex conjugate anymore and hence belong to different Kramer’s doublets. We infer that Kramer’s doublets have to switch partners along \( \mathbf{p} \), and a band crossing has to appear in the glide-invariant plane. Since the argument holds for any in-plane path \( \mathbf{p} \), there is a line of band crossings separating \( \mathbf{\Gamma}_{1,2} \) within the plane: the NSNL.

In the absence of additional symmetries, the band structure is built up of the quadruplets illustrated in Fig. 2b of the main text. Simple electron counting suggests that the NSNL if formed by occupied and unoccupied whenever there are

\[
\nu_{\text{filled}} = 4n + 2, \quad n \in \mathbb{N},
\]

(8)

filled bands (see Section A4 for the discussion of the stability of NSNLs at the Fermi level). Additional symmetries may lead to additional spectrum degeneracies and change the above filling criterion. For example, in the presence of inversion symmetry \( I \) the whole argument becomes not applicable, since \( \Theta \circ I \) leads to spin degeneracy of all bands throughout the Brillouin zone (BZ). Table I lists all 47 non-centrosymmetric space groups (SGs) that contain a glide plane fulfilling criterion of Eq. (6).

### 2. Drumhead surface states

It is known [2] that the presence of accidental NL (ANL) leads to the existence of a drumhead surface state that resides within the projection of the ANL to the surface. Here we argue that this is also the case for NSNLs.

To see this, note that in the presence of spin-orbit coupling ANLs appear in mirror-invariant planes of the Brillouin zone, while, as argued above, the NSNLs reside in glide-symmetric planes. Let us assume that ANL or NSNL is formed by bands \( N \) and \( N + 1 \). A topological invariant defining the presence of a NL exists for both ANLs [3] and NSNLs. Indeed, a mirror (glide) symmetry leads to the quantization of the Berry phase accumulated by \( N \) lower lying bands around any mirror- (glide-) symmetric loop enclosing the ANL (NSNL) into values 0 or \( \pi \). More precisely, the Berry phase on such a loop is equal to \( \pi \) times the number of NLS enclosed by the loop.

Due to the periodicity of \( \mathbf{k} \)-space, a particular example of such a loop is a one-dimensional straight line threading across the BZ, orthogonal to the glide plane. For 1D insulators with spatial symmetries quantizing the Berry phase to either 0 or \( \pi \) (like mirror or glide), it is known that in the latter case a metallic end mode of half an electron charge has to exist [4, 5]. Considering a 3D crystal as a collection of coupled 1D chains, one arrives at the conclusion that the projection of the NSNL on a crystal surface has to enclose a topological metallic surface state, which is similar to the drumhead state of ANLs [2].

### 3. Nodal chains

We further focus on systems with (1) a pair of mutually orthogonal glide planes \( g_{1,2} = \{\sigma_{1,2} \mathbf{t}_{1,2}\} \). According to the discussion above, each of them may create a NSNL in a mirror-invariant plane. These NSNLs necessarily touch if (2) the suitable choice of the TRIMs \( \mathbf{\Gamma}_{1,2} \) fulfilling Eq. (6) for both \( \mathbf{t}_{1,2} \) coincides with the two TRIMs along an intersection of the two mirror-symmetric planes. Moreover, (3) the high-symmetry line connecting
\( \Gamma_1 \) and \( \Gamma_2 \) should support at least two 1D IRs in the \( \Theta \)-symmetric case for the presented eigenvalue argument to be valid. Of the SGs listed in Table I, only nine satisfy criteria (1-3). Eight of them preserve the filling condition of Eq. (8) and are listed in Fig. 1 of the main text. The additional space group \#110 (\( I_4 1 cd \)) is more complicated since the minimal number of detached bands is eight rather than four [6, 7], and because it supports only 2D IRs at \( P = (\Gamma_1 + \Gamma_2)/2 \) [8]. This leads to a rather complicated nodal line structure illustrated in Fig. 1b.

4. Tuning non-symmorphic nodal loops and nodal chains to the Fermi energy

While the appearance of the NSNLs formed by conduction and valence bands requires the filling of Eq. (8), the experimental observation of the transport properties of NSNLs and nodal chains would require their proximity to the Fermi level. Notice that in general in metals the condition of Eq. (8) does not guarantee this proximity. Indeed, additional carrier pockets can provide the necessary charge compensation in the undoped materials even when the topologically protected degeneracy is away from the Fermi level.

For example, in nodal chain metals, such pockets would generally appear around the double Weyl point, accompanying the nodal chain. Thus, candidate materials for experimental probes of nodal chains and NSNLs should be chosen such that the nodal loops are realized reasonably close to the Fermi level, like in the case of IrF\(_4\). In other materials, some additional fine tuning of the nodal loops location relative to \( E_F \) may be required. This fine tuning can be done by straining, applying pressure or doping the compound.

Moreover, in materials with additional Fermi pockets a nodal chain or a NSNL can be probed experimentally even when the condition of Eq. (8) is not fulfilled. For \( \nu_{\text{filled}} = 4n \) a NSNL or a nodal chain formed by conduction or valence bands can still have drastic effects on transport provided that it appears sufficiently close to the Fermi level. Examples of such materials are provided by the CuTISe\(_2\) material class of space group \#122 (\( I_4 1 md \)). These materials were recently predicted to host Weyl points occurring between the valence and conduction bands [9], but the presence of the NSNLs formed by conduction or valence bands was missed. Since in many of these compounds the NSNLs are located close to the Fermi level, we expect both the Weyl points and the NSNLs to be relevant for transport properties of these materials.

5. Generalization to antiferromagnets

Let us finally generalize the argument for the appearance of a NSNL to antiferromagnetic (AFM) systems. For such systems the time reversal \( \Theta \) is not a good symmetry anymore, but its "non-symmorphic" analogue \( \mathcal{T} = \{ \Theta | t_\sigma \} \) is, where \( t_\sigma \) is a vector connecting the two spin-polarized sublattices of the AFM. We denote the glide plane as \( g = \{ \sigma_n | t_\sigma \} \). The two operators square to \( \mathcal{T}^2 = \{ E | 2t_\sigma \} \) and \( g^2 = \{ E | 2t_\sigma \} \), thus being equivalent to translations by Bravais vectors \( 2t_\Theta \) and \( 2t_\sigma \) correspondingly. The action of the squares of these operators on Bloch wave functions at \( k \) is

\[
T^2(k) = -e^{-2i k \cdot t_\sigma} \mathbb{1} \quad \text{and} \quad g^2(k) = -e^{-2i k \cdot t_\sigma} \mathbb{1},
\]

being equal to \( \pm \mathbb{1} \) at mirror-invariant TRIMs. The commutation relation between the operators is

\[
\mathcal{T} \circ g = \lambda(k) g \circ \mathcal{T}
\]

where

\[
\lambda(k) = e^{-2i k_\perp \cdot t_\Theta}
\]

and \( k_\perp \) denotes the momentum component orthogonal to the mirror plane. We observe from (11) that at TRIMs the operators either commute or anticommute.

To guarantee a two-fold degeneracy at a TRIM \( \Gamma \), its little co-group has to contain an antiunitary operator commuting with \( \mathcal{H}(k) \) and squaring to \( -\mathbb{1} \), i.e. either \( \mathcal{T}^2(\Gamma) = -\mathbb{1} \) or

\[
(g \circ \mathcal{T})^2 = \lambda(\Gamma) g^2(\Gamma) \mathcal{T}^2(\Gamma) = -\mathbb{1}.
\]

We say that a TRIM \( \Gamma \) is type-\( n \) if it contains \( n \) such operators. All the possibilities are summarized in Table II. The possible glide eigenvalues at a TRIM \( \Gamma \) are

![FIG. 1. Nodal chains along the high-symmetry line.](image)
\[ \eta_{\pm}(\Gamma) = \pm \sqrt{g^2(\Gamma)}, \] and the (anti)commutation relation of Eq. (10) forces the Kramer’s doublets to carry eigenvalues
\[ (\eta_1, \eta_2)_{\pm} = \pm \left( \sqrt{g^2(\Gamma)}, \lambda(\Gamma) \sqrt{g^2(\Gamma)} \right). \] (13)

Since all glide eigenvalues change their phase along an in-plane path \( p \) connecting \( \Gamma_1 \) and \( \Gamma_2 \) by the same increment \( \Delta \varphi = (\Gamma_1 - \Gamma_2) \cdot \tau_{s,i} \), a NSNL has to appear if \( \eta_1 = \eta_2 \) at one and \( \eta_1 = -\eta_2 \) at the other of the TRIMs. This is equivalent to \( g^2(\Gamma) \lambda(\Gamma) \) being positive at one and negative at the other TRIM. We observe in Table II that this occurs if one TRIM is type-1 and the other type-2.

**B. A RELATION BETWEEN NON-SYMMORPHIC NODAL LOOPS AND NON-SYMMORPHIC DIRAC POINTS**

Introducing inversion symmetry \( \mathcal{I} \) into a time-reversal symmetric SOC system results in spin degeneracy of all bands. Thus, if the inversion-breaking terms in the Hamiltonian of a NSNL are taken to zero, the NSNL shrinks into a four-fold degeneracy at either \( \Gamma_1 \) or \( \Gamma_2 \). In a system with time-reversal and glide-plane symmetries this four-fold degeneracy corresponds to one of the non-symorphic Dirac points (NSDP) classified in Ref. [10] [or to a Dirac line (that is, a line of four-fold degeneracy) along a high-symmetry axis], uncovering a relation between NSNLs and NSDPs.

Here we consider the following question: Is it *always* possible to obtain a NSNL by a suitable distortion of a system possessing a NSDP? We show in the following that there are situations when it is *not* possible to distort a NSNL into a NSNL.

As shown in the work of Ref. [10], a NSDP located at a TRIM on the BZ boundary requires a simultaneous presence of time-reversal \( \Theta \), inversion \( \mathcal{I} \), and an even \( n \)-fold rotational symmetry \( C_{nz} \) (set along the \( z \)-axis by convention). For low order expansion in \( k \), the non-symorphic symmetry matrices can be considered to be \( k \)-independent, so that rotation and screw axes become identical for low order \( k \cdot p \) expansions. The point group corresponding to these symmetries then contains a twofold rotational symmetry
\[ C_{2z} = (C_{nz})^{n/2} \] (14)
and a mirror symmetry
\[ \sigma_z = \mathcal{I} \circ C_{2z}. \] (15)

The NSDP appears in the mirror-invariant plane (again, there is no difference between a mirror and a glide for low order \( k \cdot p \) expansions, in contrast to tight-binding models). Breaking \( C_{2z} \) while keeping \( \sigma_z \) allows for the appearance of a NSNL (note that breaking \( C_{2z} \) also breaks inversion and lifts the spin degeneracy of bands). To find how such a crystal distortion modifies the spectrum, we consider additional terms appearing in the Dirac Hamiltonian that are consistent with the symmetries left.

The Dirac Hamiltonian is
\[ \mathcal{H}^{(s)}(\Gamma) = \hbar \left[ v_x \left( k_x^c + k_y^c \right) \gamma_1 + v_y \left( k_y^c - k_x^c \right) \gamma_2 + v_z k_z \gamma_3 \right] \] (16)
where \( k_x^c = (k_x \pm i k_y)^s \), and \( \gamma_1 \) to \( \gamma_5 \) are mutually anti-commuting Hermitian matrices squaring to \( 1 \). Together with the commutators \( \gamma_2 = -\frac{1}{2} [\gamma_1, \gamma_3] \) they form a basis of traceless \( 4 \times 4 \) Hermitian matrices. The value of the parameter \( s = 1 \) (\( s = 3 \)) corresponds to linear (cubic) Dirac Hamiltonians. Terms in the Hamiltonian that are independent of \( k \) and consistent with \( \Theta \) and \( \sigma_z \) can only be proportional to those of the 15 Dirac matrices that commute with both of the symmetries. For \( \Theta \) we find [3]
\[ [\Theta, \gamma_a] = 0 \quad \text{for} \quad a \in \{4,14,24,34,45\} \] (17)
and \( [\Theta, \gamma_a] = 0 \) for the remaining Dirac matrices. The classification developed in Ref. [10] allows us to check the anti-/commutation relations of the operator \( \sigma_z \) for all possible NSDPs, which we present in Table III.

We find that for a NSDP located along a 2-fold or 6-fold rotation axes
\[ \mathcal{H}^{(n=2,6)}_{\text{pert.}} = w \gamma_{34}, \] (18)
leading to a NSNL in the mirror-invariant plane [3]. The bands forming the NSNL have different eigenvalues of \( \sigma_z \), hence the nodal loop is stable against including higher-order symmetry-preserving perturbations to the Hamiltonian. This situation corresponds to both, the NSDPs in \( \beta \)-cristobalite \( \text{BiO}_2 \) [11] and in distorted spinels \( \text{Ba}_2\text{SiO}_4 \) [12]. Such a distortion might be induced by a structural phase transition at low temperature [13] or by strain.

For NSDPs that occur on 4-fold rotational axes, the corresponding perturbation is
\[ \mathcal{H}^{(n=4)}_{\text{pert.}} = m \gamma_4 + u_x \gamma_{14} + u_y \gamma_{24} \] (19)
and the spectrum is gapped whenever \( m \neq 0 \), therefore not leading to a NSNL in general [3]. In the presence of an additional mirror plane \( \parallel \) to the rotation axis, like in the case of \( \beta \)-cristobalite BiO\(_2\) [11], a NSNL can still appear in this plane. However, the existence of such a mirror is not in general guaranteed, examples being the A and Z points of the simple tetragonal space group \#84.

Combining Eqs. (16) and (18) we find a \( \mathbf{k} \cdot \mathbf{p} \) expansion for a NSNL to be

\[
\mathcal{H}_{\text{NSNL}}(\mathbf{k}) = \hbar \left[ v_x k_x \gamma_1 + v_y k_y \gamma_2 + v_z k_z \gamma_3 + w \gamma_{34} \right]. \tag{20}
\]

Using this Hamiltonian we can analytically compute the topological \( \mathbb{Z}_2 \) charge of the NSNL defined as

\[
z_2(c) = \frac{1}{\pi} \oint_c \mathbf{k} \cdot \mathbf{A}(\mathbf{k}) \mod 2. \tag{21}
\]

Here \( c \) is a mirror-symmetric path enclosing the NSNL and \( \mathbf{A}(\mathbf{k}) \) is the Berry connection of the occupied bands. Choosing a specific set of Dirac matrices

\[
\begin{align*}
\gamma_1 &= -\tau^\sigma y^g, & \gamma_2 &= \tau^\tau \sigma^x, & \gamma_3 &= \tau^y, \\
\gamma_4 &= \tau^x, & \gamma_5 &= \tau^z \sigma^z.
\end{align*} \tag{22}
\]

consistent with \( \Theta = i \sigma^y \kappa \) (where \( \kappa \) is the complex conjugation), and a path enclosing the NSNL

\[
c = \left\{ \left( \frac{w + u \cos \alpha}{\hbar v_x}, 0, \frac{u \sin \alpha}{\hbar v_z} \right) \mid \alpha \in [0, 2\pi) \right\}. \tag{23}
\]

We find smoothly gauged valence band wave functions

\[
|\psi(\alpha)\rangle = \frac{e^{-i\alpha/2}}{\sqrt{2}} \left( -\sin \frac{\alpha}{2}, i \sin \frac{\alpha}{2}, i \cos \frac{\alpha}{2}, \cos \frac{\alpha}{2} \right)^T. \tag{24}
\]

The corresponding Berry connection is

\[
\mathbf{A}_\alpha = i \langle \psi(\alpha) | \partial_\alpha | \psi(\alpha) \rangle = \frac{1}{2} \tag{25}
\]

which, upon integration over \( \alpha \), yields the topologically non-trivial value \( z_2(c) = 1 \), as expected for the NSNL.

### C. Landau Levels of Non-Symmorphic Nodal Loops

We consider the effects of magnetic field on the \( \mathbf{k} \cdot \mathbf{p} \) Hamiltonian of a NSNL presented in Eq. (20).

#### 1. Out-of-plane field

We first consider a perpendicular magnetic field \( \mathbf{B} = (0, 0, B) \) with \( B > 0 \). The Peierls substitution gives

\[
\langle h k_x, h k_y, h k_z \rangle \rightarrow (-i \hbar \partial_x + e A_x, -i \hbar \partial_y + e A_y, h k_z)
\]

\[
\equiv (\Pi_x, \Pi_y, h k_z) \tag{26}
\]

so that the commutator

\[
[\Pi_x, \Pi_y] = i \hbar e (\partial_y A_x - \partial_x A_y) = -i \hbar e B. \tag{27}
\]

This allows us to express the \( \Pi \)-operators using the usual ladder operators \(|a, a^\dagger\rangle = 1\) as

\[
\Pi_x = \sqrt{\frac{e h v_y B}{2v_x}} (a + a^\dagger), \quad \Pi_y = i \sqrt{\frac{e h v_x B}{2v_y}} (a - a^\dagger). \tag{28}
\]

Adopting Dirac matrices of Eq. (22) and representing \( \tau \)-matrices as \( 2 \times 2 \) blocks and \( \sigma \)-matrices as elements within the blocks, we obtain the matrix Hamiltonian

\[
\tilde{\mathcal{H}}^2 = \begin{pmatrix}
- w & i \sqrt{b} a & -i h v_z k_z & 0 \\
- i \sqrt{b} a^\dagger & - w & 0 & - i h v_z k_z \\
i h v_z k_z & 0 & w & - i \sqrt{b} a \\
0 & i h v_z k_z & i \sqrt{b} a^\dagger & w
\end{pmatrix} \tag{29}
\]

where we introduced a rescaled field \( b = 2 v_y v_z \hbar e B \). When squared, this Hamiltonian has a block-diagonal form

\[
\tilde{\mathcal{H}}^2 = \tilde{\mathcal{H}}^2(k_z) - (w^2 + \hbar^2 v_z^2 k_z^2) \mathbb{1}_r \otimes \mathbb{1}_\sigma.
\]

Clearly, the eigenvalues of \( \tilde{\mathcal{H}}^2(k_z) \) and of \( \tilde{\mathcal{H}}^2 \) are related through

\[
\tilde{\mathcal{E}}^2(k_z) = \tilde{\mathcal{E}}^2 + w^2 - \hbar^2 v_z^2 k_z^2.
\]

The eigenfunctions (that is, Landau levels) of \( \mathcal{H} \) are found in the form

\[
|\tilde{\psi}\rangle = \sum_{n=0}^{+\infty} \tilde{\psi}_{n}^{+} |n\rangle
\]

where \(|n\rangle\) is the eigenstate of a number operator \( a^\dagger a |n\rangle = n |n\rangle \). Using the standard algebra of the ladder operators

\[
a |n\rangle = \sqrt{n} |n - 1\rangle, \quad a^\dagger |n\rangle = \sqrt{n+1} |n + 1\rangle \tag{31}
\]
we find the eigenstates of $\tilde{H}^2$ corresponding to the eigenvalue $\tilde{\varepsilon}^2$ to satisfy conditions

$$b(n + 1)\tilde{\psi}_n^{s,+} - 2i\sqrt{b}\sqrt{n + 1}\tilde{\psi}_{n+1}^{s,-} = \tilde{\varepsilon}^2\tilde{\psi}_n^{s,+}$$

$$2i\sqrt{b}\sqrt{n}\tilde{\psi}_n^{s,+} + bw_0\tilde{\psi}_n^{s,-} = \tilde{\varepsilon}^2\tilde{\psi}_n^{s,-}$$

where $n \geq 0$ and $s = +, -$. This leads to solutions of the form

$$\begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

for the lowest eigenvalue $\tilde{\varepsilon}^2 = 0$, and to solutions

$$\frac{1}{\sqrt{2}} \begin{pmatrix} |n| \\ \pm i |n+1| \\ 0 \end{pmatrix} \quad \text{and} \quad \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 0 \\ |n| \pm i |n+1| \end{pmatrix}$$

with eigenvalues $\tilde{\varepsilon}^2 = b(n + 1) \pm 2w_0\sqrt{b}\sqrt{n + 1}$, where $n$ is any non-negative integer. It is now easy to check that suitable linear combinations of states in Eq. (34) form eigenstates of $\mathcal{H}$ with the corresponding Landau level energies

$$\varepsilon_{0,\pm} = \pm \sqrt{(hv_zk_z)^2 + w^2}$$

while linear combinations of states in Eq. (35) gives the eigenstates of $\mathcal{H}$ with the Landau level energies

$$\varepsilon_{n,\pm} = \pm \sqrt{(hv_zk_z)^2 + \left(w \pm \sqrt{n}b\right)^2}$$

where $n$ is any positive integer. Results of Eqs. (36)-(37) can be written using a single equation

$$\varepsilon_{n,\pm}(k_z) = \pm \left[(hv_zk_z)^2 + \left(w \pm \text{sign } n\sqrt{|n|b}\right)^2\right]^{\frac{1}{2}}$$

where $n \in \mathbb{Z}$. The resultant spectrum is gapped unless $w^2/b \in \mathbb{Z}$, i.e. for magnetic fields

$$B_e = \frac{w^2}{2ehv_z\nu n}, \quad n \in \mathbb{Z}\setminus\{0\}.$$ (39)

As mentioned in the main text, these gap closings correspond to topological phase transitions, in which a charge $e/2$ is topologically pumped to the surface of the sample, orthogonal to the direction of the field. To see this, notice that the perturbation of Eq. (18) is proportional to the mirror operator $\sigma_z = i\gamma_3\gamma_4$. As a consequence, tuning the magnitude of the perturbation $w$ shifts the energy of the eigenstates with different mirror eigenvalues in opposite directions, and thus a gap closure in the LL spectrum interchanges “valence” and “conduction” LLs with different mirror eigenvalues. Assuming, in the flavor of $k \cdot p$ theory, that the LLs are gapped at other momenta, this gap closing corresponds to a 1D topological phase transition, in which the Berry phase of the LL (considered as a band in the $k_z$ direction) changes by $\pi$. This change corresponds to pumping a charge of $e/2$ to the surface of the sample parallel to the plane of NSNL [4]. For this reason, a change in the Hall response of the metallic surface states is expected to occur at the critical values of the magnetic field, corresponding to the gap closure in the LL spectrum.

2. In-plane field

Now we consider the case of an in-plane magnetic field $\mathbf{B} = (B, 0, 0)$ with $B > 0$. The corresponding Peierls substitution is

$$(hk_x, hk_y, hk_z) \mapsto (hk_x, -ih\partial_y + eA_y, -ih\partial_z + eA_z)$$

$$\equiv (hk_x, \Pi_y, \Pi_z)$$

with the commutation relationship

$$[\Pi_y, \Pi_z] = i\hbar e(\partial_z A_y - \partial_y A_z) = -i\hbar eB.$$ (41)

In this case we express the $\Pi$ operators as

$$\Pi_y = \sqrt{\frac{ehv_zB}{2\nu_y}} (a + a^\dagger), \quad \Pi_z = i\sqrt{\frac{ehv_zB}{2\nu_z}} (a - a^\dagger).$$ (42)

Substituting this into the Hamiltonian of Eq. (20) and using a set of Dirac matrices

$$\gamma_1 = \tau^y, \quad \gamma_2 = \tau^z\sigma^z, \quad \gamma_3 = \tau^z\sigma^y,$$

$$\gamma_4 = \tau^x, \quad \gamma_5 = \tau^z\sigma^z$$

(43)
we arrive at the following Hamiltonian matrix

\[
\mathcal{H}(k_x) = \begin{pmatrix}
0 & \sqrt{b}a & -w \\
\sqrt{b}a^\dagger & 0 & -i\hbar v_z k_x \\
i\hbar v_z k_x & w & 0
\end{pmatrix}. \tag{44}
\]

Applying the parametrization of Eq. (30) and setting \(k_x = 0\), we find recurrence equations for the eigenstates of \(\mathcal{H}(k_x = 0)\) with zero energy

\[
\psi_{s+}^{n+1} = -\psi_{s-}^{n+1} \sqrt{n + 1} \frac{w}{\sqrt{b}} \tag{45}
\]

\[
\psi_{s-}^{n+1} = \psi_{s-}^{n+1} \frac{1}{\sqrt{n + 1}} \frac{w}{\sqrt{b}}. \tag{46}
\]

We can construct four linearly independent solutions for this system, starting with a single non-trivial component, \(\psi_0^s = 1\). The solutions generated for \(r = +\) are not normalizable because of the cumulative divergent factor \(\sqrt{n}\), and are therefore non-physical. The normalized solutions for \(r = -\) are

\[
|\psi^+_{s,-} \rangle = e^{-\frac{a^2}{b}} \left( \begin{array}{c}
0 \\
\cosh \left( \frac{wa^2}{\sqrt{b}} \right) \\
0
\end{array} \right) |0 \rangle \\
|\psi^-_{s,-} \rangle = e^{-\frac{a^2}{b}} \left( \begin{array}{c}
0 \\
\sinh \left( \frac{wa^2}{\sqrt{b}} \right) \\
0
\end{array} \right) |0 \rangle 
\]

where we used

\[
\sum_{n=0}^{+\infty} \frac{1}{n!} \frac{w^{2n}}{b^n} = e^{w^2/b} \tag{47}
\]

to obtain the normalization factor.

For \(k_x \neq 0\) the first order correction to zero energy can be obtained by diagonalizing the matrix

\[
M_{rs} = \hbar v_z k_x \langle \psi^r_{s,-} | (\tau^y \otimes \mathbb{1}_\sigma) | \psi^s_{s,-} \rangle. \tag{48}
\]

Evaluating the matrix leads to

\[
M = \hbar v_z k_x e^{-\frac{2a^2}{b}} \begin{pmatrix}
0 & -i \\
i & 0
\end{pmatrix} \tag{49}
\]

and the first order correction to the energy becomes

\[
\Delta \varepsilon(k_x) = \pm \hbar v_z k_x e^{-\frac{2a^2}{b}}. \tag{50}
\]

We see that the dispersion of the zeroth LLs is exponentially suppressed for weak magnetic fields \(b \lesssim w\). This is confirmed by the numerical analysis presented in Fig. 2d.

We now show that the crossing of the lowest LLs is protected by system symmetries. Notice that the composition of the time-reversal and the glide plane

\[
\Xi(k) = \Theta \circ g(k) \tag{51}
\]

remains a symmetry of the system even in the presence of an in-plane magnetic field. Using the Dirac basis of Eq. (22), the glide symmetry is represented as

\[
g(k) = e^{i\varphi_k \gamma_{34}} = e^{i\varphi_k \tau^z}. \tag{52}
\]

where \(\varphi_k\) is a \(k\)-dependent phase factor due to the non-symmetric nature of the system, starting with a single non-trivial component, and are therefore non-physical. The normalized solutions

\[
\Xi(k) = ie^{-i\varphi_k \tau^z \sigma^y K} \tag{53}
\]

which squares to

\[
\Xi[(\Theta \circ g)k] \Xi(k) = ie^{-i\varphi_k (\Theta \circ g)k} \tau^z \sigma^y K ie^{-i\varphi_k \tau^z \sigma^y K} = -\exp \left[ i \left( \varphi_k - \varphi_k (\Theta \circ g)k \right) \right]. \tag{54}
\]

For an applied in-plane magnetic field, only the momentum parallel to the field is a good quantum number. If this component is set to zero, \(k_x = 0\), then (54) evaluates to \(-1\), hence, by Kramer’s theorem, the twofold degeneracy is enforced at this point. (As a consistency check, remember that the case of \(w = 0\) corresponds to a Dirac semimetal, where the zero-energy crossing of the chiral LLs is well-known).

Let us briefly compare the response of NSNLs discussed here to that of accidental nodal loops (ANLs). ANLs in a mirror-invariant plane of a time-reversal symmetric system inevitably appear in pairs centered around points \(\pm k_0\), and the symmetry (51) relates LLs of one ANL to the LLs of the other, thus avoiding the two-fold degeneracy at zero energy. As a consequence, ANLs do not produce chiral LLs and therefore should have transport properties qualitatively different from those of NSNLs.

## D. NODAL CHAIN MATERIAL CANDIDATES

In this section we present a detailed discussion of the methods used to identify real material candidates for the nodal chain phase, and present the identified materials. We used two complementary approaches: first principles calculations and tight-binding modeling. The latter was done using the Wannier-based tight-binding models with long range hoppings, derived directly from first principles calculations, and also by creating a model with short range hoppings based purely on symmetry analysis and fitting it’s parameters to the \textit{ab initio} band structure.

### 1. Crystal structure and symmetry

With the aid of the Materials Project [15], the material candidates for the nodal chain realization identified in this work are all from the class of Iridium tetrafluoride (IrF\(_4\)). This parent compound crystallizes in space group \#43 (Fd\(_{3d}\)) with the conventional unit cell parameters [16]

\[
a = 9.64(1) \text{ Å}, \quad b = 9.25(1) \text{ Å}, \quad c = 5.67(1) \text{ Å}. \tag{55}
\]

The primitive unit cell contains two structural units.

In this crystal structure, shown in Fig. 3a-b, every Ir site is surrounded by an octahedral cage of six F atoms,
### FIG. 3. Crystal structure of unstrained and strained IrF\textsubscript{4}.

(a) Crystal structure of unstrained IrF\textsubscript{4} in space group \#43. (b) Same as (a) shown along the [001] direction. (c) Crystal structure of IrF\textsubscript{4} strained along the [011] direction. The symmetry is reduced to that of space group \#9 with only one glide plane. The nodal chain reduces to NSNLs under this strain. (d) Same as (c) shown along the [001] direction. The crystal structures were plotted using VESTA 3 [14].

Four of which are shared with the neighboring octahedra, while the remaining two belong solely to one iridium site. These octahedra form a bipartite lattice indicated in color in Fig. 3a–b of the main text. Appropriate straining of the crystal shown in Fig. 3c–d will transform the nodal chain into a single NSNL.

Other representatives of the IrF\textsubscript{4} material class were considered. The lattice constants of XY\textsubscript{4} (X=Ir, Ta, Re; Y=F, Cl, Br, I) were obtained by optimizing numerically both the lattice constants and the atomic positions of the compounds, starting from the IrF\textsubscript{4} structure. The resultant lattice parameters are listed in Table IV. Band structures of several such compounds are presented in Fig. 6. Nodal chains are clearly visible in all of these materials.

### FIG. 4. Construction of the tight-binding model.

The numbers indicate sites related by corresponding hoppings in Hamiltonian of Eq. (56).

### FIG. 5. Band structure of IrF\textsubscript{4}.

The solid red and dotted green lines correspond to the band structure calculated from first-principles and from the chiral symmetric model, respectively, and were already presented in Fig. 3f of the main text. The dashed blue line represents the tight-binding model constructed in subsection D3.

### 2. First-principles calculations

The electronic structure calculations have been performed within the framework of density functional theory (DFT) [17], using generalized gradient approximation (GGA) [18] with the projector augmented-wave [19] implemented in VASP (Vienna ab-initio simulation program) [20, 21]. Spin-orbit coupling was included into consideration via the pseudopotentials. For all the materials presented the band structures were obtained using a 500 eV energy cutoff for the plane waves and the energy precision of \(10^{-8}\) eV. The Brillouin zone was sampled using a \(10 \times 10 \times 10\) Gamma-centered mesh. The lattice constants and atom positions listed in Table IV are fully relaxed until the total energy is converged to \(10^{-7}\) eV and the forces on atoms are below \(10^{-3}\) eV/Å.

Wannier90 [22–24] code was used to construct a Wannier-based tight binding model. The 20\(\times\)20 model was obtained by projecting the band structure around the Fermi level onto the five \(d\)-orbitals of both Ir atoms in the unit cell. The surface band structures and densities of states were calculated using this tight-binding model and the iterative Green’s function technique of Ref. [25], which was implemented in Wannier\textsubscript{tools} package [26].

### 3. Tight-binding model

We now discuss a short-ranged symmetry-based tight-binding model of IrF\textsubscript{4}. The DFT calculations predict the set of bands with \(5d\)-Ir character to be separated from the \(5s\)-Ir bands above and the \(2p\)-F bands below. The local octahedral crystal field splits the \(5d\)-Ir orbitals into a partially filled lower-lying \(t_{2g}\) manifold and an empty higher energy \(e_g\) states. The spin-orbit coupling further
The body-centred tetragonal group from the face-centred orthogonal set of Pauli matrices assume a perfect band tight-binding model. To simplify the analysis, we assume a perfect $C_{4z}$ screw rotational symmetry, which is only mildly broken in IrF$_4$. This increases the space group from the face-centred orthogonal #43 ($Fdd2$) to the body-centred tetragonal #109 ($I4_1md$).

The resultant tight-binding Hamiltonian can be written compactly, using a set of Pauli matrices $\sigma = (\sigma^x, \sigma^y, \sigma^z)$ for the spin degrees of freedom, and another set of Pauli matrices $\tau = (\tau^x, \tau^y, \tau^z)$ for the sublattice degrees of freedom. The electron annihilation operator at site $i$ with position vector $\mathbf{r}_i$ is given by $c_i = (c_i^\dagger, c_i)$.

The real space Hamiltonian reads

$$\hat{H} = \sum_{\langle i,j \rangle \in 1} c_i^\dagger (t_1 \mathbb{1} + i T_1 \frac{\mathbf{r}_{ij} \times e_z}{\mathbf{r}_{ij}^2} \cdot \sigma) c_j + t_2 \sum_{\langle i,j \rangle \in 2} c_i^\dagger c_j + t_3 \sum_{\langle i,j \rangle \in 4} c_i^\dagger c_j + i T_3 \sum_{\langle i,j \rangle \in 3} c_i^\dagger [(e_z \cdot \mathbf{r}_{ij})(e_z \times \mathbf{d}_{ij})] \cdot \sigma c_j$$

where $\mathbf{d}_{ij} = \mathbf{r}_{ik} + \mathbf{r}_{jk}$, $k$ is the common nearest neighbor of sites \{i,j\} $\in 3$, and $|\mathbf{v}| = |\mathbf{v}|/|\mathbf{v}|$ is the unit vector in a specified direction.

We remark that further hopping terms are possible and that symmetries allow for other spin-orbit terms [27], but we found the fitted amplitudes for such processes to be small compared to the terms already included in Eq. (56). The fitted values of the TB parameters and the corresponding value of the chemical potential in eV are

$$t_1 = 0.0548, \quad T_1 = -0.0577, \quad t_2 = -0.0153$$
$$T_3 = 0.0071, \quad t_4 = 0.0068, \quad \mu = 0.0179.$$  (57)

Note that the hoppings between the two sublattices $(t_1, T_1)$ strongly dominates over intra-sublattice hoppings $(t_2, T_3)$. This indicates that the chiral symmetry of the system is only weakly broken. Indeed, neglecting the intra-sublattice hoppings leads to an ideal chiral symmetry of the model, while still producing reasonable band structure, shown in Fig. 5. The parameters of the chiral tight-binding model are

$$t_1 = 0.0548, \quad T_1 = -0.0577, \quad t_2 = 0$$
$$T_3 = 0, \quad t_4 = 0, \quad \mu = 0.$$  (58)
The chiral symmetry (CHS) operator is $\mathcal{C} = \tau^z$. Comparison of the DFT results with the two approximations is shown in Fig. 5.

### E. TOPOLOGICAL INVARIANT ON THE CURVED PLANE

In the main text we introduced a $Z_2$ topological invariant of a curved plane, the projection of which onto the (100) surface is shown with a magenta line in Fig. 3f of the main text. The invariant was computed using the method of Refs. [28, 29] as implemented in the Z2Pack software package (https://z2pack.ethz.ch) [30]. Its value was found to be non-trivial, suggesting an odd number of Kramers pairs of edge states to cross the magenta line of Fig. 3f at some energies. The corresponding surface spectral function shown indeed exhibits a single Kramers pair of edge (surface) states, as shown in Fig. 7a.

The value of the $Z_2$ invariant is also constrained to be non-trivial by crystalline symmetries. To see this, we apply an established technique of Refs. [28, 29] to compute the value of topological invariants by tracking the changes in Wannier charge center (WCC) positions (or, alternatively, a Wilson loop) on cuts of the Brillouin zone. In particular, we consider a cut $P = (k_x, k_z)$, shown as a magenta plane in Fig. 7b. The cut is formed by $k_x$ and a curved line $k_{\ell}$, and it exhibits a gapped spectrum. The projection of this cut onto the (100) surface is shown with a magenta line in Fig. 3f of the main text. Importantly, this cut $P$ of the Brillouin zone is symmetric under the glide $g_z$, and contains four inequivalent time-reversal invariant momenta (TRIMs), shown as dark points on $P$.

We now construct the WCCs $\ell(k_{\ell})$ by carrying out the non-Abelian parallel transport of Bloch states along $k_{\ell}$ at different values of $k_x$ (some of such parallel transport paths are shown as yellow dashed lines in Fig. 7b) (see Refs. [22, 28] for details of the procedure). The $k_x$ lines that connect TRIMs at $k_x = A$ or $k_x = C$ are mapped onto themselves by time-reversal symmetry, and hence the WCCs at these values of $k_x$ should appear in Kramers degenerate pairs [28, 31]. At values of $k_x$ other than $A$ and $C$ the degenerate centers split, as shown in Fig. 7c. Since lines located at $B \pm k_x$ are related by $g_x$ containing vertical shift by half-unit cell, the WCCs at $B \pm k_x$ are themselves displaced by half-unit cell along $\ell$, as indeed can be seen in Fig. 7c. Due to this shift the connectivity of the WCCs between $B$ and $C$ is constrained in such a way that the $Z_2$ invariant is trivial (non-trivial) if there are $4n$ ($4n+2$) occupied bands [32], meaning that the WCCs do not exchange (do exchange) partners when $k_x$ goes from $A$ to $C$. This proves the existence of the topological phase for the filling $4n+2$.

### F. CHIRAL SYMMETRIC MODEL

Consider the Hamiltonian of Eq. (56) with parameters of Eq. (58). As discussed in Sec. D3, such a choice of parameters corresponds to admitting only inter-sublattice (NN) processes. Representing the spin degree of freedom by Pauli matrices $\sigma = (\sigma^x, \sigma^y, \sigma^z)$ and the sublattice degree of freedom by $\tau = (\tau^x, \tau^y, \tau^z)$, the chiral symmetry (CHS) operator $\mathcal{C} = 1_\sigma \otimes \tau^z$ fulfills

$$\mathcal{C}^2 = 1 \quad \text{and} \quad \{\mathcal{C}, \mathcal{H}(k)\} = 0. \quad (59)$$

The symmetry manifests itself in the particle-hole symmetric spectrum of $\mathcal{H}(k)$ in Fig. 3c of the main text.

In the sublattice basis, the chiral-symmetric Hamiltonian has the block-off-diagonal form

$$\mathcal{H}(k) = \begin{pmatrix} 0 & M(k) \\ M(k)^\dagger & 0 \end{pmatrix}. \quad (60)$$

At momenta, where a spectral gap exists between the conduction and valence bands, $\det M(k) \neq 0$. We can

---

**Table IV. Crystal structure of IrF$_4$, material class $XY_4$, with space group #43.** The numbers next to the chemical formula indicate the conventional unit cell parameters $a$, $b$, $c$, respectively. Listed below are the coordinates of atoms. The Wyckoff positions are 8$a$ for the $X$ atom and 16$a$ for both inequivalent $Y$ atoms. In all cases, the crystals contain two formula units per primitive unit cell.

<table>
<thead>
<tr>
<th>Material</th>
<th>$a$ (Å)</th>
<th>$b$ (Å)</th>
<th>$c$ (Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td>ReF$_4$</td>
<td>9.710</td>
<td>9.050</td>
<td>5.630</td>
</tr>
<tr>
<td>F$_1$</td>
<td>0.0052</td>
<td>0.0052</td>
<td>0.9948</td>
</tr>
<tr>
<td>F$_2$</td>
<td>0.4506</td>
<td>0.5023</td>
<td>0.8193</td>
</tr>
<tr>
<td>IrF$_4$</td>
<td>9.764</td>
<td>9.479</td>
<td>5.778</td>
</tr>
<tr>
<td>F$_1$</td>
<td>0.0052</td>
<td>0.0052</td>
<td>-0.0052</td>
</tr>
<tr>
<td>F$_2$</td>
<td>0.4506</td>
<td>0.5023</td>
<td>0.8193</td>
</tr>
<tr>
<td>IrCl$_4$</td>
<td>11.082</td>
<td>10.947</td>
<td>7.541</td>
</tr>
<tr>
<td>Cl$_1$</td>
<td>-0.0039</td>
<td>0.0201</td>
<td>0.2961</td>
</tr>
<tr>
<td>Cl$_2$</td>
<td>0.4547</td>
<td>0.4737</td>
<td>0.8212</td>
</tr>
<tr>
<td>IrBr$_4$</td>
<td>11.772</td>
<td>11.506</td>
<td>8.021</td>
</tr>
<tr>
<td>Br$_1$</td>
<td>-0.0125</td>
<td>0.0278</td>
<td>0.2981</td>
</tr>
<tr>
<td>Br$_2$</td>
<td>0.4481</td>
<td>0.4813</td>
<td>0.8175</td>
</tr>
<tr>
<td>TaF$_4$</td>
<td>10.134</td>
<td>9.887</td>
<td>5.861</td>
</tr>
<tr>
<td>Ta</td>
<td>0.0015</td>
<td>0.0015</td>
<td>0.9985</td>
</tr>
<tr>
<td>F$_1$</td>
<td>0.0013</td>
<td>0.0142</td>
<td>0.2818</td>
</tr>
<tr>
<td>F$_2$</td>
<td>0.4589</td>
<td>0.4841</td>
<td>0.8322</td>
</tr>
<tr>
<td>TaCl$_4$</td>
<td>11.481</td>
<td>11.468</td>
<td>7.862</td>
</tr>
<tr>
<td>Cl$_1$</td>
<td>0.0203</td>
<td>0.0203</td>
<td>-0.0203</td>
</tr>
<tr>
<td>Cl$_2$</td>
<td>0.4550</td>
<td>0.4560</td>
<td>0.8292</td>
</tr>
<tr>
<td>TaBr$_4$</td>
<td>12.153</td>
<td>12.102</td>
<td>8.425</td>
</tr>
<tr>
<td>Br$_1$</td>
<td>0.0227</td>
<td>0.0227</td>
<td>-0.0227</td>
</tr>
<tr>
<td>Br$_2$</td>
<td>0.4533</td>
<td>0.4575</td>
<td>0.8266</td>
</tr>
<tr>
<td>TaI$_4$</td>
<td>13.149</td>
<td>13.088</td>
<td>9.046</td>
</tr>
<tr>
<td>I$_1$</td>
<td>0.0212</td>
<td>0.0212</td>
<td>0.9788</td>
</tr>
<tr>
<td>I$_2$</td>
<td>0.0097</td>
<td>0.0129</td>
<td>0.2951</td>
</tr>
<tr>
<td>I$_3$</td>
<td>0.4559</td>
<td>0.4603</td>
<td>0.8237</td>
</tr>
</tbody>
</table>
therefore define a winding number \( z(c) \) for any closed path \( c \), along which the spectrum is gapped

\[
z(c) = \frac{1}{2\pi} \text{Im} \oint_c dk \cdot \nabla_k [\log \det M(k)] \quad (61)
\]

which presents a \( Z \)-valued topological charge [33].

For a mirror-symmetric loop \( c \), the invariants of Eqs. (21) and (61) are related by [4, 34, 35]

\[
z(c) = z_2(c) \mod 2. \quad (62)
\]

Any two paths \( a_b \) with \( z(a_b) = \pm 1 \) are topologically distinct in the chiral case, but the distinction is lost once the CHS is broken. Thus, if one-dimensional lines perpendicular to the mirror plane crossing the three-dimensional Brillouin zone of a chiral-symmetric system have distinct chiral charges, they need to be separated by a gapless line in the momentum space. If the chiral charge of the lines is different by 2, this line becomes gapped upon breaking the chiral symmetry (but preserving mirror/glide).

Furthermore, we show in the present section that in a crystal with a symmetry \( S \), the winding numbers \( z(c) \) and \( z(Sc) \) are related by

\[
z(Sc) = \zeta z(c) + \frac{N_{\text{occ}}}{2\pi} \oint_c dk \cdot \nabla_k [\arg (v_k)] \quad (63)
\]

where \( N_{\text{occ}} \) is the dimension of \( M(k) \) and the appropriate form of \( v_k \) and \( \zeta \) is listed in Table V. The integral in (63) vanishes if \( c \) is contractible (i.e. if it does not wind across the BZ). Relations (62) and (63) provide handy tools to explain the appearance of the nodal net in Fig. 4c of the main text.

To outline the derivation of (63), we discuss the case of a unitary symmetry \( S \) that exchanges the two crystal sublattices, corresponding to the first row of Table V. Such a symmetry is off-diagonal in the sublattice basis, i.e.

\[
S_1(k) = U(k) \otimes (a_k \tau^x + b_k \tau^y) \quad (64)
\]

The \( k \)-dependence of \( U(k) \in U(N_{\text{occ}}) \) and \( a_k, b_k \in C \) is assumed to be continuous. The unitarity of (64) implies \( |a_k|^2 + |b_k|^2 = 1 \) and \( a_k b_k^* - b_k a_k^* = 0 \). Operator (64) alters the upper right block of (60) as

\[
M(Sk) = v_k U(k) M^\dagger(k) U^\dagger(k). \quad (65)
\]

from which we conclude the relation (63) with \( \zeta \) and \( v_k \) given in the first row of Table V. We can similarly find \( \zeta \) and \( v_k \) for symmetries that do not exchange the two sublattices and for antiunitary symmetries that (anti)commute with \( C \).

The presence of a nodal chain in Fig. 1c of the main text is compatible with relations of Eqs. (62) and (63). To see this, consider two loops \( c_{1,2} \) in Fig. 8a related by \( c_2 = -C_2 c_1 = g_z c_1 \). The relation of Eq. (63) implies \( z(c_2) = -z(c_1) \). Loops \( c_{1,2} \) enclose a NL so that \( z_2(c_2) = z_2(c_1) = 1 \). The last two relations imply

\[
|z(c_2) - z(c_1)| = 2. \quad (67)
\]

This means that for the CHS model deforming \( c_1 \) onto \( c_2 \) must be associated with encountering at least two NLs. This is indeed true – the red NL in Fig. 8a needs to be intersected twice. We can analogously consider loops \( c_{3,4} \) in Fig. 8a related by \( c_4 = -C_2 c_3 = g_y c_3 \), and infer

\[
|z(c_4) - z(c_3)| = 2. \quad (68)
\]
Therefore, deforming \( c_3 \) onto \( c_4 \) is associated with encountering at least two Weyl lines in the CHS case. This time it is the blue NL in Fig. 8a that needs to be intersected twice to connect the two loops.

To explain the appearance of the additional NL imposed by CHS, consider a pair of horizontal loops \( c_{5,6} \) in Fig. 8a related by \( c_6 = - (g_x \circ \Theta) c_5 \). The relation of Eq. (63) implies that \( z(c_6) = - z(c_5) \), and we obtain

\[
|z(c_6) - z(c_5)| = 2. \tag{69}
\]

Hence, a deformation of \( c_5 \) into \( c_6 \) is accompanied by crossing two nodal lines. In this case, the presence of the nodal chain itself is not sufficient to satisfy this constraint. Thus, CHS imposes an additional NL located in the \( k_z = 0 \) plane and separating \( c_{5,6} \). We indicate such possible NLs by dashed green lines in Fig. 8a.

A suitable choice of considered paths can explain the actual topology of the additional NL. First, note that Eq. (69) implies that the additional NL cannot terminate at the red NL, because that would correspond to just a single gap closing between \( c_5 \) and \( c_6 \), so that it would not be possible to change the topological invariant by 2. Instead, the NL necessarily has to touch the red NL, having a ring-like shape. This leaves us with only two possibilities indicated by the dashed green and magenta lines in Fig 8b. We now show that it is the first option to be realized.

Consider a path \( c_7 = C_{2z}c_5 \), such that \( z(c_7) = z(c_5) \). The paths \( c_{5,7} \) can be merged into \( c_8 \) with \( |z(c_8)| = 2 \). If we finally consider a path \( c_9 = - (g_x \circ \Theta) c_8 \), we conclude using Eq. (63) that

\[
|z(c_9) - z(c_8)| = 4. \tag{70}
\]

Therefore, deforming \( c_8 \) onto \( c_9 \) is accompanied by crossing of four NLs. This implies that the topology of the nodal net cannot take the form (2) of Fig. 8b. More careful argumentation determines the topology of the nodal chain uniquely to that of Fig. 4c of the main text. We expect analogous findings for all eight space groups listed in Fig. 1 of the main text.

Let us finally tackle the distinction of the regions designated as “0” and “2” in Fig. 3h of the main text. The labels correspond to the winding numbers of straight paths traversing the Brillouin zone in the [100] direction. The two regions are related by \( C_{2z} \). Since these loops are non-contractible, we have to take into account the integral term in Eq. (63). We adopt the tight-binding convention with phase factors \( e^{ik \cdot R} \) where \( R \) are the Bravais vectors. With such a choice, \( \mathcal{H}(k) = \mathcal{H}(k + G) \). The representation of \( C_{2z} \) in this convention is

\[
C_{2z}(k) = -i \sigma_z \otimes \begin{pmatrix} e^{-i(k_x-k_y)/2} & 0 \\ 0 & e^{-i(k_x+k_y)/2} \end{pmatrix}. \tag{71}
\]

and the phase \( v_k \) in Eq. (63) becomes

\[
v_k = (a_k^* - b_k^*) (a_k + b_k) = e^{i(k_x+k_y)/2} \tag{72}
\]

which winds once for any one-dimensional path threading the Brillouin zone in the [100] direction. Since in our case \( N_{occ.} = 2 \), we obtain from Eq. (63) that

\[
c(k_y, k_z) = -c(-k_y, k_z) + 2 \tag{73}
\]

compatible with the region labels in Fig. 3h of the main text.

Finally, note that the appearance of an additional nodal line in the \( k_z = 0 \) plane is compatible with the symmetries of the system in the CHS case. The little group of any point in the \( k_z = 0 \) plane contains at least two symmetry operations: the CHS and the product symmetry \( C_{2z} \cdot \mathcal{T} \), where \( \mathcal{T} \) is the time-reversal operator. Due to the presence of these two symmetries, the existence of double degeneracies in the \( k_z = 0 \) plane corresponds to vanishing of a general \( 2 \times 2 \) Hamiltonian, subjected to the two symmetry constraints. As a result, one has a single equation to satisfy by tuning two parameters (in-plane momenta), and hence a general solution admits the appearance of nodal lines in the \( k_z = 0 \) plane.

### G. MINIMAL \( k \cdot p \) MODELS

A minimal model Hamiltonian of a NSNL is given by Eq. (20) of Section B. That Hamiltonian, however, only includes \( k \)-independent perturbations to a \( k \)-linear Dirac Hamiltonian. A more complete \( k \cdot p \) expansion should also include all possible perturbations linear in \( k \). The full list of such perturbations is given by the following 11 terms that can be included into the Hamiltonian of Eq. (20) of Section B:

\[
k_x \gamma_5, k_x \gamma_12, k_x \gamma_15, k_x \gamma_25, k_y \gamma_5, k_y \gamma_12, k_y \gamma_15, k_y \gamma_25, k_z \gamma_23, k_z \gamma_13, k_z \gamma_35. \tag{74}
\]
A minimal Hamiltonian of a nodal chain is somewhat more complicated. This is because such a model cannot take the form of a \( k \cdot p \) expansion, since finite order polynomials cannot reproduce the periodic structure of the chain. Instead, the minimal model of a nodal chain can be obtained by combining a polynomial expansion in the momenta perpendicular to the axis of the chain with the fully periodic function of momentum parallel to the chain.

To derive such a nodal chain Hamiltonian, we start again with the model of Eq. (20) developed in Section B that contains a glide \( g_z \) commuting with \( \gamma_1, \gamma_2, \gamma_5 \) and anticommuting with \( \gamma_3, \gamma_4 \) matrices. To obtain a nodal chain running in the \( k_y \) direction, we have added a glide \( g_z \) that commutes with \( \gamma_2, \gamma_3, \gamma_4 \) and anticommutes with \( \gamma_1, \gamma_5 \) matrices. Assuming the simplest possible \( k_y \)-dependence in the form of cosine and sine functions, the complete \((k_x, k_z)\)-linear model of a nodal chain is given by combining the following 11 terms

\[
\begin{align*}
    & k_x \gamma_1, \sin k_y \gamma_2, k_z \gamma_3, \\
    & \cos \frac{k_x}{2} \gamma_4, \sin \frac{k_x}{2} \gamma_5, k_x \gamma_12, k_z \gamma_23, \\
    & k_x \cos \frac{k_x}{2} \gamma_5, k_z \sin \frac{k_x}{2} \gamma_4, k_z \cos \frac{k_x}{2} \gamma_25, k_z \sin \frac{k_x}{2} \gamma_24.
\end{align*}
\]

Assuming further that the two NSNLs making up the nodal chain are related by symmetry (as is the case in space groups #109 and #122) the number of independent parameters in the minimal model can be reduced to six. In this case the Hamiltonian of a nodal chain is

\[
\mathcal{H}_{\text{NC}}^{\text{sym}}(\mathbf{k}) = hv \left( k_x \gamma_1 + k_z \gamma_3 \right) + v_\parallel \sin k_y \gamma_2 \\
+ w \left( \cos \frac{k_x}{2} \gamma_4 - \sin \frac{k_x}{2} \gamma_5 \right) \\
+ a \left( k_x \gamma_12 + k_z \gamma_23 \right) \\
+ b \left( k_x \cos \frac{k_x}{2} \gamma_5 + k_z \sin \frac{k_x}{2} \gamma_4 \right) \\
+ c \left( k_x \cos \frac{k_x}{2} \gamma_25 - k_z \sin \frac{k_x}{2} \gamma_24 \right)
\]

where an additional condition \( |w/v_\parallel| > \sqrt{2} \) needs to be imposed to guarantee a band ordering compatible with a nodal chain in the center of the band quadruplet. Note that in both Eqs. (75) and (76), we omitted possible terms proportional to the identity matrix.

Alternatively, one can construct a true \( k \cdot p \) expansion around the touching point (TP) of the two NSNLs in the nodal chain. The model captures only the two bands that form the nodal chain. Up to second order in momentum the corresponding Hamiltonian is

\[
\mathcal{H}_{\text{TP}}(\mathbf{k}) = \left( c_0 k_y + c_1 k_x^2 + c_2 k_y^2 + c_3 k_z^2 \right) \sigma_z \\
+ k_x k_z \left( c_4 \sigma_x + c_5 \sigma_y \right)
\]

where a representation, in which both glide operators \( g_x \) and \( g_z \) are proportional to \( \sigma_z \) is chosen. Such a model has lost the periodicity in \( k_y \), and depending on the choice of the parameters \( c_i \) it may replace one or both closed nodal loops by open nodal lines of parabolic/hyperbolic shape. Note that we also omitted terms proportional to the identity matrix: \( k_y \mathbb{1}, k_x^2 \mathbb{1}, k_y \mathbb{1}, k_z^2 \mathbb{1} \).

FIG. 8. Paths considered in the discussion of the chiral symmetric model. (a) The difference of \( z(c_1) \) and \( z(c_2) \) can be explained by the red NL separating them. Similarly, the blue NL explains the difference between \( z(c_3) \) and \( z(c_4) \). However, the nodal chain alone does not explain the difference between \( z(c_5) \) and \( z(c_6) \), and an additional NL in the \( k_z = 0 \) plane is imposed. (b) The invariants for paths \( c_8, c_9 \) are related by Eq. (70), which is consistent with the green NL (1), but not with the magenta NL (2). This uniquely fixes the topology of the nodal net.