Topological Node-Lines in Mechanical Metacrystals

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Topological acoustic and elastic waves have recently emerged as an exciting interdisciplinary field which is still mainly focused on low-dimensional structures and model systems. Here we demonstrate numerically an elastic-wave analogue of topological node-lines in three-dimensional mechanical metacrystals with ribbon- or drumhead-like surface states. These two-dimensional topological surface states offer unprecedented, robust subwavelength confinement of elastic waves. Design principles for topological mechanical metamaterials, from both material and symmetry aspects, are unveiled and connected to fundamental conservation laws and nonsymmorphic space group. Our study paves the way toward the synergy between three-dimensional mechanical metamaterials and topological wave dynamics.

Introduction.—The discovery of topological insulators and quantized edge transport has renewed our understanding of quantum phases of condensed matters [1, 2]. Recently, the exploration of topological physics has been extended from electronic [1, 2] and matter [3] waves to classical waves such as acoustic [4, 5] and photonic [6] waves. As benefited from good controllability and measurability in broad frequency ranges and enriched by its vectorial nature, classical waves emerge as intriguing media for the study of topological phenomena [4–22]. Photonic, acoustic, and elastic topological edge states provide robust wave propagation which are ideal for guiding energy and information flow against noisy, imperfect environments.

To date, the rich physics of three-dimensional (3D) topological elastic waves remains unexplored (with only two recent exceptions [23, 24]). Owing to the full polarization degrees of freedom and the larger wavevector space, 3D mechanical waves can support versatile topological states that do not have analog in low-dimensional systems [23, 24]. Surprisingly, 3D mechanical metacrystals and metamaterials, despite their important roles and very broad range applications in the cutting-edge material technologies [25], have not yet been considered as hosts for topological elastic waves.

In this Letter, we present numerical discovery of mechanical topological node-lines in a class of 3D mechanical metacrystals of tetragonal symmetry. A topological node-line is a line-degeneracy between two bands in 3D wavevector space as described by [26]

\[ \mathcal{H} = \omega_0 + \delta \mathbf{k}_\perp \cdot \hat{v} \cdot \mathbf{\sigma}. \] (1)

Here \( \omega_0 \) is the frequency of a degeneracy point on the node-line, \( \delta \mathbf{k} \) denotes the difference wavevector with respect to the wavevector of the degeneracy point, where \( \delta \mathbf{k}_\perp \) is its component perpendicular to the tangent of the node-line. \( \hat{v} \) represents the group velocity tensor, and \( \mathbf{\sigma} \) is the Pauli-matrix vector.

We find that the mechanical node-lines give rise to topological edge states which enable unprecedented subwavelength confinement of elastic waves on 2D surfaces of 3D mechanical metamaterials. The emergent edge states manifest ribbon- or drumhead-like dispersions, which slow down the surface wave propagation. A unique partner switching scenario is uncovered, which leads to node-
lines guaranteed by the crystalline symmetry and fundamental conservation laws. Design principles for 3D topological mechanical metacrystals are unveiled, which paves the avenue toward the synergy between 3D mechanical metamaterials and topological phenomena—an interdisciplinary field full of opportunities for fundamental researches and applications.

**Mechanical metacrystal architecture.**—Consider a tetragonal mechanical metacrystal with lattice constant \( a \) along all three directions [Fig. 1(a)]. The Brillouin zones (BZs) for the bulk and surface states are given in Fig. 1(b). The metacrystal architecture is designed from both the “scatters” and the space symmetry aspects. There are two “scatters” of “H” shape in each unit-cell [Fig. 1(c)], as inspired by the tuning fork. The three principal axes are the \( x, y, z \) axes.

The six indices in the above matrix are 1 \( \equiv x \), 2 \( \equiv y \), 3 \( \equiv z \), 4 \( \equiv xy \), 5 \( \equiv xz \), and 6 \( \equiv yz \). The material parameters are given in the Supplemental Materials [29].

**Symmetry-induced band degeneracy.**—We now introduce a unique property of the phononic spectrum: at the \( k_z = 0 \) plane, all phononic bands are doubly degenerate. To reveal the underlying mechanism, we construct an anti-unitary operator \( \hat{\Theta}_x = \mathcal{S}_x \ast \mathcal{T} \) (\( \mathcal{T} \) is the time-reversal operator) which transforms the wavevector as \( (k_x, k_y, k_z) \rightarrow (-k_x, k_y, k_z) \). Thus, \( \hat{\Theta}_x \) is an invariant operator at the \( k_x = \frac{\pi}{a} \) plane where it has the special property,

\[
\hat{\Theta}_x \varphi_{n\mathbf{k}} = e^{-ik_xa} \varphi_{n\mathbf{k}} = -\varphi_{n\mathbf{k}},
\]

for an arbitrary band index \( n \). According to the Kramers
Parity evolution and mechanical node-lines.—The topological node-line resides in the \( k_z = 0 \) plane, where the phononic states can be labeled by the mirror eigenvalues \( M_z \hat{\varphi}_{n\vec{k}} = m_z \hat{\varphi}_{n\vec{k}} \) with \( m_z = \pm 1 \). We find that
\[
M_z \hat{\Theta}_z \hat{\varphi}_{n\vec{k}} = e^{-ik_z \hat{a}} \hat{\Theta}_z M_z \hat{\varphi}_{n\vec{k}} = m_z \hat{\Theta}_x \hat{\varphi}_{n\vec{k}},
\]
for \( k_z = 0 \). This property indicates that at the BZ boundary, the two degenerate Bloch states, \( \hat{\varphi}_{n\vec{k}} \) and \( \hat{\Theta}_x \hat{\varphi}_{n\vec{k}} \), have the same mirror eigenvalue [see Supplemental Materials [29] for numerical confirmation]. Fig. 2(a) indicates degeneracies between the second and the third bands of opposite mirror parity along three lines from the BZ center to boundary, \( \Gamma X, \Gamma M, \) and \( \Gamma Q \). These degeneracies are found to form node-lines rather than Weyl or Dirac points.

To illustrate this, we examine the evolution of phononic bands. Starting from \( \omega = 0 \), three acoustic-phonon branches evolve from the \( \Gamma \) point to an arbitrary point on the \( XM \) line and evolve back to form higher-frequency bands of the same \( m_z \). Remarkably, there is an unavoidable crossing between the second and the third phononic bands, regardless of their group velocities [see Fig. 2(b) for a case different from Fig. 2(a)]. These arguments hold for band-evolution from the \( \Gamma \) point to an arbitrary point on the BZ boundary lines at \( k_z = 0 \) plane [e.g., see the inset of Fig. 2(a)]. Therefore, such unavoidable band-crossing must extend from a point to a line enclosing the \( \Gamma \) point, i.e., a node-line (denoted as “the first node-line”) [see Fig. 2(c)]. This node-line, discovered at finite frequencies, is distinct from the Weyl lines at zero frequency as found in Ref. 29.

The above scenario also reveals the deterministic nature of the first node-line: it must appear due to the degeneracy-partner switch between the \( \Gamma \) point which has degeneracy between bands of opposite \( m_z \) and the BZ boundary lines which have leads degeneracy between bands of the same \( m_z \). We emphasize that this scenario is unique to elastic (and electromagnetic) waves which have two branches of different mirror properties in the limit of \( \omega \to 0 \) and \( \vec{k} \to 0 \). There is no such analog in electronic or atomic systems.

In Fig. 2(d) we present the phononic dispersion around one point [the \( P \) point as labeled in Figs. 2(a) and 2(c)] on the node-line. We find that the dispersion along the tangential direction (i.e., \( k_y \) direction) of the node-line is very weak, whereas along the other two directions a Dirac dispersion emerges as shown in Fig. 2(d). The Hamiltonian for the \( P \) point is
\[
\mathcal{H} = \omega_0 + v_x \delta k_x \hat{\sigma}_x + v_z \delta k_z \hat{\sigma}_y,
\]
where \( \omega_0 \) is the frequency of the Dirac point (we set \( \hbar = 1 \)) and \( v_x (v_z) \) is the group velocity along the \( x (z) \) direction. The space-time reversal operation is manifested as \( \mathcal{PT} = \hat{\sigma}_z \mathcal{K} \) where \( \hat{\sigma}_z \) represents the mirror operation \( M_z \) and \( \mathcal{K} \) is complex conjugation. The Hamiltonian satisfies Eq. (1) and the \( \mathcal{PT} \) symmetry.

Mechanical topological surface waves.—The 3D phononic crystal can be reduced to the 1D Su-Schrieffer-Heeger [30] model using the dimensional reduction procedure [31]: for given \( k_x \) and \( k_y \) the metacrystal is equivalent to a 1D system along the \( z \) direction. The \( \mathcal{PT} \) symmetry and the \( M_z \) symmetry guarantee that such an effective 1D system has trivial or nontrivial Zak phase, i.e., \( \theta_{Zak}(k_x, k_y) = 0 \) or \( \pi \). It has been proven [32] that with these symmetries, the Zak phase for each given \((k_x, k_y)\) can be simplified into (for phononic analog, see Supplemental Materials [29])
\[
\frac{\theta_{Zak}}{\pi} = \left\{ \frac{1}{2} \sum_n \left[ m_z \left( \frac{\pi}{a}, n \right) - m_z(0, n) \right] \right\} \mod 2.
\]

The first and second arguments of the \( m_z \)'s are the wavevector \( k_z \) and the band index \( n \), while the summation over \( n \) includes all bands below the node-line. The node-lines are the boundaries between the regions with trivial and nontrivial Zak phases. Crossing the node-line is equivalent to a topological pumping which transfers a pair of phonon states from bulk to the two edges [31].
Materials [29] is presented in Fig. 3(a), together with the projection of the first node-line. The topological surface states appear outside the node-line where the Zak phase is nontrivial. A finite bulk band gap is also required to observe the topological surface states. Therefore, the second and the third bands must be well-separated, which is realized by using anisotropic elastic materials. Due to the requirement of finite band-gap, topological surface states are found in a fraction of the region outside the first node-line, forming ribbon-like spectrum with mild dispersions [see Fig. 3(a)]. The topological surface spectrum and the node-line have the $C_{4v}$ symmetry which is a projective representation of the tetragonal space group. The projected bulk bands and surface states along the high-symmetry lines are presented in Fig. 3(b). The displacement-profile of the topological surface wave for $k = \frac{\pi}{a}(1, 0.6)$ point in the surface BZ is shown in Fig. 3(c), which indicates strong subwavelength wave confinement due to topological mechanism.

**Node-lines from mechanical metamaterials.** We now show that topological node-lines can also be realized by using anisotropic metamaterials as the background medium and steel as the scatterers. The elastic metamaterial is made of a multilayer structure of epoxy and steel which is compatible with 3D printing technologies [see the inset of Fig. 4(a)]. The effective elastic modulus and mass density of the metamaterial are derived from the effective medium theory [28] (for details, see Supplemental Materials [29]). We calculate the phononic band structure and topological surface states [presented in Fig. 4]. The bulk band structure shows band-evolution resembling that in Fig. 2(c). Beside the deterministic node-lines, there are accidental node-lines at higher frequencies. It turns out that the projective band gap is finite for a node-line formed by the sixth and seventh bands [indicated by the arrows in Fig. 4(a)]. The region inside this node-line has nontrivial Zak phase which leads to the drumhead-like topological surface elastic waves [see Fig. 4(b)]. The topological surface states are strongly confined around the interface and have small group velocity as indicated by their weak dispersions.

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