Phononic Weyl Nodal Straight Lines in High-Temperature Superconductor MgB$_2$

Qing Xie$^{1,2}$, Jiangxu Li$^{1,3}$, Min Liu$^{1,3}$, Lei Wang$^{1,3}$, Dianzhong Li$^{1}$, Yiyi Li$^{1}$, and Xing-Qiu Chen$^{1,4}$

$^1$Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, Shenyang 110016, China
$^2$University of Chinese Academy of Sciences, Beijing 100049, China
$^3$School of Materials Science and Engineering, University of Science and Technology of China, 110016 Shenyang, Liaoning, China

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Based on first-principles calculations, we predict that the superconducting MgB$_2$ with a AlB$_2$-type centrosymmetric lattice host the so-called phononic topological Weyl nodal lines (PTWNLs) on its bulk phonon spectrum. These PTWNLs can be viewed as countless Weyl points (WPs) closely aligned along the straight lines in the $\sim$H–K–H direction within the three-dimensional Brillouin zone (BZ). Their topological non-trivial natures are confirmed by the calculated Berry curvature distributions on the planes perpendicular to these lines. These lines are highly unique, because they exactly locate at the high-symmetry boundary of the BZ protected by the mirror symmetry and, simultaneously, straightly transverse the whole BZ, in different from known classifications including nodal rings, nodal chains or nets, and nodal loops. On the (1010) crystal surface, the PTWNLs-induced drumhead-like non-trivial surface states appear within the rectangular area confined by the projected lines of the PTWNLs with opposite chirality. Moreover, when the mirror symmetry is broken, the double-degenerate PTWNLs are further lifted to form a pair WPs with opposite chirality. Our results pave the ways for future experimental study on topological phonons on MgB$_2$ and highlights similar results in a series of isostructural AlB$_2$-type metallic diborides.

As accompanying with extensive studies of topological insulators, topological semimetals and even topological superconductors in their electronic structures [1–3], topological phonons [4–8] have been most recently attracted attentions in condensed matter physics and material sciences. This is mainly because the topological phononic states will be interesting for potential applications. In different from various electronic fermions, phonons, as one of bosons, are not limited by the Pauli exclusion principle. This fact demonstrates that the whole frequency zone of phonon spectrum can be physically probed. In similarity to topological properties of electrons, the topological effects of phonons can induce the one-way edge phonon states or topologically protected surface phononic states. Physically, these states will conduct phonon with little or no scattering [4, 5], suggesting possible applications for designing phononic circuits [6]. For instance, utilizing the one-way edge phonon states an ideal phonon diode [6] was proposed with a fully 100% efficiency in a multi-terminal transport system. It was even theoretically uncovered that the chirality of topological phonons excited by polarized photons can be detected by a valley phonon Hall effect in monolayer hexagonal lattices [8]. In particular, it needs to be emphasized that in similarity to various fermions of electrons, the exciting progresses of the bosons (vibrational phonons) have been also predicted [7] or observed in the 3D momentum space of solid crystals with the topological vibrational states, such as Dirac, Weyl and line-node phonons in phononic crystals with macroscopic acoustic systems of kHz frequency [4, 5, 7, 9–21] and theoretically predicted doubly-Weyl phonons in transition-metal monosilicides with atomic vibrations at THz frequency [22]. Most recently, also in a series of WC-type family of materials (i.e., ZrS, ZrSe and ZrTe) with atomic vibration at THz frequency, the single topological Weyl phonons are predicted and they exist opening topological arcs of surface phonons, connecting pairs of surface-

FIG. 1. Known main classifications of topological nodal lines: (a) isolated nodal ring, (b) nodal chain, (c) nodal link, (d) nodal knot, and (e) nodal straight lines extending the whole BZ in an one-way direction.

projected Weyl points with opposite chirality [23]. However, to date no phononic topological Weyl nodal lines have been reported in macroscopic acoustic systems at kHz frequency or in atomic vibrational periodic lattices at THz frequency.

It needs to be emphasized that topological nodal lines [24] have been already and extensively studied in electronic band structures, optical lattices, photonic and acoustic systems. It has been found that symmetries, i.e., both $\mathcal{P}$ and $\mathcal{T}$ ones, can protect the presence of various nodal lines. Once these symmetries are broken, nodal lines would be gapped out or form Dirac points (DPs) or WPs. To date, nodal lines have been classified into various categories, such as (i) isolated closed nodal rings (Fig. 1(a)) in alkaline earth metals of hcp Be and Mg [25], of fcc Ca and Sr [25, 26], TiSi-family [27], 3D carbon allotropes [28], antiperovskite Cu$_3$(Pb,Zn)N [29, 30], Ca$_3$P$_2$ [31], photonic crystals [7], and a hyperhoneycomb
FIG. 2. (a) Crystal structure of MgB$_2$. Three shadowed planes are the mirror planes. (b) The Brillouin zone and (1010) surface. The PTWNLS transverse the whole BZ along both the $-H$ to $H$ and the $-H'$ to $H'$ directions. Red (blue) lines have negative (positive) chirality. Each PTWNL extends through the whole BZ 1 times along one of the direction and carries a topological charge $Q = \gamma/\pi = \pm 1$ using the input of the Berry phase. The surface states at about 14.2 THz are schematically depicted on the surface. (c) The phonon dispersion of MgB$_2$ along the high-symmetry momentum paths in the BZ. Three red thick bands (as marked by the 1st, 2nd, and 3rd) along the H-K direction transverse the whole BZ along both the $-\pi$ and $+\pi$ momenta. Three double-degenerate phonon bands along the directions from $-H(\frac{1}{3}, \frac{1}{3}, -\frac{1}{3})$ to $H(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$ in the bulk BZ as illustrated in Fig. 2(b). The calculations demonstrate that these double-degenerate phonon bands exactly are PTWNLS. The Berry phases of the defined loops around these PTWNLS are derived to be $\pm \pi$, indicating their non-trivial topological nature. Berry curvature distributions uncover their chirality. In addition, on the (1010) surface, we observe PTWNLs-induced drumhead-like non-trivial surface states, which are indeed very similar with the topological surface states found in topological Dirac nodal line systems. When the inversion symmetry is broken, the double-degenerate PTWNLS can be further lifted up and WPs can be formed. Afterwards, the surface states form opening Fermi arc structure connecting these WPs. In addition, we have noted that the other three doubly-degenerate phononic bands form $-A(0,0,-\frac{1}{3})$ to $A(0,0,\frac{1}{3})$ in the bulk BZ are topologically trivial, without appearance of any phononic topological surface states.

Methods.— We perform first-principles calculations based on density functional theory (DFT) [53, 54] with generalized gradient approximation (GGA) in the form of Perdew-Burke-Ernzerhof function [55, 56] for exchange-correlation potential. The calculations are performed using the Vienna ab initio simulation package (VASP) [51, 52]. A self-consistent field method (tolerance $10^{-5}$ eV/atom) is employed in conjunction with planewave basis sets of cutoff energy of 500 eV. Atomic structure optimization is implemented until the remanent Hellmann-Feynman forces on the ions are less than 0.001 eV/Å. We use a Γ-centered $11 \times 11 \times 17$ k point mesh in the Brillouin zone.
FIG. 3. Phononic states on the (1010) surface of MgB$_2$. (a) The surface phonon spectrum along high symmetry lines. (b) The evolution of the surface phonon spectra and the topologically protected phononic non-trivial surface states by increasing the $k_z$ value along the $\Gamma - \bar{X} - \Gamma$ direction. (c) The frequency-dependent evolution of the phononic surface states of the (1010) BZ as defined in Fig. 2(b) to show the change of the phononic drumhead non-trivial surface states in the rectangular region confined by the projected lines of two PTWNLs with opposite chirality.

to sample the BZ. Phonon spectra are obtained using the density functional perturbation theory (DFPT) with a Born-Karman boundary condition implemented in the Phonopy package [57]. The force constants are calculated using a $3 \times 3 \times 3$ supercell and are taken as the tight-binding parameters to build the dynamic matrices. The surface DOS are obtained by using the iteration Green’s function method [59].

Structure.— The optimized lattice constants are $a = 3.074$ Å and $c = 3.513$ Å. These values are in good agreements with previous experimental [40–42] and computational [43–47] results. The structure is shown in Fig. 2(a).

Phonon spectra.— Figure 2(c) presents the phonon spectrum of MgB$_2$ along high symmetry momentum paths, which are in nice agreement with previous calculations [43–47] and experimental characterizations [48–50]. At the high-symmetry $K(\frac{1}{3}, \frac{1}{3}, 0)$ and $H(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$ points, there are three double-degenerate points each. Phonon spectrum along $-H$ to $H$ in Fig. 2(c) evidences the existence of the three double-degeneracy bands, which are PTWNLs in the strictly straight lines traversing the whole BZ. In Figs. 2(d) and 2(e), we depicted the phonon dispersions along a PTWNL on the $xz$-plane and around a specified point, $(1/3, 1/3, 0.2)$ in an unit of reciprocal lattice vector, of a PTWNL on the $xy$-plane. It can be seen that their dispersion around any point of the PTWNLs exhibits a linear dispersion on the $xy$-plane. It is a hallmark of a WP. In other words, these 1st, 2nd, and 3rd PTWNLs in Fig. 2(c) are highly unique. In the first, they along the $-H-K-H$ direction can be viewed as countless WPs closely aligned in the straight lines in its three-dimensional BZ. In the second, each PTWNL can extend through the whole BZ along this high-symmetry direction in the momentum space. In particular, all of them exactly lie at the BZ boundary along the one-way high-symmetry direction, which are indeed protected by the mirror symmetry. In addition, it needs to be emphasized that, although such Dirac-line behaviors stretching the whole BZ along the one direction has been recently outlined in the electronic structures of rhombohedrally stacked honeycomb lattices [60] and of nanostructured carbon allotropes [61], these symmetry-protected PTWNLs along the one-direction high-symmetry lines in the phonon spectrum of MgB$_2$ is still recognized for the first time. Mechanically, these three different PTWNLs are associated with three distinct phonon modes. The 1st PTWNL mainly involves the in-plane vibrational mode of Mg atoms, the 2nd one is totally determined by the out-of-plane vibrational mode of two boron atoms moving in opposite or same directions along the $c$ axis while the Mg is stationary, and the 3rd one only involves the in-plane motion in which boron moves along the $x$ or $y$ axes and Mg along almost the diagonal direction of the $xy$ axes. Another difference for these three PTWNLs is that the 2nd
PTWNL shows an apparent $k$-dependent dispersion of the frequencies, whereas both the 1st and 3rd PTWNLs are nearly flat in the frequencies against $k$ vector along the $-H-K-H$ or $-H'-K'-H'$ directions as shown in Fig. 2(c).

Topological properties of phonon.—To determine the topological nature of these PTWNLs, we have derived the corresponding Berry phases and Berry curvature distributions. For a closed loop in 3D BZ, the berry phase is defined as

$$\gamma_n = \oint_C \mathbf{A}_n(k) \cdot dl,$$

where $\mathbf{A}_n(k) = i \langle u_n(k) | \nabla_k | u_n(k) \rangle$ is the Berry connection and $u_n(k)$ is the Bloch wavefunction of $n$-th band. As illustrated in Fig. 2(b), we have first selected a closed circle on the $xy$-plane centered at a momentum position of the PTWNL (see the circle marked by the green curves). Note that the radius of the closed circles going around each PTWNL can be selected to be arbitrary large, as long as it does not also cover another PTWNL. Interestingly, we have found that their Berry phase for all three PTWNLs along the $-H-K-H$ direction are $\pi$, whereas the other three PTWNLs along the $-H'-K'-H'$ direction have an opposite Berry phase of $-\pi$. This means that these PTWNLs are topological non-trivial and it also proves that the topological nature of the PTWNLs along the $-H-K-H$ direction and $-H'-K'-H'$ direction are opposite in their chirality. As a further supporting evidence, we can directly visualize the source or sink effects by deriving the Berry curvature distributions, $\Omega_n(k) = \nabla \times \mathbf{A}_n(k)$, on the $xy$-plane, as shown in Figure 2(f).

In addition, as shown in the phonon spectrum from $\Gamma$ to $\Lambda$ in Fig. 2(c) there are also two-fold degenerate lines. However, the analysis of their Berry phases and Berry curvatures confirm that these three lines are indeed topological trivial. Their associated vibrational phonon modes were already discussed in a previous publication [47].

Phononic drumhead-like surface states.—Furthermore, we have identified the surface phonon spectrum of the (10\bar{1}0) surface of MgB$_2$. As expected, there should have topologically protected phononic non-trivial drumhead-like surface states in the rectangular region confined by the projected lines of the PTWNLs along the K to H direction and along the K' to H' direction. We calculate surface phononic density of states (PDOSs) by using the iteration Green’s function method [59]. After Fourier transforming the force constants, surface Green’s function is built from dynamical matrix and the surface DOS is taken from the imaginary part of surface Green’s function. Figure 3 presents the surface states on the MgB$_2$ (10\bar{1}0) surface. In Fig. 3(a), we depict the surface PDOSs along high symmetry moment paths on the surface BZ ranging from 12.0 THz to 16.0 THz to clearly show the phononic surface states associated with the 2nd PTWNL. It can be seen in Fig. 3 that in the $\bar{X}-\bar{M}$ direction the bright phononic non-trivial surface states are clearly observable. In Figs. 3(b) and 3(c), we further show the evolutions of drumhead-like surface states with respect to increasing $k_z$ and frequency, respectively. We observe that the surface states are confined well in the rectangular region outlined by the projected lines of two 2nd PTWNLs with opposite chirality. In Fig. 3(b), with increasing $k_z$, the downward parabolic-shape non-trivial surface states climb up to a higher frequency and the depth of the parabola becomes smaller and smaller. At $k_z = 0.5$ in Fig. 3(b), the shallow parabolic non-trivial surface state is completely above the surface state at $k_z = 0.0$. This leads to an interesting evolution of the phononic non-trivial surface states as the frequency increases. We have observed three typical types of non-trivial surface states associated with the 2nd PTWNL in Fig. 3(c). When the frequency $13.3 \lesssim f \lesssim 13.9$ THz, the surface states looks like to connect two points on the same projected line of the bulk PTWNL. When $13.9 \lesssim f \lesssim 14.8$ THz, the surface states clearly connect two points on the two projected lines of the bulk PTWNLs with opposite chirality. When $14.8 \lesssim f \lesssim 15.1$ THz, the surface states form a ring on the 2D surface BZ and do not intersect with any projected lines of the bulk PTWNLs. Indeed, in another two different frequency regions below 12 THz or above 16 THz, we can certainly observe the phononic non-trivial surface states which are associated with the 1st and 3rd PTWNLs along the bulk K-H directions.

Phononic Weyl points and surface arcs.—Interestingly, our calculations also reveal that the double detergency of these
PTWNLS can be lifted, possibly resulting in the appearance of WPs, when both the mirror and inversion symmetries are broken. To elucidate this feature, we have substituted one boron atom with a carbon atom in the MgB$_2$ unit cell, leading to the composition of MgBC. With such a treatment, the MgBC structure now belongs to the space group of $P6_3$ (No. 187) because the inversion symmetry is broken and, simultaneously, the mirror symmetry of the K-H direction is also broken. As illustrated in Fig. 4(a), the derived phonon dispersion along the H to K direction does not exhibit any PTWNLS due to the lifting up of double degeneracy. In contrast, a pair WPs appear because of the phonon band crossings. We also analyzed their topological nature using the Berry curvature distributions around each WP, obtaining the nonzero topological charges of ±1 as shown in Fig. 4(a). Additionally, on the (1010) surface we have clearly observed the opening phononic surface arc states connecting to such a pair WPs with opposite chirality in Fig. 4(b,c and d).

Finally, we have found that a series of metallic diborides, which are isostructural to MgB$_2$ in the AlB$_3$ family, host similar PTWNLS in their phonon spectra. These materials include the prototype material AlB$_2$, BeB$_2$, CaB$_2$, CuB$_2$, NaB$_2$, OsB$_2$, ScB$_2$, SrB$_2$, TaB$_2$, TiB$_2$, YB$_2$, and ZrB$_2$. For each of them, there are three double-degenerate PTWNLS along $\bar{H}$ to H in the 3D BZ. These PTWNLS transverse the whole BZ and act as source or sink of the Berry curvatures. On their (1010) crystal surface, we observed drumhead-like non-trivial phononic surface states. At certain frequencies, the drumhead-like surface states form isolated arc structures and should serve as clear signature for experimental verifications. Available experimental techniques [62–65] to probe these states include neutron scattering, electron energy loss spectroscopy and X-ray thermal diffuse scattering.

Note added.—During the preparation of this work, we became aware of a very recent manuscript proposing the electronic topological Dirac nodal lines in MgB$_2$ through first-principles calculations [66].

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These authors contributed equally to this work.
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