Dual topological–nonsymmetric Dirac semimetal in three dimensions

Yun-Tak Oh,1 Hong-Guk Min,1 and Youngkuk Kim1,∗

1Department of Physics, Sungkyunkwan University, Suwon 16419, Korea
(Dated: January 4, 2019)

Previously known three-dimensional Dirac semimetals (DSs) occur in two types – topological DSs and nonsymmetric DSs. Here we present a novel three-dimensional DS that exhibits both features of the topological and nonsymmetric DSs. We introduce a minimal tight-binding model for the space group 100 that describes a layered crystal made of two-dimensional planes in the $p4g$ wallpaper group. Using this model, we demonstrate that double glide-mirrors allow a noncentrosymmetric three-dimensional DS that hosts both symmetry-enforced Dirac points at time-reversal invariant momenta and twofold-degenerate Weyl nodal lines on a glide-mirror-invariant plane in momentum space. The proposed DS allows for rich topological physics manifested in both topological surface states and topological phase diagrams, which we discuss in detail. We also perform first-principles calculations to predict that the proposed DS is realized in a set of existing materials $\text{BaLaXYB}_2$, where $X = \text{Cu or Au}$, and $Y = \text{O, S, or Se}$.

Dirac semimetals (DS) refer to a class of topological semimetals, characterized by hosting massless Dirac fermions in momentum space [1]. First identified in graphene with the vanishingly weak spin-orbit coupling (SOC), the massless Dirac fermion system has attracted a surge of interest, exhibiting exotic properties and potential applications for future electronic devices [2, 3]. Notably, with the advent of topological insulators [4, 5], the three-dimensional (3D) DS with strong spin-orbit coupling has reinforced their status as an important class of topological semimetals. It was first noted that a 3D DS can occur at the phase boundary between the topological and the normal insulators in the presence of inversion symmetry [6, 7]. Later, Young et al. found that the 3D DS can be stabilized by crystalline symmetries and time-reversal symmetry [8], and Wang et al. theoretically proposed the material realizations in $\text{Na}_3\text{Bi}$ and $\text{Cd}_3\text{As}_2$ [9, 10], which were confirmed experimentally [11–15]. Currently, the DSs are expected to exist in a variety of forms, such as two-dimensional (2D) DSs [16], double DSs [17], type-II DSs [18], and Dirac-Weyl semimetals [19].

In spite of this variety, it is surprising to notice that all the previously known DSs fall into two disjoint classes, dubbed topological and nonsymmetric DSs, respectively [20]. The nonsymmetric class of the DSs is characterized by hosting Dirac points (DPs) that are pinned at the time-reversal invariant momenta (TRIMs) of the Brillouin zone (BZ). On the other hand, the topological class of the DSs distinguish themselves from the nonsymmetric DSs by having a pair of DPs off TRIMs. Another distinguishing feature of the topological DSs is the coexistence of nontrivial band topology in the bulk, manifested as gapless excitations on the surface [21, 22]. In contrast, the bulk bands of the nonsymmetric DSs are expected to be topologically trivial. Instead, a topological nature of the nonsymmetric class is reflected in topological phase transitions, driven by symmetry-lowering perturbations from the nonsymmetric DS into either a topological insulator or a normal insulator [8, 20, 23–25].

In this Letter, we provide an exception to this disjoint a priori classification of 3D DSs. Developing a minimal tight-binding model for space groups (SGs) $P4bm$ (# 100), we establish the existence of a novel type of 3D DSs, characterized by featuring both the topological and nonsymmetric DSs. It is shown that the DS hosts the DPs that reside at TRIMs, which is a characteristic feature of the nonsymmetric DSs. Simultaneously, the bulk bands carry nontrivial band topology, giving rise to topological surface states, which is a characteristic feature of the topological DSs. A striking consequence of this dual nonsymmetric and topological nature of the DS is the rich topological physics manifested not only in the surface energy spectrum but also in topological phase transitions driven by symmetry-breaking perturbations. Drumhead-like topological surface states arise due to the nontrivial band topology in the bulk, characterized by hosting Weyl nodal lines (WNLs). Moreover, symmetry-lowering perturbations derive a topological phase transition from the proposed DS to distinct topological phases, including a weak topological insulator (WTI) and Weyl and double Weyl semimetal (WS) phases. Using first-principles calculations, we also discuss its material realization in an existing compound, $\text{BaLaCuBO}_5$.

Let us begin with elucidating the role of symmetries in SG 100 to protect degeneracies of the Bloch states. SG 100 has the distinguishing feature that it is generated by a glide-mirror $g_x$ and a fourfold rotation $C_{4z}$ without inversion symmetry. As emphasized in [26, 27], the double glide-mirrors, $g_x$ and $g_y = \frac{1}{2} C_{4z} g_x C_{4z}$, together with time-reversal symmetry $T$, span four-dimensional irreducible representations (FDIRs) at $M = (\pi, \pi, 0)$ and $A = (\pi, \pi, \pi)$, where $g_x$ and $g_y$ satisfy the minimal algebras for a FDIR, $g_x^2 = g_y^2 = 1$ and $[T, g_x(y)] = \{g_x, g_y\} = 0$. Moreover, the linear dispersion of the bands is generic at $M$ and $A$ since a $T$-odd vector representation of the point group at the $M$ and $A$ points is present in the tensor product of the FDIRs [8, 17, 26]. Therefore, the presence
The location of the twofold-degenerate WPs and fourfold-degenerate WNLs are present on the projected nodal lines, where red and blue, respectively. The DP is indicated by a dashed (green) circle. (d) Bulk (grey) and slab (red) energy bands. Topological surface states emerge in the interior region of the red and blue, respectively. The DP is indicated by a dashed (green) circle. (e) Topological characterization of twofold-degenerate nodal lines in SG 100.

describes the nearest hopping of electrons, and

\[
V(k) = v_0 \cos \frac{k_x}{2} \cos \frac{k_y}{2} \tau_y \sigma_z + v_1 (\sin k_x \sigma_x + \sin k_y \sigma_y) \tau_z \\
+ v_2 (\sin k_x \sigma_y - \sin k_y \sigma_x) + v_3 \sin k_z \tau_x \\
+ v_4 \left( \sin \frac{k_x}{2} \cos \frac{k_y}{2} \sigma_y - \cos \frac{k_x}{2} \sin \frac{k_y}{2} \sigma_x \right) \tau_x
\]

describes the potential terms that lower the transnational symmetry of \( \mathcal{H}^t(k) \) into SG 100. \( V(k) \) is constructed, such that it preserves the generators of SG 100, \( g_x = \tau_x \exp(-i\frac{\pi}{2} \sigma_z) \) and \( C_{4z} = \exp(-i\frac{\pi}{2} \sigma_z) \), and time-reversal symmetry \( \mathcal{T} = i \sigma_y K \), where \( \{\sigma_1, \tau_x, \tau_y, \tau_z\} \) are the Pauli matrices for spins. We adopted a gauge, in which the Hamiltonian \( \mathcal{H}^0(k) \) transforms under the translation of a reciprocal lattice vector \( \mathbf{G} \) according to

\[
\mathcal{H}^0(k + \mathbf{G}) = e^{-i d(\tau_z) \cdot \mathbf{G}} \mathcal{H}^0(k) e^{i \mathbf{G} \cdot d(\tau_z)}
\]
degeneracy at $M$. Note that the bands are linearly dispersing in the vicinity of $M$ point. Therefore, the bands feature a nonsymmorphic DP at $M$. We also have confirmed that an additional DP is present at $A$, as we expected from the symmetry-analysis. Based on the Wilson bands calculations [30], we find that the DPs carry the zero Chern number [31]. This indicates that the fourfold degeneracy is a genuine DP, in the sense that it is a composite of two WPs with $\pm 1$ Chern numbers, respectively.

Besides the fourfold degeneracy, we find that the bands also feature twofold-degeneracy WNLs, the hourglass-like band connectivity on the high-symmetry $\Gamma-X$ ($Z-R$) line. This guarantees the presence of a twofold degeneracy on the $k_y = 0$ plane, as shown in Fig. 2(c). A close inspection in the entire BZ reveals that one-dimensional nodal lines are present in the vicinity of $X$ ($R$) lying on the $k_y = 0$ plane. We have confirmed that a Weyl line node carries the $\pi$ Berry phase, calculated along a $C_2 T$-invariant path that threads the nodal line [See the left panel of Fig. 2(f),] where the Berry phase is $Z_2$-quantized. As a consequence of the $\pi$ Berry phase, drumhead-like states emerge on the surface where the projected interior region of a nodal line has non-zero area, such as the (001) surface. As shown in Fig. 2(d), the slab band calculation results in the topological surface states at $E = 0$ near the $\Gamma(R)$, which constitute a part of the drumhead-like surface states on the (010) surface.

The WNL hosted in SG 100 is of a hourglass-type [32–34], which is robust against the band inversion at $M$ ($R$). As illustrated in Fig. 2(e), the band inversion at $X$ shrinks the size of the nodal line into a fourfold-degenerate DP. However, instead of annihilating it, the band inversion reverts the DP to a nodal line due to the hourglass-like band connectivity. We assert that this type of WNLs can be characterized by a non-trivial $Z_2$ topological invariant, calculated on the time-reversal invariant sphere that encloses a nodal line [See the right panel of Fig. 2(f).]. The Wilson bands calculation results in the same connectivity of the Wilson bands as those of a 3D Dirac point [35]. The nontrivial $Z_2$ invariant, again, reveals that the WNL can be shrunk to form a 3D DP.

Having demonstrated the topological aspect of the DS, we now move to its nonsymmorphic aspect, captured in a topological phase diagram shown in Fig. 3. From the DS phase, we consider symmetry-lowering perturbations [36]. Among diverse possibilities, as a representative example, here we consider a combination of the inversion symmetric $E_g$- and $B_{2g}$-mode strains and an $m_{A_2u}$-mode staggered potential. These perturbations are described by a perturbed Hamiltonian $H^1(k)$, where

$$H^1(k) = m_{E_g} \sin \left( k_x + k_y \right) \tau_y + m_{B_{2g}} \sin \frac{k_x}{2} \sin \frac{k_y}{2} \tau_x + m_{A_2u} \tau_z.$$  

For simplicity, we assume the mass parameters are equivalent between the inversion-symmetric perturbations ($m_s \equiv m_{E_g} = m_{B_{2g}}$). Furthermore, we decompose the pristine Hamiltonian $H^0(k)$ (Eq. 1) into the inversion-symmetric part $H^0_+ (k)$ and inversion-asymmetric part.
\[ H^0_+ = t_1 \cos \frac{k_x}{2} \cos \frac{k_y}{2} \tau_x + v_1 (\sin k_x \tau_z \sigma_x + \sin k_y \tau_z \sigma_y) + v_3 \sin k_x \tau_z \sigma_z, \]

and

\[ H^0_- = v_- \left[ v_0 \cos \frac{k_x}{2} \cos \frac{k_y}{2} \tau_y \sigma_z + v_2 (\sin k_x \sigma_y - \sin k_y \sigma_x) + v_4 \left( \sin \frac{k_x}{2} \cos \frac{k_y}{2} \sigma_y - \cos \frac{k_x}{2} \sin \frac{k_y}{2} \sigma_x \right) \tau_x \right]. \]

Here, \( v_- \) is introduced to parametrize the overall strength of the inversion-asymmetric part.

Figure 3(a) shows a topological phase diagram that is obtained from \( H^0 + H^1 \) in the \((v_-; m_s; m_{z\mu})\) space. We first note that the DS phase in SG 100 resides along the \( |v_-| \) (red) axis. From this DS phase, a centrosymmetric strain, described by \( m_s \), drives a topological phase transition; positive (negative) \( m_s \) induces a WTI (normal insulator), characterized by \( Z_2 \) topological indices \((\mu_0; \mu_1; \mu_2; \mu_3) = (0;001)(0;000)\). Therefore, the DS phase defines a phase boundary between the normal and topological insulator phases, thus exhibiting the nonsymmetric nature of the DS. In addition to the WTI phase, we find that a Weyl semimetal (WS) can also be induced from the DS phase by applying the staggered potential \((|m_{z\mu}| > 0)\). Interestingly, we find that the three distinctive WS phases are allowed: (1) one having regular (single) WPs with the Chern number \(|C| = 1\), (2) another having double WPs with \(|C| = 2\), and (3) the other having both single and double WPs. We also note that an archetypal centrosymmetric DS phase is restored from the DS phase by turning off the noncentrosymmetric interactions \( v_\sigma = 0 \), from which a WNL semimetal phase is induced by the \( m_s \) strains, represented by a vertical green line in the figure.

Figure 3(b) illustrates the detailed process of topological phase transition via the creation and annihilation of WPs along the vertical (yellow) path indicated in Fig 3(a). When varying \( m_{z\mu} \) from 0.1 to 0.4 in the unit of \( t_1 \), the in-plane \( C = 1 \) WP near \( X \) (\( Y \)) and the in-plane \( C = -1 \) WP near the DP of \( M \) fuse and annihilate eventually, while the WPs residing on the \( k_z \)-axis find their anti-chiral partners by moving along the \( k_z \) axis. This inter-TRIM WP annihilation results in the trivial insulator phase. On the other hands, Fig. 3(c) illustrates the evolution of the WPs during the topological phase transition from the WS with \( C = 2 \) to the WTI phase that occurs along the horizontal (yellow) path indicated in Fig. 3(a). Apart from zero, \( m_{z\mu} > 0 \) splits a WP with \( C = 2 \) into two \( C = 1 \) WPs off the \( k_z \)-axis. One of the two \( C = 1 \) WPs encounters with other two \( C = -1 \) WPs from the \( k_z = 0 \) plane. This event results in a single \( C = -1 \) WP, indicated by a solid green circle. The resultant \( C = -1 \) WP is eventually annihilated on the \( k_z = 0 \) plane by meeting with another WP with \( C = 1 \), which originates from the double WP on the \( k_z \)-axis. This annihilation results in a WTI \[37\].

Finally, searching for materials that realize the DS in SG 100, we have found an existing material BaLaCuBO\(_5\) \[38\]. BaLaCuBO\(_5\) is a layered system in SG 100 as shown in Fig. 4(a). It comprises \( p4g \) multilayers with an each layer preserving \( C_{4z} \) rotation and double glide-mirrors \( g_x \) and \( g_y \) symmetries. Our first-principles calculations support that BaLaCuBO\(_5\) realizes the proposed DS phase \[39\]. Figs. 4(b) and 4(c) show the first-principles electronic energy bands of BaLaCuBO\(_5\). The sticking of four bands is clear from the band structure. A fourfold-degenerate \( DP \) is present at \( M \), and the hourglass-like band connectivity appear on the \( \Gamma-X \) line. The hourglass-like band connectivity leads to a band crossing on the \( \Gamma-X \) line, as shown in the magnified view in Fig. 4(d). The presence of band crossing signals the presence of a WNL that encircles the \( M \) point lying on the \( k_z = 0 \) plane, which we have confirmed throughout the band calculations performed in the entire BZ.

In conclusion, we have established the existence of a novel type DSs in three dimensions, characterized by hosting topological surface states and mediating topological phase transitions. These characteristics are dis-
tistinguishing features of the topological DSs and the nonsymmorphic DSs, respectively. In this sense, the proposed DS is beyond the current classification of 3D DSs into the topological and nonsymmorphic types. The surface energy spectrum should give rise to drumhead-like topological surface states, which should be feasible to observe in the BaLaCuBO$_5$ compound using a known experimental technique, such as angle-resolved photoemission spectroscopy (ARPES). Moreover, defining a symmetry-tuned topological critical point between a normal insulator and a WTI, the proposed DS can transform to diverse topological phases by symmetry-lowering perturbations. Serving as the first example of the dual topological–nonsymmetric DS, the proposed DS can be an ideal platform for rich topological phenomena.

Y.-T.O. was supported from the Global Ph.D. Fellowship Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education (No. NRF-2014H1A2A1018320). Y.K. was supported from the NRF grant funded by the Korean government (MSIP; Ministry of Science, ICT & Future Planning) (No. NRF-2017R1C1B5018169). The computational resource was provided from the Korea Institute of Science and Technology Information (KISTI).

* youngkuk@skku.edu

[1] N. P. Armitage, E. J. Mele, and A. Vishwanath, Rev. Mod. Phys. 90, 015001 (2018).
[2] A. K. Geim, Science 324, 1530 (2009).
[3] M. J. Allen, V. C. Tung, and R. B. Kaner, Chem. Rev. 110, 132 (2010).
[4] M. Z. Hasan and C. L. Kane, Rev. Mod. Phys. 82, 3045 (2010).
[5] X.-L. Qi and S.-C. Zhang, Rev. Mod. Phys. 83, 1057 (2011).
[6] L. Fu, C. L. Kane, and E. J. Mele, Phys. Rev. Lett. 98, 106803 (2007).
[7] S. Murakami, New J. Phys. 10, 029802 (2008).
[8] S. M. Young, S. Zaheer, J. C. Y. Teo, C. L. Kane, E. J. Mele, and A. M. Rappe, Phys. Rev. Lett. 108, 140405 (2012).
[9] Z. Wang, Y. Sun, X.-Q. Chen, C. Franchini, G. Xu, H. Weng, X. Dai, and Z. Fang, Phys. Rev. B 85, 195320 (2012).
[10] Z. Wang, H. Weng, Q. Wu, X. Dai, and Z. Fang, Phys. Rev. B 88, 125427 (2013).
[11] Z. K. Liu, B. Zhou, Y. Zhang, Z. J. Wang, H. M. Weng, D. Prabhakaran, S.-K. Mo, Z. X. Shen, Z. Fang, X. Dai, Z. Hussain, and Y. L. Chen, Science 343, 864 (2014).
[12] S.-Y. Xu, C. Liu, S. Kushwaha, T.-R. Chang, J. Kirzlan, R. Sankar, C. Polley, J. Adell, T. Balasubramanian, K. Miyamoto, et al., arXiv preprint arXiv:1312.7624 (2013).
[13] S. Borisenko, Q. Gibson, D. Evtushinsky, V. Zabolotnyy, B. Büchner, and R. J. Cava, Phys. Rev. Lett. 113, 027603 (2014).
[14] M. Neupane, S.-Y. Xu, R. Sankar, N. Alidoust, G. Bian, C. Liu, I. Belopolski, T.-R. Chang, H.-T. Jeng, H. Lin, A. Bansil, F. Chou, and M. Z. Hasan, Nat. Commun. 5, 3786 (2014).
[15] Z. K. Liu, J. Jiang, B. Zhou, Z. J. Wang, Y. Zhang, H. M. Weng, D. Prabhakaran, S.-K. Mo, H. Peng, P. Dudin, T. Kim, M. Hoesch, Z. Fang, X. Dai, Z. X. Shen, D. L. Feng, Z. Hussain, and Y. L. Chen, Nat. Mater. 13, 677 (2014).
[16] B. J. Wieder and C. L. Kane, Phys. Rev. B 94, 155108 (2016).
[17] B. J. Wieder, Y. Kim, A. M. Rappe, and C. L. Kane, Phys. Rev. Lett. 116, 186402 (2016).
[18] T.-R. Chang, S.-Y. Xu, D. S. Sanchez, W.-F. Tsai, S.-M. Huang, G. Chang, C.-H. Hsu, G. Bian, I. Belopolski, Z.-M. Yu, S. A. Yang, T. Neupert, H.-T. Jeng, H. Lin, and M. Z. Hasan, Phys. Rev. Lett. 119, 026404 (2017).
[19] H. Gao, Y. Kim, J. W. F. Venderbos, C. L. Kane, E. J. Mele, A. M. Rappe, and W. Ren, Phys. Rev. Lett. 121, 106404 (2018).
[20] B.-J. Yang and N. Nagaosa, Nat. Commun. 5, 4898 (2014).
[21] M. Kargarian, M. Randeria, and Y.-M. Lu, Proc. Natl. Acad. of Sci. 113, 8648 (2016).
[22] G. Bednik, Phys. Rev. B 98, 045140 (2018).
[23] J. A. Steinberg, S. M. Young, S. Zaheer, C. L. Kane, E. J. Mele, and A. M. Rappe, Phys. Rev. Lett. 112, 036403 (2014).
[24] L. M. Schoop, M. N. Ali, C. Straßer, A. Topp, A. Varykhalov, D. Marchenko, V. Duppel, S. S. P. Parkin, B. V. Latsch, and C. R. Ast, Nat. Commun. 7, 11696 (2016).
[25] B.-J. Yang, T. A. Bojesen, T. Morimoto, and A. Furusaki, Phys. Rev. B 95, 075135 (2017).
[26] S. Zaheer, Three dimensional Dirac semimetals, Ph.D. thesis, University of Pennsylvania (2014).
[27] B. J. Wieder, B. Bradlyn, Z. Wang, J. Cano, Y. Kim, H.-S. D. Kim, A. M. Rappe, C. L. Kane, and B. A. Bernevig, Science 361, 246 (2018).
[28] S. M. Young and C. L. Kane, Phys. Rev. Lett. 115, 126803 (2015).
[29] Z. Wang, A. Alexandradinata, R. J. Cava, and B. A. Bernevig, Nature 532, 189 (2016).
[30] R. Yu, X. L. Qi, A. Bernevig, Z. Fang, and X. Dai, Phys. Rev. B 84, 075119 (2011).
[31] See the Supplemental Materials for the details of the Wilson bands calculations.
[32] T. Bzdusek, Q. Wu, A. Rüegg, M. Sigrist, and A. A. Soluyanov, Nature 538, 75 (2016).
[33] L. Wang, S.-K. Jian, and H. Yao, Phys. Rev. B 96, 075110 (2017).
[34] S.-S. Wang, Y. Liu, Z.-M. Yu, X.-L. Sheng, and S. A. Yang, Nat. Commun. 8, 1844 (2017).
[35] See the Supplemental Materials for the detailed results of the topological invariants.
[36] See the Supplemental Materials for the classification of the perturbations by the point group D$_{4h}$.
[37] See Supplemental Material at http:// for the detailed calculations of the associated topological invariants.
[38] R. Norrestam, M. Kritikos, and A. Sjoedin, Acta Crystallographica, Section B: Structural Science 50, 631 (1994).
[39] See Supplemental Material at http://xxxxxx for the details of computational methods and the first-principles results for other candidates.