New type of hybrid nodal line semimetal in Be$_2$Si

Z H Li$^{1,}$ W Wang$^{1,}$ P Zhou$^{1,3}$, Z S Ma$^{2}$ and L Z Sun$^{1,3}$

Abstract

Following Dirac and Weyl semimetals, nodal line semimetals represent a new type of topological semimetal and attracted extensive interest in modern condensed matter physics. Recently, a kind of hybrid nodal lines have been proposed (Zhang et al 2018 Phys. Rev. B 97 125143) and it mainly come from anisotropy interaction. Based on the first-principle calculations and k-p model, we predict a cubic Be$_2$Si with topological nontrivial electronic states exhibiting fascinating type-I and type-II hybrid nodal line around Fermi level. Unexpectedly the low energy electronic states of Be$_2$Si are isotropy in $k_x$ and $k_y$ directions and a new effective model has been proposed for the appearance of this new type hybrid nodal line. The four-fold degenerated type-I and type-II nodal points in the hybrid nodal lines along the high symmetry lines of $\Gamma$–$K$ and $\Gamma$–$X$ are protected by mirror reflection, time reversal and space inversion symmetry. The spin–orbit coupling effect only induces slight band gap in the hybrid nodal lines in Be$_2$Si whose nontrivial nature remains. Moreover, the nontrivial hybrid nodal lines in Be$_2$Si are robust to external strain. The results in present work indicate that Be$_2$Si are promising candidates for future experimental studies of nontrivial topological semimetals and an excellent platform to study the interaction between the two types Dirac fermions.

Introduction

In recent years, topological semimetals have attracted enormous attention of researchers due to their intrinsic topological nature and fascinating potential in future nano-electronics. In comparison with topological insulators [1,2], topological semimetals have gapless bulk states and topologically protected surface states. Up to now, the well-known topological semimetals include Dirac semimetals (DSMs) [3–10], Weyl semimetals (WSMs) [11–21], and node-line semimetals (NLSMs) [22–30]. For DSMs and WSMs, their nontrivial band crossing points distribute at separate $k$ points in the Brillouin zone (BZ). The single Dirac node of DSMs can separate into two Weyl nodes by breaking either the time reversal symmetry or inversion symmetry. And both the DSMs and WSMs have been verified theoretically and experimentally so far, for instance, the DSMs Na$_3$Bi [7], Cd$_3$As$_2$ [31], the WSMs TaAs-family [20], WTe$_2$ [32], and MoTe$_2$ [33].

As for NLSMs, their band crossing points either take the form of an extended line running across the BZ, whose ends meet at the BZ boundary, or wind into a closed loop inside the BZ, or even form a chain consisting of several connected loops (nodal chain) [34,35]. There are also nodal net semimetals [36], nodal-link semimetals [37], and nodal-knot semimetals [38] proposed theoretically. So far, three types of symmetry protected mechanisms for NLSMs have been proposed: (i) mirror reflection symmetry protected NSLMs [39,40]; (ii) NLSMs derives from combined protection of time reversal symmetry and space inversion symmetry [22,23,41–46]; (iii) NLSMs determined by non-symmorphic space group with glide plane or screw axes symmetries [27,47]. Although many different crystalline symmetries can stabilize the NLSMs, few materials including pure Be [46], PbTaSe$_2$ [48], ZrSiS [30], PtSn$_4$ [49], InBi [29], and ZrSiSe/ZrSiTe [50] were
experimentally verified as topological NLSMs by angle-resolved photoemission spectroscopy (ARPES). There are challenges to experimental realization and observation of NLSMs. The most important challenge is that most of the NLSMs proposed theoretically are fragile to the spin–orbit coupling (SOC) effect of the systems. Moreover, most NLSMs are proposed or designed theoretically, the realization of the materials itself in experiments is difficult. Finally, trivial bulk bands often coexist near the Fermi level and interfere with the nontrivial states, making a definitive experimental study of the topological properties challenging [30]. Therefore, searching for NLSMs with weak SOC, simple crystal structure, and flexible synthesis or experimental existence are still significant issues in the area.

The nodal points of the topological semimetals according to its degree of tilting can be classified as two types: type-I and type-II nodal points. Just like the WSMs have been proposed to be classified as type-I WSMs, type-II WSMs [51], and hybrid (type-I.5) WSMs [52, 53] by the tilting degree of Weyl points, the NLSMs can also be classified into type-I and type-II categories. Up to now, type-I and type-II nodal line materials have been attracted plenty of attention recently. Thereinto, type-I nodal line materials have been intensively studied in the past few years. Meanwhile, the type-II NLSMs have also been proposed in K$_4$P$_3$ [54] and Kagome compound Mg$_6$Bi$_2$ [55], whose linear dispersion at every points of the nodal line is strongly tilted along one transverse direction leading to remarkable anisotropic in magnetic, optical, and transport properties compared with conventional type-I NLSMs. Very recently, Zhang et al [56] proposed hybrid nodal loop semimetal in the existing electride material Ca$_2$As, whose nodal loops composed of both type-I and type-II points. Their results indicate that for the hybrid nodal loop metal their Fermi surface consists of coexisting electron and hole pockets that touch at isolated points for an extended range of Fermi energies, without the need for fine-tuning. Interestingly, such system will show momentum-space Klein tunneling processes between the electron and hole orbits depending on the field orientation as well as the peculiar anisotropy in the cyclotron resonance. However, the electride material Ca$_2$As is unfortunately sensitive to the SOC and external strain hampering its experimental observation and realization. It is significant to identify more feasible materials that host such nontrivial topological hybrid loops and facilitate for future experimental research. Moreover, it is interesting to explore whether other types of hybrid nodal lines exist.

In present work, we proposed that cubic antifluorite material Be$_2$Si is a hybrid nodal loop semimetal with type-I and type-II hybrid nodal line around its Fermi level. For the nodal points of this nodal line in the high symmetry lines $\Gamma$–$K$ and $\Gamma$–$X$, type-I and type-II four-fold degenerate points are formed and protected by mirror reflection symmetry, as well as time reversal and space inversion symmetry. Excitingly, the hybrid nodal lines are insensitive to SOC and robust to external strain. Considering the synthesis of the antifluorite material family for several decades [57], Be$_2$Si is hoping to be feasible for experimental realization. Our results indicate that Be$_2$Si provides us an excellent platform to study the interaction between type-I and type-II Dirac fermions.

Computational methodology

Our first-principles calculations were carried out with Vienna $ab$ initio simulation package [58, 59]. The generalized gradient approximation [60] of Perdew–Burke–Ernzerhof (PBE) type exchange-correlation functional was used to simulate electronic interactions. The hybrid function (HSE06) [61] was adopted to check the low energy electronic structure obtained by PBE. The cutoff energy for wave-function expansion was 520 eV and $9 \times 9 \times 9$ Monkhorst-Pack $k$-mesh [62] was used for the BZ sampling in the self-consistent. The criteria of total energy convergence were set to $10^{-6}$ eV and the crystal structures were fully relaxed until the residual force on each atom was less than 0.01 eV Å$^{-1}$. With the help of tight-binding Hamiltonian from the maximally localized Wannier functions (MLWFs) [63, 64], projected surface states were calculated from surface Green function from WannierTools code [65].

Results and discussions

The Be$_2$Si crystal belongs to the cubic antifluorite structure, and it can also be considered as the zinc-blende-like lattice whose space group is Fm$\overline{3}$m (No. 225). Its electronic structure has been studied in previous works [66–68]. The Be$_2$C, sharing with same crystal structure with Be$_2$Si [69], has been synthesized several decades ago [57]. We present the conventional and primitive unit cell of Be$_2$Si in figures 1(a) and (b), respectively. As shown in figure 1(a), in the cubic conventional cell of Be$_2$Si, there are twelve atoms with four Si atoms occupy fcc sites and each Si atom is surrounded by eight Be atoms at ($\pm 1/4$, $\pm 1/4$, $\pm 1/4$) positions. The optimized lattice constant is $a = 5.285$ Å, which is well in agreement with previous report [66].

The energy band structure of Be$_2$Si along high symmetry lines without SOC is presented in figure 2(a). The high symmetry points in the reciprocal space are indicated with black points in figure 1(c). When SOC is not considered, there are three energy band crossing points around Fermi level, and we label them as $C_7(0.633$ eV),
C₂ (0.376 eV), and C₃ (0.500 eV) in figure 2(a). Taking no account of the spin degeneracy, the three band crossing points are two-fold degenerate. More importantly, the tilting degree of the three crossing points shows that C₁ and C₃ are type-I crossing points whereas C₂ is type-II crossing point. To reveal the orbital contribution of the three crossing bands around Γ point, orbital projected energy bands of Be₂Si are calculated and shown in figure 2(b). The results indicate that low energy electronic states mainly come from Si-p and Be-p states. Because of different bonding interactions of different directions for p orbitals, we expect the energy bands dispersion are also anisotropic. To elucidate either the band crossing points C₁, C₂ and C₃ around Γ point are accidental crossing or symmetry protected one, we identify the irreducible representations (IRs) of the energy bands around Γ points and their IRs are denoted in figure 2(a). The point group of Γ points in reciprocal space is Oₐh and the two energy bands around Fermi level belong to the T₂g and T₁u IRs. The two representations have opposite parity ensuring the band crossing is protected by spatial inversion symmetry and time reversal symmetry. In addition, the high symmetry lines Γ–X, Γ–K, and Γ–W are in the Γ–X–K–W planes that are the mirror symmetric planes of the BZ of Be₂Si. The IRs along the high symmetry lines as shown in the figure 2(a) and inset of figure 2(a) indicate that the two bands for the crossing points of C₁, C₂ and C₃ have opposite mirror eigenvalues. Furthermore, we also investigate the crossing points of the nodal lines do not in the high symmetry lines of the BZ, the results can be found in figure S1 in the supplementary materials available online at stacks.iop.org/NJP/21/033018/mmedia. The results indicate that all the bands forming the crossing points in the hybrid nodal line show opposite mirror eigenvalues. Such results confirm that the band crossings of the hybrid nodal line are stably protected by the
mirror symmetry. Therefore, Be$_2$Si is typical NLSMs protected by time reversal symmetry, spatial inversion symmetry, and mirror symmetry.

The three-dimensional (3D) energy band in plane of $\Gamma$–$K$–$X$ as shown in figure 3(a) reveals that the band crossing points in the plane form a closed nodal line. Moreover, as mentioned above, the nodal line is made up with type-I and type-II regions. To clarify the feature of the type-I and type-II hybrid nodal line, the energy difference between the two crossing bands closed the nodal line around $\Gamma$ point is shown in figure 3(b). And the zoom in view of the zero energy difference circle is shown in figure 3(c). The blue and red segment represent type-I and type-II Dirac fermions, respectively. The sectional view along $G$–$K$ direction (d) and $G$–$X$ direction (e) of the 3D energy bands.

Figure 3. (a) 3D energy bands around Fermi level in $\Gamma$–$K$–$X$ plane. (b) The difference of energy for the two crossing bands around Fermi level in $X$–$W$–$K$ plane, the blue circle indicate the position of nodal line. (c) Zoom in of the zero energy difference circle, the blue and red segment represent type-I and type-II Dirac fermions, respectively. Sectional view along $G$–$K$ direction (d) and $G$–$X$ direction (e) of the 3D energy bands.

The topological nontrivial characteristics of nodal lines can be well described by the Berry phase along a closed loop. With the help of MLWFs Hamiltonian, we found the Berry phase of closed loop in reciprocal space, which pass through the nodal lines, are $+\pi$ or $-\pi$. Thus, the hybrid nodal lines are protected against from perturbation by certain crystal symmetries. The presence of topological surface state is also a remarkable feature of nontrivial topological semimetal properties. So we calculated the surface states of density for semi-infinite edge. The surface states in (001) Si terminal surface are shown in figure 4. The surface states in (001) Be termination surface can be found in figure S2 in the supplementary materials. We can see that the nontrivial surface states connect the projected type-I (0.5 eV) and type-II (0.376 eV) energy band crossing points. Moreover, the dispersion of the surface states in (001) Be terminal surface is largely different from Si terminal.
The results indicate that the surface potential induced by the surface configuration will greatly impact on the surface states. In the figure S6 and figure S7, we present the surface states in (111) and (110) surfaces with MLWFs Hamiltonian. The topological surface states can be well distinguished from projected bulk states in Si terminal (111) surface, but not other cases due to the different surface potential. In the following sections, we will discuss the k·p model for the hybrid nodal lines in Be2Si.

The point group of \( \Gamma \) is \( O_{\text{h}} \). The generators of this point group are \( C_{\text{x} y z}, C_{\text{x} y z}, C_{\text{z} x y} \), rotation along (111) direction, \( C_{\text{y} x z} \), rotation along (110) direction, and \( I \), time reversal, \( \text{xyz} \), ---.

Certainly, the time reversal symmetry must be additionally considered. The symmetry representations around Fermi level at \( \Gamma \) point are \( T_{1u} \) and \( T_{2g} \), the definitions of the notation of the representations can be found in book of Bradley and Cracknell [70]. Clearly, this two three order representations have opposite parity characters. With the basis function of odd-parity \( (p_x, p_y, p_z) \) and even-parity \( (d_{xy}, d_{yz}, d_{zx}) \) to the representation \( T_{1u} \) and \( T_{2g} \) [71], we can construct following 3-order k·p model for the bands around \( \Gamma \) point. The three bands model for \( T_{1u} \) and \( T_{2g} \) have different coefficient \( A_n \) and \( B_n (n = 0 – 3) \):

\[
H_{\Gamma} = \begin{pmatrix}
D(k) + M_z(k) & A_3 k_x k_z & A_3 k_y k_z \\
A_3 k_x k_z & D(k) + M_z(k) & A_3 k_y k_z \\
A_3 k_y k_z & A_3 k_x k_y & D(k) + M_z(k)
\end{pmatrix}
\]

(1)

where \( D(k) = A_0 + A_z(k_x^2 + k_y^2 + k_z^2), M_z(k) = A_z(k_x^2 + k_y^2 - 2k_z^2), M_y(k) = A_y(k_x^2 + k_z^2 - 2k_y^2), \) and \( M_x(k) = A_x(k_y^2 + k_z^2 - 2k_x^2) \). The k·p model hamiltonian for valence bands(\( T_{2g} \) in figure 2(a)) share the same form with \( H(\Gamma) \) but with different coefficient \( A_n \rightarrow B_n \). If we set the three mutually perpendicular high symmetry lines \( \Gamma-X \) as the direction of \( k_x, k_y, \) and \( k_z \) primitive vector, the hybrid nodal lines are located in the \( k_z = 0 \) planes and they can symmetric transform with each others. In order to simplify the form of eigenvalues of \( H(\Gamma) \), we neglect the effect of \( A_z \) (set to 0). When we only consider \( k_z = 0 \) plane, by diagonalizing the \( H(\Gamma) \) matrix and comparing the 3D bands in figure 3, we find \( A_z \) exactly have little impact on the characteristics of hybrid nodal lines. The hybrid nodal lines around Fermi level are formed with the band

![Figure 4. Surface states in (001) Si terminal surface with the energy of (a) 0.376 eV and (b) 0.500 eV and the enlarged figures around the \( \Gamma \) point.](image)
dispersion of $E_i(k_x, k_y) = A_0 + \frac{1}{2}((2A_i - A_2)(k_x^2 + k_y^2) - 3[A_2(k_x^2 - k_y^2)]){1)}$ and $E_2(k_x, k_y) = B_0 + \frac{1}{2}((2B_1 - B_2)(k_x^2 + k_y^2) - 3[B_2(k_x^2 - k_y^2)]){1)$. By fitting the first-principle bands around $\Gamma$ point, we obtain the values of parameters are $A_0 = 0.7883$ eV, $A_1 = 0.9654$ eV $\text{Å}^2$, $A_2 = 5.9145$ eV $\text{Å}^2$, $B_0 = 0.3849$ eV, $B_1 = 1.2733$ eV $\text{Å}^2$ and $B_2 = 1.1859$ eV $\text{Å}^2$, respectively. The 3D bands with $E_1$ and $E_2$ are presented in supplementary materials (figure S8). We found it can well reproduce the main characters of first-principle bands in figure 3(a).

In the high symmetry lines $k_x = \pm k_y$, the last term of $E_1$ and $E_2$ turn to zero and the band crossing comes from two curves with opposite sign of quadratic coefficients. Therefore, the band crossing of them are type-I. However, in the high symmetry lines $k_x = 0$ (or $k_y = 0$), the sign of the coefficients for $k_x^2$ or $k_y^2$ in both $E_1$ and $E_2$ are negative. Therefore, the bands in these two high symmetry lines form type-II crossing point. If we rotate the high symmetry lines from $k_x = 0$ to $k_y = k_x$, namely $\Gamma$–$X$ rotate counterclockwise to $\Gamma$–$K$ in figure 3(c), the equation of high symmetry lines can be set as $k_y = \alpha k_x$ ($\alpha$ change from 0 to 1). We replace this relationship into $E_1$ and $E_2$, and we obtain $E_i(k_x, k_y) = A_0 + (A_1(1 + \alpha^2) + (\alpha^2 - 2)A_2)k_x^2$ and $E_2(k_x, k_y) = B_0 + (B_1(1 + \alpha^2) + (\alpha^2 - 2)B_2)k_x^2$. When $\alpha$ change from 0.0 to 1.0, the coefficients of $k_x^2$ for $E_1(k_x, k_y)$ always keep negative. However, the coefficient of $k_y^2$ for $E_2(k_x, k_y)$ vary from negative to positive values, namely the band crossing change from type-II to type-I and form hybrid nodal lines around Fermi level.

According to previous discussions, we can abstract an two bands effective model with two diagonal eigenvalues: $E_{12} = e_{12} + \alpha_{12}(k_x^2 + k_y^2) + \beta_{12}(k_x^2 - k_y^2)$, and the coefficients of $\alpha_{12}$ and $\beta_{12}$ determine the type of nodal lines. If $\alpha_1 \times \alpha_2 < 0$ and $\alpha_1 + \beta_2 > 0$, which means the crossing bands form type-I nodal points in $k_x = \pm k_y$ and type-II nodal points in $k_x = 0$ and $k_y = 0$. This situation and its opposite case($\alpha_1 \times \alpha_2 > 0$ and $\alpha_1 + \beta_2 < 0$) indicate hybrid nodal lines are formed. For other cases energy band crossing between these two bands would form pure type-I or type-II nodal lines. Here we will comparing the hybrid nodal lines between Zhang’s [56] and ours. The main difference between these two cases is the shape of energy bands dispersion. The two bands in their model are saddle-type with strong anisotropy between $k_x$ and $k_y$ directions. In our case, hybrid nodal lines are formed from two oppositely oriented deformed quadric surface. Depending on our model discussed above, the electronic states in our case along $k_x$ and $k_y$ are equivalent to each others, which lead to higher symmetry ($C_{4v}$) in $k_x = 0$ plane in ours case. Secondly, comparing with the hybrid nodal line of Ca$_2$As, hybrid nodal lines in Be$_2$Si can well exist under hybrid exchange-correlation function (figure S9) or applied ±5% strain (figure S10), which ensure its existence in different experimental situations.

One of the most interesting characteristics of the hybrid nodal line, besides momentum-space Klein tunneling effect and further zero-field magnetic breakdown as mentioned above, is that type-I or type-II DSM states or both of them can be relatively easy obtained in the system due to the nodal line usually disperse within an energy window. The intersection between the Fermi surface and finite type-I or type-II crossing points will happen as long as the energy position of the Fermi surface tuned in the energy window. Furthermore, for hybrid nodal line, there must be a flat crossing band in a specific energy, the contact between type-I and type-II crossing lines. The energy band dispersion of Be$_2$Si in this specific contact has been denoted in figure S11 in the supplementary materials. This kind of semimetal recently is named as type-III Dirac fermion [72]. A critical chiral anomaly effect and the black-hole-horizon analog in solid-state can be realized when the Fermi level of Be$_2$Si tuned to this specific energy.

We known that SOC always turns the symmetry of bands from single group representation to double group representation, and NLSM generally changed into other nontrivial or trivial topological phase [23]. When the SOC is considered, we find that only type-II crossing point $C_2$ in figure 2 remain. The representations of the two bands around the $C_2$ are $\Gamma_4$ and $\Gamma_7$ of $C_{4h}$ double point group. They are two order representations and the values and characters for them have opposite sign under $C_2$ operator. So the crossing of them is protected by $C_2$ rotation symmetry. As a result, the Be$_2$Si is a kind of DSM when considering the effect of SOC. Namely, SOC turn hybrid nodal lines semimetal into type-II DSM. However, The computed SOC splitting is only about 1.5 meV (figure S12 in supplemental materials), it can be neglected as long as the temperature is higher than 17.4 K. Therefore, we expect the hybrid nodal lines of Be$_2$Si can be detected in experiment.

Finally, we will discuss the experimental synthesis of the Be$_2$Si and the observation of the topological states and surface states in experiments. Because of isovalent to the group-IV semiconductor, $\text{A}_2(\text{IIA})\text{B}(\text{IV})$ antifluorite compounds receive attentions in potential semiconductor technological application. At the same time, they are potential materials with high hardness and fascinating optical properties. However, these properties are closely related to their semiconductor electronic structure, that is why four of the semiconductor compounds(Be$_2$C, Mg$_2$Si, Mg$_2$Ge and Mg$_2$Sn) receive much attentions and have already been reported to be experimental synthesized [57, 73]. Due to pristine properties of metallicity, few researchers have noticed the compound Be$_2$Si. Due to similar structure and elemental composition with other antifluorite compounds, we expect Be$_2$Si can be synthesized with similar experimental method. As mentioned above, the nodal line crossing points range from 0.376 to 0.634 eV above the Fermi level. However, such separation between the topological
states and Fermi level is not a hinder to detection in experiments. For example, the topological states of non-symmorphic topological semimetal InBi\(^{29}\), NLSM ZrSiS\(^{30}\) and Dirac nodal links materials TiB\(_2\)\(^{74}\) depart from the Fermi level larger than 0.5eV could be well resolved by ARPES through tuning the photon energy. Moreover, electric gating can routinely tune the Fermi level of the 2D system with electron or hole doping. Besides the electric gating, strain engineering is another effective approach to tune the electronic state of 3D system. In figure S10(a) in the supplemental material, the band structures under 5% compressive strain indicate that the topological states along \(\Gamma-\Gamma\) are lowered close to the Fermi level. In experiment, such strain can be achieved by choosing appropriate substrate. To observe and apply the surface states, we need to cleave the system and expose surface. Surface atomic relaxation and polarization are inevitable. To consider the effect of surface atomic relaxation and polarization on the energy dispersion of the surface states, we cleave Be\(_2\)Si slabs along [001], [111], and [110] directions with the thickness of 51.480 Å, 61.739 Å, and 35.468 Å, respectively, and the results can be found in the supplementary materials. The results of (001) slab as shown in figure S3 indicate that the surface states of both Si and Be terminals show large dispersion and intersect with the Fermi level due to the influence of the surface potential ensuring the experimental observation. Part of surface states in other orientations also intersect with the Fermi level (see the results in figures S4 and S5). In conclusion, there are no problem to detect the bulk semimetal state and surface states of Be\(_2\)Si in experiments although the topological states are above the Fermi level. Moreover, further magnetic responses research in theory and experiment are also important topic to this new type of hybrid nodal lines semimetals.

**Conclusion**

In summary, based on the first-principle calculations and the space group theory analysis, we predict a cubic Be\(_2\)Si with topological nontrivial electronic states by exhibiting fascinating type-I and type-II hybrid nodal line around Fermi level. It is predicted that the type-I and type-II four-fold degenerate points of this nodal line are protected by time reversal symmetry, space inversion symmetry and mirror reflection symmetry, which provide an appropriate platform to study the interaction and different characters between these two Dirac fermions. In addition, a new \(k-p\) model have been proposed for the appearance of hybrid nodal lines. The topological property is verified by presence of topological surface states in this structure. And the slight gap induced by the SOC effect indicates that Be\(_2\)Si is a promising candidate for future experimental studies of nontrivial topological semimetals.

**Acknowledgments**

This work is supported by the National Natural Science Foundation of China (Grant No.11574260 and 11804287). ZHL and WW contributed equally to this work.

**ORCID iDs**

P Zhou ◼️ https://orcid.org/0000-0002-5570-2427

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