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RESEARCH HIGHLIGHT

New topological semimetal candidate of nonsymmorphic $PdSb_2$ with unique six-fold degenerate point

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Since the discovery of Majorana fermions in condensed matter systems, new quasiparticle predictions of novel fermions have been predicted in solid state systems which exhibit three, six or eight fold degenerate band crossings protected by crystal symmetry in presence of spin orbit coupling and time reversal symmetry [1]. The nontrivial topology in condensed matter systems results from the crossings of conduction and valence bands. And the cases of $g = 3$, 6, and 8 are of particularly interesting as they can only be found in condensed matter systems, having no high energy analogues as constrained by Poincare symmetry [2].

Dirac and Weyl fermions have already been observed in many solid state systems with unique properties [1–9]. At this point, we note that Dirac points are four-fold degenerate whereas Weyl points are two-fold degenerate, which always come in pairs. In contrast to the well-known Weyl and Dirac semimetals, which exhibit two- and four-fold degeneracies respectively at the band crossing [shown in Figs. 1(a, b)], a different type of fermion has been realized recently in symmorphic MoP [10], which possesses three-fold degeneracy at the crossing point [shown in Fig. 1(c)]. In fact, while the three-fold points can be realized in both nonsymmorphic [2] and symmorphic crystal systems [10], nonsymmorphicity is essential for stabilizing six- and eight-fold degenerate points [2].

It is also interesting that by using angle-resolved photoemission spectroscopy, unconventional chiral fermions with long Fermi arcs in CoSi have recently been observed [11], which reveal two types of unconventional chiral fermions — spin-1 and charge-2 fermions — at the band-crossing points near the Fermi level in CoSi. Moreover, these chiral fermions are enforced at the center or corner of the bulk Brillouin zone by the crystal symmetries, making CoSi a system with only one pair of chiral nodes with large separation in momentum space and extremely long surface Fermi arcs, in sharp contrast to Weyl semimetals, which have multiple pairs of Weyl nodes with small separation. At this point, some interesting pyrite compounds have been identified for their topological features in the band structures. For example, $PtBi_2$ is a Dirac semimetal and could also host tripple point fermions [12]. The isoelectronic $PdSb_2$ is also a semimetal which is known to superconduct below 1.25 K, which is a candidate for hosting 6-fold-degenerate exotic fermions (beyond Dirac and Weyl fermions) [13]. It is worthwhile noting that the nontrivial band crossing protected by the non-symmorphic symmetry plays a crucial role in physical properties.

Jin *et al.* [13] have recently grown $PdSb_2$ single crystals for the first time, confirming its nonsymmorphic structure. Moreover, they reported its electrical and magnetic properties under various stimuli [temperature (T), magnetic field (H), and quasihydrostatic pressure (p)]. While it is a diamagnetic Fermi-liquid metal under ambient pressure, $PdSb_2$ exhibits a large magnetoresistance with continuous increase up to 14 T, which follows the Kohler's scaling law at all temperatures.

$PdSb_2$ is diamagnetic resulting from atom core contributions [13]. Applying H either parallel or perpendicular to the current I, it is found that there is positive MR. In the transverse ($H \perp I$) MR_{bc} at indicated temperatures, it is found that the MR_{bc} increases with decreasing temperature. At a fixed temperature, the MR increases with increasing field without any sign of saturation, reaching 174% at 2 K and 14 T. For $H//I$, the MR_{bc} is about one order of magnitude smaller. By applying magnetic field along the [111] direction, there are de Haas–van Alphen oscillations with frequency of 102 T when field is applied along the [111] direction, revealing nearly zero effective electron mass and a nontrivial Berry phase. The effective mass is nearly zero ($0.045m_0$) with the Berry phase close to π, confirming that the band close to the R point has a nontrivial character. Since the MR_{bc} for $H//I$ is much smaller than that for $H \perp I$, there is little contribution from spin scattering. The positive MR in a nonmagnetic metallic system is attributed to the modification of electron tra-

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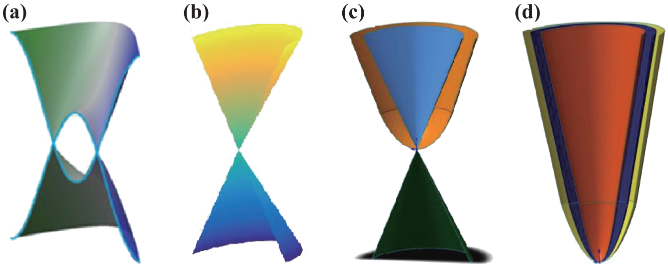

Fig. 1 Schematic representation of different band crossings for the topological semimetals. **(a)** Dirac semimetal (DSM); **(b)** Weyl semimetal (WSM); **(c)** Tripple point; **(d)** Sextuple point with 6-fold.

jectories due to the application of H. This effect is more significant at low temperatures in pure metallic systems where charge carriers effectively follow the cyclotron motion around the magnetic field. They also found that the MR_{bc} displays quadratic field dependence in the low-field regime of magnetic field (when $H < 3$ T), as expected for conventional metals with a single band. On the other hand, at higher fields, MR_{bc} gradually deviates from H^2 dependence, while continuously increasing. Such a non-saturating MR has been attributed to exotic mechanisms. They further noticed that the MR_{bc} data taken at different temperatures collapse into a single curve when plotting MR_{bc} versus H/ρ, which means that Kohler's law is also valid for $PdSb_2$ within/in a single-band transport scenario [14, 15]. As a result, contrary to the multiband nature of $PdSb_2$ [2, 16], it is inferred that only one band plays a dominant role in the transport. Here it is worth noting that the effective single-band transport in multiband systems is a common feature of topological materials [15, 17].

Another interesting property is that it becomes superconducting under the application of quasi-hydrostatic pressure p with the maximum superconducting transition temperature at $T_c^{max} \sim 2.9$ K. They further argued that the formation of Cooper pairs (bosons) is the consequence of the redistribution of the 6-fold-degenerate fermions under pressure.

Furthermore, based on *ab-initio* calculations, two six-fold band crossings have been predicted to be existing in the nonsymmorphic compound $PdSb_2$, completely distinct from other topological semimetals. As shown in Fig. 1(d), the two sextuple points (SP) are formed at the corner of the Brillouin zone by three two-fold-degenerate parabolic bands, which might provide a platform for exploring new topological materials with extremely large magnetoresistance (XMR) among noble metal compounds for spintronics [17]. In fact, the six fold degeneracy results from three bands that is doubly degenerate due to the presence of TR symmetry and appears at the time reversal invariant R-point. The *ab-initio* calculations with spin–orbit coupling further reveal that the three two-fold-degenerate bands predominantly result from the Pd $d_{x^2-y^2}$ and Pd d_{z^2} orbitals with small contribution from other Pd d orbitals.

The ARPES measurement investigation on $PdSb_2$, which might provide the first experimental evidence of six component fermions in a condensed matter system, should be planned in future, in order to stimulate further studies in the field of new fermions to identify unusual physical properties resulting from quadratic band crossing distinctly different from the so-called Dirac and Weyl fermions. Similarly, in isoelectronic and isostructural $PtBi_2$ the sextuple point is predicted to occur just above the Fermi energy. As a result, herein it is proposed that a solid solution of $PdSb_2$ and $PtBi_2$ would be an ideal candidate, which is protected by time reversal symmetry, and thereby the breaking of time reversal symmetry by applying external magnetic field would be possible, leading to the splitting of the sextuple point into two tripple points. We however expect that the characteristics of such a triply degenerate point will be markedly different compared to the already known tripple point fermion metals, for example, MoP.

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