A new member of the topological semimetals family

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In topological semimetals (TSMs), the quasi-particle excitations of electrons can be described by the Dirac or Weyl equation, mimicking the elusive massless Dirac or Weyl fermions in the low-frequency regime as emergent phenomena. The realization of elementary excitations, with and even without counterparts in high-energy field theory, in solids is possible and fundamentally important. This perspective introduces the brief history of this rising field to celebrate the birth of a new member of the star family of TSMs.

In 1928, P.A.M. Dirac proposed a $4 \times 4$ matrix equation to describe relativistic free electrons at the quantum level. From its solution, one can derive the origin of charge and spin, and even predict the existence of anti-matter. In the second year, H. Weyl reconsidered this Dirac equation by setting the mass term zero. He obtained two decoupled $2 \times 2$ matrix equations, describing a pair of new massless particles with opposite chiralities. They are now known as Weyl fermions. Thus, the massless Dirac fermion can be looked at as a superposition of a pair of Weyl fermions. The power of the Dirac equation is further demonstrated by E. Majorana, who found a set of real solutions representing yet another new type of fermions: the Majorana fermions.

A Majorana fermion is neutral in charge and is its own antiparticle. However, until now, neither the Weyl fermion nor the Majorana fermion has been discovered as a fundamental particle in any high-energy physics experiment.

On the other hand, in condensed-matter physics, which frequently borrows concepts from high-energy particle physics, recently there has been active searching for the ‘cousins’ of these fermions among the quasi-particle excitations in solids as emergent phenomena. In solids, electrons dressed by particle-hole excitations due to interactions among themselves and the potential periodicity of a lattice are called quasi-particles. People have found that, in some compounds, the motion of quasi-particles can be described using the massless Dirac/Weyl equation. The first well-known example is the Dirac cone-like energy dispersion in $2D$ graphene, where the electron energy depends linearly on its crystal momentum. A similar low-energy excitation was also realized on the boundary and surface of topological insulators (TIs). In $3D$ space, S. Murakami noticed that both the massless Dirac and Weyl fermions could be found in the region of the topological phase transition between a TI and a normal insulator.

Such a metallic state is a special $3D$ metal where the conduction and the valence bands cross at discrete nodal points in the Brillouin zone. The nodal points at the Fermi level are either four-fold degenerate (Dirac nodes) or double degenerate (Weyl nodes) and the corresponding $3D$ metal is called Dirac semimetal (DSM) or Weyl semimetal (WSM). For WSM at zero or small doping, the Fermi surface consists of several disconnected pieces of spheres and each encloses a single Weyl node. In fact, Weyl nodes are the monopoles of Berry curvature in momentum space, which was studied in 2003 in the context of the anomalous Hall effect. The Berry flux passing through each sphere is quantized to be the net charge of the Weyl node enclosed within it. This quantized flux can serve as the topological invariant, Fermi Chern number, for metallic states. In this way, the topological classification of matters has been extended from insulators to metals. According to different number and distribution of Weyl nodes in momentum space [1], the TSM family is classified and shown in Fig. 1.

The Dirac semimetal (DSM) and WSM at the phase transition region are hard to realize for experimental measurements. Young et al. have proposed to find Dirac nodes at high-symmetrical momenta where the four-fold degeneracy is protected by crystalline symmetry. Inspired by the band-inversion mechanism in TIs, Wang et al. proposed that crystal symmetry could protect accidental degeneracy at the band-crossing point if the four (including the spin degree of freedom) inverted bands belong to different irreducible representations. This leads to success in predicting two DSM materials: $\text{Na}_3\text{Bi}$ and $\text{Cd}_3\text{As}_2$. They are the two eldest TSM family members, experimentally confirmed in 2014.

As early as in 1937, Herring studied accidental two-fold degeneracy of band-crossing in a $3D$ lattice and found it robust even without any symmetry protection within the Weyl equation. In 1969, the chiral anomaly of Weyl fermions was discussed and it was found that the Weyl fermions should come in pairs in any lattice realization. However, it was 40 years later in 2011 when Wan et al. proposed the first specific compounds $\text{Re}_2\text{Ir}_2\text{O}_7$ ($\text{Re} = \text{rare earth element}$) to be WSMs. They further pointed out one unique property of Weyl fermions in a lattice, namely the Fermi arc on the surface, which does not exist for Weyl fermions in a vacuum. In the same year, Xu et al. proposed double Weyl fermions with topological charges of two in ferromagnetic $\text{HgCr}_2\text{Se}_4$. However, these two proposals have yet to be verified experimentally. The first discovered WSM materials are the TaA family compounds including TaAs, TaP, NbAs and NbP. All of them are nonmagnetic, noncentrosymmetric and WSM without any tuning. They were predicted in numerics and soon after discovered in experiments in 2015.

The quasi-particle analogue of the Majorana fermion is the zero-energy
Majorana mode. In 2016, Sun et al. reported their experimental evidence of its existence in the vortex of a topological superconductor. This means that all three fundamental particles might have been realized in the ‘material universe’. People also get to know that the fermions in a lattice can have different properties from their cousins in a vacuum. In addition to the surface Fermi arc, the violation of Lorentz invariance due to discrete lattice symmetry has led to exploration of ‘new fermions’ [2] that have no counterpart in high-energy particle physics, such as the Node-Line semimetal (NLSM), type-II WSM and the multiply degenerate nodal-point semimetal [3–6].

In 2016, Bradlyn et al. [2] found that lattice symmetry can stabilize three-, six- and eight-fold degenerate band crossings in addition to two- and four-fold ones in WSM and DSM, respectively. They exhausted these types of band crossings in all 230 space groups with time-reversal symmetry. They found that these multiply degenerate energy nodes could be protected by non-symmorphic symmetries at high-symmetrical momenta. Differently from their proposal, Weng et al. [3,4] found that the combination of band inversion and proper symmorphic crystal symmetries can also lead to triply degenerate nodal points (TDNP) in TaN and ZrTe with hexagonal WC crystal structure. In this case, TDNP can move freely along the rotation axis instead of being fixed at specific momenta. This is similar to the difference between class-one and class-two DSM. Zhu et al. [5] and Sun et al. [6] have also proposed similar compounds, including WC, MoC, WN, MoP, MoN, NbN, NbS, etc. Among them, MoC, WC, TaN, NbN and ZrTe have TDNPs very close to the Fermi level, which are TDNP semimetals (TDNPSM) that are ideal for exploring unique properties related to the three component fermions excited around TDNPs. Weng et al. [3] proposed that the longitudinal magnetoresistivity is anisotropic in contrast to the isotropic one in DSM and WSM.

Soon after the theoretical prediction, Lv et al. [7] reported their experimental observation of TDNPs in MoP. Though the TDNPs in MoP are around 1.5 eV below the Fermi level, this is the first experimental verification or birth of such distinct fermions in the ‘material universe’. Extremely low resistivity and high mobility of carriers in MoP have also been reported [8], though the relationships to TDNPs remain elusive. Other most notable progress is the anisotropic longitudinal magnetoresistivity observed in WC [9], which has TDNPs close to the Fermi level. Therefore, these distinguished quantum phenomena related to the unconventional three component fermions are very interesting and studies in this direction are just at their very beginning. Exploring these intriguing fermions in a different ‘universe’ will, it is hoped, lead to better and deeper understanding.

Figure 1. The family of topological semimetals. The upper panel is the band structure for each family member and the corresponding Fermi surface is shown in the lower panel. In the new member TDNPSM, the electron and hole pockets are drawn in solid and dashed circles, respectively. The magnetic monopoles of opposite charges are denoted by red and blue dots. Adapted and reprinted from [10].

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