Experimental Observation of Weyl Semimetals

1. **Experimental observation of Weyl points**
   Authors: Ling Lu, Zhiyu Wang, Dexin Ye, Lixin Ran, Liang Fu, John D. Joannopoulos, Marin Soljacic. arXiv:1502.03438.

2. **Experimental realization of a topological Weyl semimetal phase with Fermi arc surface states in TaAs**
   Authors: Su-Yang Xu et al. arXiv:1502.03807.

3. **Discovery of Weyl semimetal TaAs**
   Authors: B. Q. Lv et al. arXiv:1502.04684.

Recommended with a commentary by Ashvin Vishwanath, UC Berkeley

In 1929, Hermann Weyl noticed that the Dirac equation can be considerably simplified for a massless particle, and written in terms of a two component field:

$$i\partial_t\Psi = c\vec{p}\cdot\vec{\sigma}\Psi \tag{1}$$

with σ^a being the usual Pauli matrices. Around the same time, von Neumann and Wigner solved the the problem of accidental degeneracies in quantum systems. Since the effective Hamiltonian for a pair of levels , in the most general case (ignoring an overall energy shift), can be written as

$$H = A\sigma_x + B\sigma_y + C\sigma_z \tag{2}$$

achieving a degeneracy requires $A = B = C = 0$, i.e. would typically require tuning three parameters to satisfy three real equations. These seemingly disparate concepts came together in Herring's 1937 work on degeneracies in band structures. A pair of energy levels could typically be brought together by tuning three crystal momenta, and the dispersion near these touching points is (with some simplifications for clarity) : $H = \pm v_F(p_x\sigma_x + p_y\sigma_y + p_z\sigma_z)$ where p now is the deviation from the degeneracy point. In analogy with Eqn. 1, it is natural to call these Weyl nodes. The $\pm$ sign indicates the handedness or chirality of each Weyl node. Consistency demands an equal number of opposite chirality nodes.

Despite these rather ancient origins there was little progress in identifying Weyl nodes in crystals. However, the recent upsurge in interest in topological band structures provided fresh perspectives. Weyl nodes are sources and sinks of Berry flux (or monopoles of Berry flux), which lead to exotic surface states, that take the form of 'Fermi arcs' or incomplete Fermi surfaces. The missing pieces of the Fermi surface live on the opposite surface of the sample.

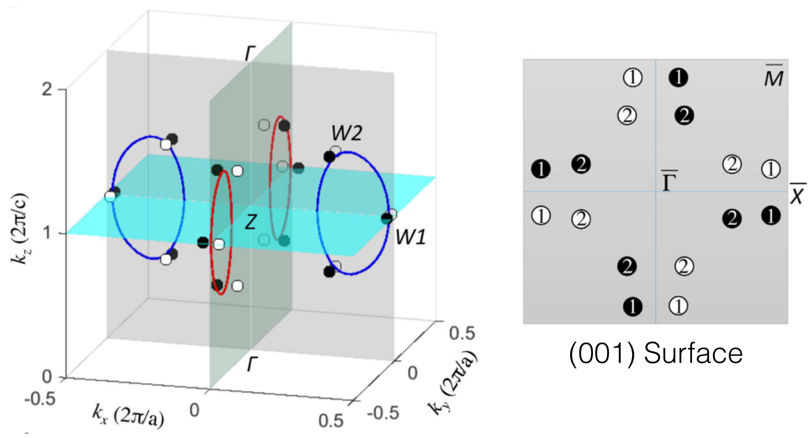

Figure 1: Calculated 3D band structure of TaAs (from [1]) showing the 12 pairs of Weyl nodes. On right, the (001) surface Brillouin zone, with projections of Weyl nodes - some Weyl nodes line up to give a net chirality of ± 2. These charges denote the number of Fermi arcs that should emanate from these points.

A key requirement is the presence of non degenerate bands, which implies that either inversion or time reversal symmetry must be broken (related 'Dirac semimetals' where both symmetries are present have also been considered and are an active topic of research, but differ in some significant ways). Early proposals relied on time reversal breaking, studying magnetic phases in pyrochlore and spinel materials. However, these remain to be experimentally confirmed.

A different and potentially easier approach is to consider non-centrosymmetric crystals with broken inversion symmetry. This avoids the complication of working with correlated materials with magnetic ground states, although the effect of inversion breaking in band structures can be relatively weak. The featured references utilize inversion breaking to realize Weyl nodes.

Reference 1 reports on a photonic material with lattice constants of order centimeters, where Weyl nodes appear in the photonic band structure. Interestingly, contrary to the solid state example discussed below, here the theoretically desired band structure was first determined and the material machined according to specifications. An inversion breaking strategy that

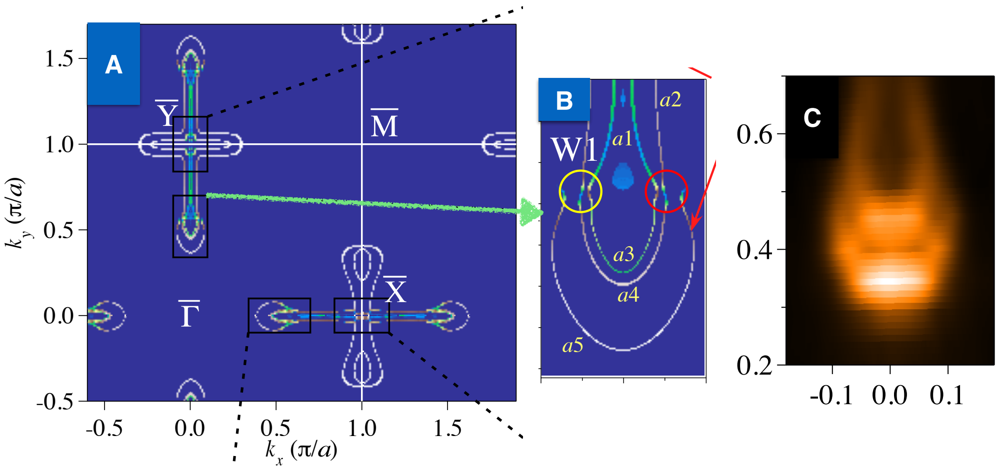

Figure 2: (A). Calculated (001) surface band structure of TaAs. (B). detailed view of part of the calculated band structure. The segment a5 is clearly a Fermi arc. (C). Fermi surface determined from ARPES data in the same part of the Brillouin Zone, showing surface states at the Fermi energy, which can be compared with panel B. (Adapted from Reference 3)

realizes 4 Weyl nodes (the minimum without time reversal breaking) was adopted.

The featured References 2, 3 both study the electronic band structure of TaAs, which crystallizes in a body centered tetragonal structure which lacks inversion. The calculated band structure is as shown in Figure 1 ([1, 2]). In the absence of spin orbit interactions, the conduction and valence bands intersect on 4 closed loops that live on mirror planes. Adding spin orbit leads to a gapping of these intersections, but the bands now intersect at points, that are opposite chirality points, slightly displaced from these planes. In all there are 24 Weyl nodes, 12 of each chirality. Since these nodes are not all related by symmetry, they are at slightly different energies, and hence there are always finite sized Fermi pockets in this semimetal. Angle resolved photoemission broadly confirms the expected bulk band structure, but the key confirmation of Weyl nodes arises by looking at surface states. The Fermi arc surface state emanate from the projection of the Weyl nodes onto the surface Brillouin zone. These take the form on the right of Figure 1, for the (001) surface.

Despite the rather complex surface band structure, the Fermi arc surface states seem to be experimentally verified. For example in Figure 2, the two left panels show a section of the calculated Fermi surfaces, while the figure on the right is the ARPES data. The experimental Fermi surfaces seen in panel C closely follow that expected from theory in panel B. Demonstrating that these are Fermi arcs needs further work, such as following them into the bulk Weyl nodes, which are discussed in detail in the references.

These are promising first steps but there are several areas that require further work. The separation between Weyl nodes is rather small in TaAs, only a few percent of the Brillouin Zone. Ideally one would like the Weyl nodes to be separated by large crystal momenta, as in graphene, to prevent scattering between nodes. Also, it would be nice to find examples where, like in graphene, the nodes are all exactly at the Fermi energy at stoichiometry. This will maximize the potential for novel transport phenomena. Similarly, the time reversal symmetry breaking version of Weyl semimetals displays some unique features related to the anomalous Hall effect and will be worth searching for. Finally, since Weyl nodes are associated with the chiral anomaly, detecting its consequences in transport would be a fruitful direction.

References

[1] S-M. Huang et al., arxiv:1501.00755

[2] Hongmin Weng et al., arxiv:1501.00060