Validity of Dirac and Weyl fermion picture for Cd_3As_2 and transition metal monopnictides

O. Pulci[1], D. Grassano[1], A. Mosca Conte[2], F. Bechstedt[3]

[1]*Universita' di Roma Tor Vergata, Via della Ricerca Scientifica 1, 00133 Rome, Italy*
[2]*Mediterranean Institute of Fundamental Physics, Via Appia Nuova, Marino, Italy*
[3]*Friedrich-Schiller-Universität, Max-Wien-Platz 1, 07743 Jena, Germany*
Corresponding author: olivia.pulci@roma2.infn.it

Topological semimetals have opened a new fascinating field for solid-state physicists. Despite strong spin-orbit interaction (SOI), significant band overlap gives rise to linear bands and Dirac cones in these three-dimensional (3D) bulk solids. Gapless electronic excitations, Dirac or Weyl fermions, which are protected by topology and symmetry, appear. While Dirac semimetals, e.g. Cd_3As_2, possess both time-reversal and inversion symmetry, one of these symmetries is broken in Weyl semimetals such as TaAs, TaP, NbAs, and NbP (see Fig. 1). The overlap of Ta5d- and Nb4d-derived conduction and valence bands leads to electron and/or hole pockets near the Fermi level at the 24 Weyl nodes. The semimetals are investigated by means of ab initio methods for atomic geometries and electronic structures but also optical properties. They are interpreted as 3D analogues of graphene. However, in contrast to two-dimensional graphene the Dirac physics does not yield to a constant IR absorbance ruled by the Sommerfeld finestructure constant [1]. Instead, in 3D a linear frequency increase is predicted for the optical conductivity. Indeed, the bct structure of the Cd_3As_2, as a Dirac semimetal, exhibits this behavior. However, the Dirac fermions appear only for small excitation energies, whereas Kane electrons are found for larger energies [2]. Weyl fermions are discussed for topological Weyl semimetals, especially bct TaAs, with 12 pairs of W1 or W2 Weyl nodes, comparing with ARPES results and measured optical spectra [3]. Linear bands lead to an optical conductivity varying linearly with frequency, thereby indicating the Weyl character for small photon energies. This behavior is, however, modified by band occupation, anisotropy, light polarization, and trivial carriers and even destroyed for larger energies.

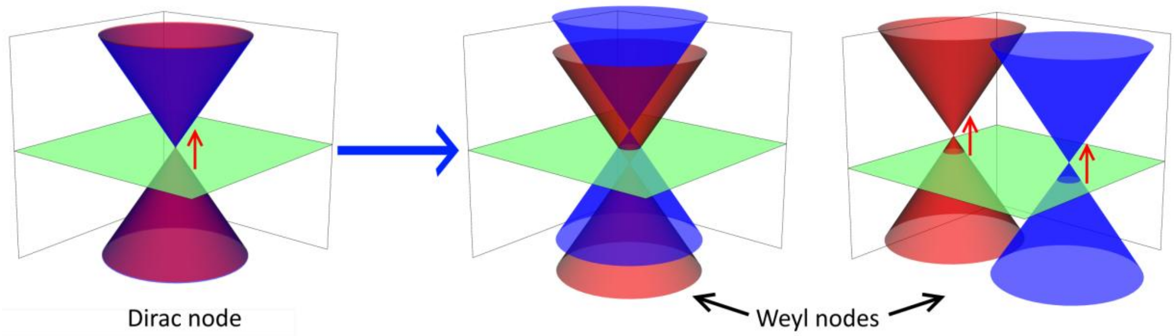

Fig. 1 Splitting of a Dirac node into Weyl nodes violating time-reversal or inversion.

References

[1] L. Matthes, O. Pulci, F. Bechstedt, Phys. Rev. B **78**, 035438 (2013).

[2] A. Mosca Conte, O. Pulci, F. Bechstedt, Scientific Reports **7**, 45500 (2017).

[3] D. Grassano, O. Pulci, F. B., Scientific Reports **8**, 3534 (2018).