TT 20: Topological Semimetals II

Time: Monday 15:00–18:45 Location: A 053

TT 20.1 Mon 15:00 A 053

Topological band crossings in hexagonal materials — •Andreas P. Schnyder — Max Planck Institute for Solid State Research, Stuttgart, Germany

Recently, topological nodal-line semimetals have become a topic of very active research, driven by the discovery of several new nodal-line materials. In this talk, I present a complete classification of all possible non-symmorphic nodal lines in hexagonal materials with strong spin-orbit coupling. The analysis is based on (i) the algebraic relations obeyed by the symmetry operators and (ii) the compatibility relations between irreducible representations at different high-symmetry points of the Brillouin zone. I present a number of existing materials where these non-symmorphic nodal lines are realized and discuss their DFT band structures. Based on these material examples, I discuss the surface states that are associated with the topological band crossings.

TT 20.2 Mon 15:15 A 053

Realizing double Dirac particles in the presence of electronic interactions — •Giorgio Sangiovanni[1], Domenico Di Sante[1], Andreas Hausoel[1], Paolo Barone[2], Jan Tomczak[3], and Ronny Thomale[1] — [1]Institut fuer Theoretische Physik und Astrophysik, Universitaet Wuerzburg — [2]Consiglio Nazionale delle Ricerche, l'Aquila (Italy) — [3]TU Wien (Austria)

Double Dirac fermions have recently been identified as possible quasiparticles hosted by three-dimensional crystals with particular nonsymmorphic point-group symmetries. Applying a combined approach of ab initio methods and dynamical mean-field theory, we investigate how interactions and double Dirac band topology conspire to form the electronic quantum state of Bi_2CuO_4. We derive a downfolded eight-band model of the pristine material at low energies around the Fermi level. By tuning the model parameters from the free band structure to the realistic strongly correlated regime, we find a persistence of the double Dirac dispersion until its constituting time-reversal symmetry is broken due to the onset of magnetic ordering at the Mott transition. Our calculations suggest that the double Dirac fermions in Bi_2CuO_4 can be restored by experimentally accessible hydrostatic pressures. In light of the growing attention to the topological quantum chemistry approach, our results on Bi_2CuO_4 show how many-body effects must be included beyond the static mean-field level for reliable predictions on new materials.

[1] Phys. Rev. B 96, 121106(R) (2017)

TT 20.3 Mon 15:30 A 053

Drumhead surface states in topological Dirac semimetal — •Andreas Leonhardt[1], Andreas Schnyder[1], Mehdi Biderang[2], Nimisha Raghuvanshi[2], and Alireza Akbari[2] — [1]Max Planck Institute for Solid State Research, D-70569 Stuttgart, Germany — [2]Asia Pacific Center for Theoretical Physics, Pohang, Gyeongbuk 790-784, Korea

Dirac nodal line semimetals (DNLSMs) host a symmetry protected band crossing along a line in the BZ. The non-trivial Berry phase of the bulk within the nodal ring leads to localized drumhead surface states (DSSs) in the interior of the projection of the line node onto the surface BZ. Promising candidates to study the physics of DNLSMs are the compounds CaAg(P/As) and $TlTaSe_2$, which provide different SOC strengths and mechanisms.

Quasi particle interference (QPI) is dominated by surface states and provides a possibility to investigate the dispersion and spin polarization of the drumhead surface states. We present spin resolved QPI patterns from an effective low energy tight binding model for the most promising candidates of nodal line semimetals, together with a symmetry analysis of the resulting patterns with respect to the spin polarization of the DSSs, with a focus on the influence of SOC onto the line node and the surface states.

Furthermore, we investigate the effect of the non-trivial topology on non-linear optical response phenomena, where the Berry connection and curvature directly appear in terms of quadratic or higher order in the electric field.

TT 20.4 Mon 15:45 A 053

Three dimensional Dirac semimetal canditate $PtBi_2$ — •Boy Roman Piening[1], Thirupathaiah Setti[1,2], Christian Blum[1], Yevhen Kushnirenko[1], Alexander Yaresko[3], Sergey Borisenko[1], Saicharan Aswartham[1], and Bernd Büchner[1,4] — [1]IFW Dresden, 01069 Dresden, Germany — [2]Indian Institute of Science, Bangalore, Karnataka, 560012, India — [3]Max-Planck-institute for Solid State Research, Heisenbergstrasse 1, 70569 Stuttgart, Germany — [4]Technical University Dresden, 01069 Dresden, Germany

From band structure calculations the pyrite-type cubic $PtBi_2$ has been predicted to be a three-dimensional Dirac semimetal, which is supported by experimental studies showing anomalous transport properties such as a non saturating extremely large linear magnetoresistance (XMR). Until now only the trigonal $PtBi_2$ was investigated in respect to electronic structure by ARPES revealing promising linearly dispersive Dirac states. We synthesized cm-sized cubic and trigonal $PtBi_2$ single crystals by selfflux method using different ratios of Pt to Bi in appropriate temperature regions in order to control the phase. For comparison trigonal $PtBi_2$ were grown with a mirror furnace leading to a several cm-long single crystal. Transport measurements, X-ray diffraction and Energy-dispersive spectroscopy confirm the high quality of the crystals which makes them suitable for further investigation. For the first time it was possible to measure the cubic $PtBi_2$ with ARPES.

TT 20.5 Mon 16:00 A 053

Planar Hall effect in half Heusler Weyl semimetal GdPtBi — Nitesh Kumar, Claudia Felser, and •Chandra Shekhar — Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany

Weyl and Dirac Fermions semimetals exhibits exotic transport properties for example high carrier mobility, large positive transverse magnetoresistance, low charge carrier density, low effective mass *etc.* However, among the very few available tools to characterize Weyl semimetals through electrical transport, negative magnetoresistance is most commonly used. Considering shortcomings of this method, new tools to characterize chiral anomaly in Weyl semimetals are desirable. We employ planar Hall effect as an effective technique in half Heusler Weyl semimetal GdPtBi to study chiral anomaly. This compound exhibits a large value of 1.5 mΩcm planar Hall resistivity at 2 K and in 9 T [1]. Our analysis reveals that the observed amplitude is dominated by Berry curvature and chiral anomaly contributions. Through the angle dependent transport studies we establish that GdPtBi with relatively small orbital magnetoresistance is an ideal candidate to observe large planar Hall effect.

[1] N. Kumar, C. Felser and C. Shekhar, *arXiv*:1711.04133, 2017.

TT 20.6 Mon 16:15 A 053

An optical investigation of the strong spin-orbital coupled magnetic semimetal $YbMnBi_2$ — •Alexander Yaresko[1], Dipanjan Chaudhuri[2], Bing Cheng[2], N. Peter Armitage[2], Quinn D. Gibson[3], and Robert J. Cava[3] — [1]Max-Planck-Institute for Solid State Research, Heisenbergstrasse 1, 70569 Stuttgart, Germany — [2]Department of Physics and Astronomy, The Johns Hopkins University, Baltimore, MD 21218, USA — [3]Department of Chemistry, Princeton University, Princeton, NJ 08544, USA

Strong spin-orbit coupling can result in ground states with non-trivial topological properties. The situation is even richer in magnetic systems where the magnetic ordering can potentially have strong influence over the electronic band structure. The class of $AMnBi_2$ (A = Sr, Ca) compounds are important in this context as they are known to host massive Dirac fermions with strongly anisotropic dispersion, which is believed to be due to the interplay between strong SOC and magnetic degrees of freedom. We report the optical conductivity of $YbMnBi_2$, a newly discovered member of this family and a proposed Weyl semi-metal candidate with broken time reversal symmetry. Comparing experimental and theoretical optical spectra we show that the complex conductivity can be interpreted as the sum of an intra-band Drude response and inter-band transitions. We find signatures of a gapped Dirac dispersion, common in other members of $AMnBi_2$ family or compounds with similar 2D network of Bi atoms.

TT 20.7 Mon 16:30 A 053

Generic Coexistence of Fermi Arcs and Dirac Cones on the Surface of Time-Reversal Invariant Weyl Semimetals —

•Alexander Lau[1], Klaus Koepernik[2], Jeroen van den Brink[2], and Carmine Ortix[3] — [1]Kavli Institute of Nanoscience, TU Delft, Netherlands — [2]Institute for Theoretical Solid State Physics, IFW Dresden, Germany — [3]Institute for Theoretical Physics, Utrecht University, Netherlands

The hallmark of Weyl semimetals is the existence of open constant-energy contours on their surface, the so-called Fermi arcs, connecting Weyl points. Here, we show that for time-reversal symmetric realizations of Weyl semimetals these Fermi arcs in many cases coexist with closed Fermi pockets originating from surface Dirac cones pinned to time-reversal invariant momenta. The existence of Fermi pockets is required for certain Fermi-arc connectivities due to additional restrictions imposed by the six $\mathbb{Z}_2$ topological invariants characterizing a generic time-reversal invariant Weyl semimetal. We show that a change of the Fermi-arc connectivity generally leads to a different topology of the surface Fermi surface, and identify the half-Heusler compound LaPtBi under in-plane compressive strain as a material that realizes this surface Lifshitz transition.

15 min. break.

TT 20.8 Mon 17:00 A 053

Weyl semimetals with single Weyl nodes, and the fate of their chiral anomaly — •Tobias Meng and Jan Carl Budich — Institute of Theoretical Physics, Technische Universität Dresden, 01062 Dresden, Germany

Weyl semimetals are defined by the presence of isolated points in the Brillouin zone at which a conduction and a valence band touch. The so-called Nielsen-Ninomiya-theorem requires these points (the "Weyl nodes") to appear in pairs. This theorem, however, is only valid for interactions of sufficiently short range. In this talk, I discuss that long-range interactions can break the Nielsen-Ninomiya-theorem, and illustrate this point by an explicit construction of an interacting tight-binding model that contains only a single Weyl node. I will then demonstrate that the chiral magnetic effect remains intact for arbitrary interactions in such a single node Weyl semimetal. In particular, already an infinitesimal magnetic field restores a pair of chiral Landau levels of opposite chirality.

TT 20.9 Mon 17:15 A 053

Quantum anomalies in strained Weyl semimetals — Sthitadhi Roy[1], •Jan Behrends[1], Michael Kolodrubetz[2], Jens H. Bardarson[3], Nathan Goldman[4], Adolfo G. Grushin[2,5], and Roni Ilan[6] — [1]Max-Planck-Institut für Physik komplexer Systeme, 01187 Dresden, Germany — [2]Department of Physics, University of California, Berkeley, California 94720, USA — [3]Department of Physics, KTH Royal Institute of Technology, Stockholm, SE-106 91 Sweden — [4]Center for Nonlinear Phenomena and Complex Systems, Université Libre de Bruxelles, CP 231, Campus Plaine, B-1050 Brussels, Belgium — [5]Institut Néel, CNRS and Université Grenoble Alpes, F-38042 Grenoble, France — [6]Raymond and Beverly Sackler School of Physics and Astronomy, Tel-Aviv University, Tel-Aviv 69978, Israel

The chiral anomaly gives the topological response of Weyl semimetals to an external perturbation, insensitive to local details of the Hamiltonian. The recent identification of strain as axial fields in these materials gives rise to other anomalies, known from high-energy theory. However, these anomalies driven by axial fields are not necessary gauge-invariant or charge-conserving; in fact, two different formulations exist, realizing just one of these conditions. In this work, we propose a way to resolve this ambiguity, supported by a lattice model that provides an intuitive picture. We identify experimental signatures and argue about their stability in presence of disorder.

TT 20.10 Mon 17:30 A 053

Creating and Controlling Weyl Fermions, Nexus Points, and Nodal Lines in the Magnetic Anti-perovskite Eu_3PbO — •Moritz M. Hirschmann[1], Alexandra S. Gibbs[2], Vahideh Abdolazimi[1], Alexander Yaresko[1], Hidenori Takagi[1,3,4], Andreas W. Rost[1,3], and Andreas P. Schnyder[1] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]ISIS Pulsed Neutron Facility, Didcot, United Kingdom — [3]FMQ, Universität Stuttgart, Germany — [4]Department of Physics, The University of Tokyo, Japan

Anti-perovskite materials A_3EO, where A denotes an alkaline earth metal, while E stands for Pb or Sn, exhibit low-energy electronic properties that are described by three-dimensional Dirac fermions, which are gapped out by spin-orbit coupling [1,2]. If A is replaced by the rare-earth element europium then magnetic order is expected due to the electron spin moment as confirmed by magnetization measurements. Neutron diffraction leads us to the conclusion that different magnetic phases appear. We studied the effect of magnetism on the electronic properties of Eu_3PbO. From DFT calculations the resulting splitting has been extracted and implemented into a tight-binding model to capture the physics close to the Fermi energy. We present the creation of Weyl points, Nexus points, and nodal lines and give their topological invariants. For the different magnetic phases we derived the respective surface states and anomalous Hall responses.

[1] T. H. Hsieh, J. Liu, L. Fu. Phys. Rev. B, 90 (2014) 08111.
[2] D. Samal, H. Nakamura, H. Takagi. APL Mater. 4 (7), 2016.

TT 20.11 Mon 17:45 A 053

Andreev reflection in time-reversal symmetric Weyl semimetals — •Jens Schulenborg[1], Uli Zuelicke[2], and Michele Governale[2] — [1]Department of Microtechnology and Nanoscience (MC2), Chalmers University of Technology, Göteborg, Sweden — [2]School of Physical and Chemical Sciences and Alan MacDiarmid Institute for Advanced Materials and Nanotechnology, Victoria University Of Wellington, New Zealand

The study of the unusual chiral properties of Weyl fermions in Weyl semimetals (WSM) has attracted enormous attention in the past decade. Most recently, reports[1,2] on simple WSM band structures with only the minimum number of Weyl nodes suggest that it might become possible to exploit the nontrivial spin-momentum locking directly through ballistic scattering. This can be useful for spectroscopy or spin-dependent quantum optics with electrons.

To explore this perspective, we theoretically study elastic Andreev reflection in a minimal model of a time-reversal symmetric WSM, at an interface between a normal and superconducting region with s-wave pairing. We show that without interface-related spin-mixing, the subgap reflection processes at the four Weyl cones completely decouple. This arguably simplest form of Andreev scattering in a time-reversal symmetric WSM can be described by a 3D analogue of graphene, with the key difference that the pseudospin becomes an effective, yet in principle accessible spin.

[1] K. Koepernik et al., Phys. Rev. B 93, 201101 (2016)
[2] I. Belopolski et al., Nat. Commun. 8, 942 (2017)

TT 20.12 Mon 18:00 A 053

Ballistic edge states in Bismuth nanowires revealed by SQUID interferometry — •Anil Murani — Laboratoire de Physique des Solides, CNRS, Univ. Paris-Sud, Université Paris-Saclay, 91405 Orsay Cedex, France — Quantronics Group, Service de Physique de l'État Condensé (CNRS UMR 3680), IRAMIS, CEA-Saclay, 91191 Gif-sur-Yvette, France

Topological insulators are materials that have electronic states lying at their edges, which are protected against backscattering by time reversal symmetry. Bismuth, a semi-metal with strong spin-orbit coupling, was predicted to be topological in the case of a bilayer thick crystal. We showed numerically that edge states still exists in Bi nanowires, and experimentally demonstrated the existence of edge conduction channels as well as their ballisticity in a recent work, by embedding the nanowire into an asymetric SQUID. The goal of the present study is to go one step further and to answer quantitatively about the topological protection against backscattering as well as the lifetime of the metastable Andreev bound states that can be formed in these topological SNS junction. This is done by inductively coupling the NS loop to a multimode superconducting resonator, with eigenfrequencies ranging from 300 MHz up to 6 GHz, and measuring the magnetic flux dependent absorbtion at the vicinity of each of these frequencies. The resulting phase dependent absorbtion spectrum is measured for different temperatures and can be analyzed using a simple low energy model taking into account two Andreev bound states that nearly anticross, in agreement with a topological protection.

TT 20.13 Mon 18:15 A 053

Breakdown of the chiral anomaly in Weyl semimetals in a strong magnetic field — •Pilkwang Kim, Ji Hoon Ryoo, and Cheol-Hwan Park — Department of Physics, Seoul National University, Seoul 08826, Korea

A Weyl semimetal is a three-dimensional material whose low-energy quasiparticles are the chiral fermions described by the Weyl equation. One of the most intriguing phenomena of Weyl semimetals is the chiral anomaly, which is the nonconservation of the chiral charge in the presence of parallel electric and magnetic fields and has been understood as an imbalance between the occupations of the zeroth Landau levels with the opposite chiralities [1]. In this presentation, we report the breakdown of the chiral anomaly in Weyl semimetals in a strong magnetic field [2]. From first-principle calculations, we demonstrate that a sizable energy gap opens up due to the mixing of the zeroth Landau levels with opposite chiralities if an applied magnetic field is sufficiently strong. Our results provide a theoretical framework for understanding a wide range of phenomena related to the chiral anomaly in topological semimetals, such as magnetotransport, thermoelectric responses, and plasmons.

[1] H. B. Nielsen, M. Ninomiya, Phys. Lett. B 130 (1983) 389.
[2] P. Kim, J. H. Ryoo, C.-H. Park, arXiv 1707.01103 (2017).

TT 20.14 Mon 18:30 A 053

Quantum oscillations in Weyl-II semimetals near magnetic breakdown — •Fabian Lambert[1], Johannes Knolle[2], and Ilya Eremin[1] — [1]Ruhr-Universität Bochum — [2]Imperial College London

The band structure of a type-II Weyl semimetal has pairs of electron and hole pockets that coexist over a range of energies and touch at a topologically protected conical point. While it is known, that in this case tunneling effects will lead to what is called a magnetic breakdown, the existence of these pairs of pockets at the Fermi energy also has an impact on the quantum oscillations associated with the topological Fermi arcs that exist on the surface of these materials. We analyze the quantum oscillations for a tight-binding model describing both Weyl I and Weyl II semimetals concentrating on the large field regime. The surface Fermi arcs coxisting with bulk electron and hole pockets lead to new experimental signatures of the quantum oscillations, which will be crucial for their experimental identification.