Fermi surface topological transitions: classification and effects on correlated systems

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Day 1

9:30-10:10 Electronic signatures of the nematic electronic phases in superconducting FeSe\textsubscript{1-x}S\textsubscript{x}. Amalia Coldea (invited).

10:10-10:50 The Uniaxial-Stress-Induced Lifshitz transition in Sr\textsubscript{2}RuO\textsubscript{4}. Clifford Hicks (invited).

10:50-11:10 s+is superconductivity triggered by topological changes of the Fermi surface in Ba\textsubscript{1-x}K\textsubscript{x}Fe\textsubscript{2}As\textsubscript{2}. Vadim Grinenko, et. al.

11:10-11:30 Manipulation of time reversal symmetry breaking superconductivity in Sr\textsubscript{2}RuO\textsubscript{4} by uniaxial strain. Hans-Henning Klauss, et. al.

11:30-11:50 The role of the d\textsubscript{xy} orbital in the nematic and superconducting state of FeSe. Luke Rhodes, et. al.


12:10-12:50 High-order Van Hove singularity and correlation effects toward a supermetal. Hiroki Isebe (invited).

Day 2


10:10-10:50 Comparison of two Superconducting phases induced by a magnetic field in UTe\textsubscript{2}. William Knafo (invited), et. al.

10:50-11:30 Quantum phase formation driven by multicritical Lifshitz transitions. Andreas Rost (invited), et al.

11:30-11:50 Transport Spectroscopy of the Field Induced Cascade of Lifshitz Transitions in YbRh\textsubscript{2}Si. Andrey Varlamov, et. al.

11:50-12:10 Fermi Surface Instabilities in the Strongly Correlated Superconductor UTe\textsubscript{2}. Alexandre Pourret, et. al.

12:10-12:50 Catastrophe theory classification of Fermi surface topological transitions in 2D. Anirudh Chandrasekaran (invited), Alex Shtyk, Joseph J. Betouras, Claudio Chamon.
Pre-recorded talks:

1. Electron-phonon coupling in superconducting 1T-PdTe$_2$. **Gloria Anemone**, et. al.


3. Uniaxial pressure induces Lifshitz phase transition in BaSn$_2$. A route to increase the number of topological nodal lines in semimetals. **Adolfo Fumega**, Victor Pardo and Alberto Cortijo.


5. Cascade of Lifshitz transitions in surface states of graphite aligned with hBN. **Sergey Slizovskiy**.

6. Direct observation of 1D-Moiré charge density wave and heavy fermion quantization in URu$_2$Si$_2$. **Edwin Herrera**, et. al.

7. Fermi Surface of Li$_x$CoO$_2$ as a function of hole doping. **Elena Salagre**, et. al.


9. Piezoelectric-driven uniaxial pressure cell for muon spin relaxation experiments. **Shreenanda Ghosh**, et. al.

Posters

Electronic signatures of the nematic electronic phases in superconducting FeSe\(_{1-x}\)S\(_x\)

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A nematic electronic state that breaks the rotational symmetry of the lattice is suggested to play an important role in the superconducting pairing of iron-chalcogenide superconductors. To understand the nature of this unique quantum phase transition, it is essential to study the key ingredients of its electronic structure and electronic correlations [1]. Here I will summarize the experimental findings from quantum oscillations [2,3] and angle-resolved photoemissions studies on FeSe\(_{1-x}\)S\(_x\) [4,5]. The distortion of the Fermi surface, induced by orbital ordering effects and electronic correlations, is suppressed at the nematic phase transition boundaries and there a subtle changes of the sizes of the smaller inner hole and electron bands across the phase diagram [4,5]. With increasing sulfur substitution, the Fermi velocities increases significantly and the band renormalizations are suppressed towards FeS [5]. Shubnikov-de Haas oscillations in high magnetic fields up to 45T below 1.5K shows that most of the Fermi surfaces monotonically increase in size. Magnetoresistance at low temperatures is dominated by a prominent low frequency oscillation associated with a small, but highly mobile band, which disappears at the nematic phase boundary near x ~ 0.17. This behavior may be indicative of a topological Lifshitz transition as a function of both chemical and applied pressure [2,3]. The quasiparticle masses are larger inside the nematic phase but they become suppressed outside it. The experimentally observed changes in the Fermi surface topology, together with the varying degree of electronic correlations and transport properties [6], suggest a fine balance between the electronic interactions in the multi-band system FeSe\(_{1-x}\)S\(_x\). These effects can promote different superconducting pairing channels inside and outside the nematic phase.

References
The Uniaxial-Stress-Induced Lifshitz transition in Sr$_2$RuO$_4$

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An in-plane uniaxial stress of 0.7 GPa, which compresses the lattice by 0.44%, drives the largest Fermi surface of Sr$_2$RuO$_4$ through a transition from a closed to an open surface. In the vicinity of this transition, the normal-state low-temperature properties of Sr$_2$RuO$_4$ are altered: the resistivity changes from a $T^2$ to a $T^{1.4}$ dependence, and the magnetic susceptibility increases measurably. The effect on the superconductivity of Sr$_2$RuO$_4$ is profound: $T_c$ increases from 1.5 to 3.5 K, while the upper critical field increases by a factor of twenty. This strong enhancement is probably not reconcilable with odd-parity pairing, which was long hypothesised for Sr$_2$RuO$_4$. In this talk I will discuss the effects of this Lifshitz transition further. I will also show some early results from uniaxial compression along the $c$ axis. Whereas in-plane uniaxial stress drives a closed-to-open transition, $c$-axis compression is predicted to drive an electron-to-hole-like transition, and an even stronger divergence in the density of states. I present evidence that, at a uniaxial compression of 4 GPa, we approach this transition.

References
s+is superconductivity triggered by topological changes of the Fermi surface in Ba$_{1-x}$K$_x$Fe$_2$As$_2$

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In general, magnetism and superconductivity are antagonistic to each other. However, there are several families of superconductors in which superconductivity coexists with magnetism, and a few examples are known where the superconductivity itself induces spontaneous magnetism. The best known of these compounds are Sr$_2$RuO$_4$ and some non-centrosymmetric superconductors. Here, we report the finding of a narrow dome of an $s+is$ superconducting phase with a broken time-reversal symmetry (BTRS) inside the broad $s$-wave superconducting region of the centrosymmetric multiband superconductor Ba$_{1-x}$K$_x$Fe$_2$As$_2$ ($0.7 \lesssim x \lesssim 0.85$). We observe spontaneous magnetic fields inside this dome using the muon spin relaxation ($\mu$SR) technique. Furthermore, our detailed specific heat study reveals that the BTRS dome appears very close to a change in the topology of the Fermi surface. With this, we experimentally demonstrate the emergence of a novel quantum state due to topological changes of the electronic system. See figure 1, adapted from the following references [1, 2].

References

Figure 1. Schematic of the change of the topology of the Fermi surface at the Lifshitz transition ($x_L$) in the Ba$_{1-x}$K$_x$Fe$_2$As$_2$ system with possible $s$-wave superconducting states. (a,b) The Brillouin zone with two-hole and one-electron Fermi pockets (optimal doping) (a) and the Brillouin zone with two-hole Fermi pockets (high doping level) (b). e–g, Possible $s$-wave pairing states in a clean limit. The relative phase $\phi$ of the superconducting order parameter components is shown by the direction of the arrows inside the circles and the magnitude is indicated by the length. A frustrated pairing $s+is$ state with arbitrary phase shifts between the components of the order parameter in a clean limit is possible in the three-band case.
Manipulation of time reversal symmetry breaking superconductivity in Sr$_2$RuO$_4$ by uniaxial strain

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Although the normal-state electronic structure of Sr$_2$RuO$_4$ is known with exceptional precision, even after two decades of research, the symmetry of its certainly unconventional superconducting state is currently under strong debate, e.g. the long time favoured spin-triplet $p_x^+ i p_y$ state is ruled out by recent NMR experiments [1]. However, in general time-reversal-symmetry breaking (TRSB) superconductivity indicates complex two-component order parameters. Probing Sr$_2$RuO$_4$ under uniaxial offers the possibility to lift the degeneracy between such components [2]. One key prediction for Sr$_2$RuO$_4$, a splitting of the superconducting and TRSB transitions under uniaxial stress has not been observed so far. Here, we report results of muon spin relaxation ($\mu$SR) measurements on Sr$_2$RuO$_4$ placed under uniaxial stress. We observed a large stress-induced splitting between the onset temperatures of superconductivity and TRSB. Moreover, at high stress beyond the van Hove singularity, a new spin density wave ordered phase is observed.

References

Figure 1. The stress-temperature phase diagram of Sr$_2$RuO$_4$ based on $\mu$SR and magnetic susceptibility data. The insets illustrate the stress-induced changes in the Fermi surfaces of Sr$_2$RuO$_4$. 

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Gapped Dirac cones and spin texture in thin film topological insulator
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The protected surface states of topological insulators (TIs) form gapless Dirac cones corresponding non-degenerate eigenstates with helical spin polarisation. The presence of a warping term deforms the isotropic cone of the simplest model into snowflake Fermi surfaces as in Bi\textsubscript{2}Se\textsubscript{3} and Bi\textsubscript{2}Te\textsubscript{3}. Their features have been identified in STM quasiparticle interference (QPI) experiments on isolated surfaces. Here we investigate the QPI spectrum for the TI thin-film geometry with finite tunnelling between the surface states. This leads to a dramatic change of spectrum due to gapping and a change in spin texture that should leave distinct signatures in the QPI pattern. We consider both normal and magnetic exchange scattering from the surface impurities and obtain the scattering t-matrix in Born approximation as well as the general closed solution. We show the expected systematic variation of QPI snowflake intensity features by varying film thickness and study, in particular, the influence on backscattering processes. We predict the variation of the QPI spectrum for Bi\textsubscript{2}Se\textsubscript{3} thin films using the observed gap dependence from ARPES results.

References

Figure 1. (a) Sketch of surface scattering processes in quasiparticle interference for thin film geometry. Isolated T, B Dirac cones with helicities $\pm$ are indicated; (b-e) The dispersion characteristics of quasiparticle interference spectrum along symmetry directions of the 2D surface Brillouin zone $M\Gamma$ and $\Gamma K$ as function of inter-surface tunnelling strength. The gap opening of the Dirac cones can clearly be followed in the quasiparticle interference dispersion.
High-order Van Hove singularity and correlation effects toward a supermetal

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The shape of a Fermi surface contains information of an electronic system as it encodes the low-energy properties of electrons. A Van Hove singularity (VHS) is tied to the topology of a Fermi surface; the singularity in the density of states (DOS) arises owing to a Fermi surface topological transition, namely a Lifshitz transition. Since the appearance of a VHS requires tuning of the Fermi energy or a material parameter, tunable materials are desirable to observe VHS-related phenomena. Such materials include strontium ruthenates (Sr$_2$RuO$_4$ and Sr$_3$Ru$_2$O$_7$) and moiré superstructures made of van der Waals materials [Fig. 1(a)].

First, we introduce a theory that describes a possible mechanism for correlated insulating and superconducting states in twisted bilayer graphene [1]. We study electronic ordering instabilities occurring near the filling of two electrons per moiré unit cell. Using a hot-spot model, we find that d- or p-wave superconductivity and charge/spin-density wave emerge from Coulomb repulsion. We further investigate the tunable nature of twisted bilayer graphene, which invokes the notion of a high-order VHS [2]. It requires only a single tuning parameter, such as a twist angle of a moiré material, pressure, and strain. At a saddle point of energy dispersion in two dimensions, the DOS shows a logarithmic divergence; however, the tunable twist angle of two graphene layers can give rise to a power-law divergence. We could attribute the origin of the so-called magic angle to the high-order VHS. Finally, we discuss correlation effects at a high-order VHS [3]. Relying on the scale invariance of a high-order VHS, we perform a renormalization-group analysis to find a nontrivial metallic state, where various divergent susceptibilities coexist, but no long-range order appears. We term such a metallic state as a supermetal. The RG analysis bears a similarity to the $\phi^4$ theory, and a controlled analysis at the interacting fixed point reveals that an interacting supermetal is a non-Fermi liquid.

References

Figure 1. (a) Moiré structure created by two layers with the honeycomb lattice, showing a longer periodicity than that of the original lattice; (b) Schematic phase diagram near a high-order Van Hove singularity.
Field-induced Lifshitz transitions: Probe of heavy fermion band structure

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The search for new types of exotic topological orders has recently rekindled the interest in Fermi surface reconstructions. Of particular interest are Electronic Topological (Lifshitz) transitions where the number of Fermi surface sheets changes abruptly under the influence of external parameters like chemical doping, pressure, or magnetic field. Lifshitz transitions are generally associated with the presence of critical points in the electronic band structure, i.e., maxima, minima, or saddle points whose presence follows directly from lattice periodicity. As their separation from the chemical potential is of the order of the bandwidth, the critical points hardly affect the low temperature behavior of “conventional” metals. In heavy-fermion materials, however, the widths of the quasi-particle bands are strongly reduced by electronic correlations and, consequently, magnetic fields can drive Lifshitz transitions. The characteristic anomalies in the equilibrium and transport properties provide a method to test the quasi-particle dispersion away from the Fermi surface. The values of the field at which the transitions occur reflects the microscopic mechanism leading to the formation of the heavy quasi-particles.

Here we demonstrate that the magnetic field-dependent anomalies in the Seebeck coefficient provide detailed information not only on the critical points, i.e., their character and position relative to the chemical potential but also on the effective mass tensor, i.e., the quasi-particle dispersion in the vicinity of the critical points. For lanthanide-based HFS, the theoretical analysis is based on Renormalized Band (RB) structure calculations assuming that the heavy quasi-particles result from a Kondo effect [1]. For U-based HFS, on the other hand, we adopt the fully microscopic model which emphasizes the role of intra-atomic Hund's rule-type correlations for appearance of heavy quasi-particle masses. The calculations reproduce the observed positions of the anomalies surprisingly well [2].

Acknowledgment
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References
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Comparison of two superconducting phases induced by a magnetic field in UTe₂

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Superconductivity induced by a magnetic field in the vicinity of a metamagnetic transition is a striking manifestation of magnetically-mediated superconducting pairing. After being observed in itinerant ferromagnets, this phenomenon was recently reported in the orthorhombic paramagnet UTe₂ [1,2]. Under a magnetic field applied along the hard magnetization axis b, superconductivity is reinforced on approaching metamagnetism at \( \mu_0 H_m \approx 35 \) T, but it abruptly disappears beyond \( H_m \) [3,4]. On the contrary, field-induced superconductivity was reported beyond \( \mu_0 H_m \approx 40-50 \) T in a magnetic field tilted by \( \approx 25-30^\circ \) from b in the (b,c) plane [5].

Here we explore the phase diagram of UTe₂ under these two magnetic-field directions. Magnetoresistivity experiments have been performed under pulsed magnetic fields up to 60 T combined with low-temperatures down to 200 mK, reached thanks to a home-developed partly-non-metallic dilution fridge. The observation of zero-resistivity permits to confirm unambiguously that superconductivity is established beyond \( H_m \) in the tilted-field direction. While superconductivity is locked exactly at fields either smaller (for \( H \parallel b \)), or larger (for \( H \) tilted by \( \approx 27^\circ \) from b to c), than \( H_m \), the variations of the Fermi-liquid coefficient in the electrical resistivity and of the residual resistivity are surprisingly similar for the two field directions. The absence of obvious differences in the normal state for the two field directions puts constraints for theoretical models of superconductivity and implies that some subtle ingredients must be in play. The questions of magnetic fluctuations and Fermi surface changes at the metamagnetic transition (see also [6,7]), as well that of the peculiar tilted field-direction, will be discussed.

References
A series of strong anomalies in the thermoelectric power is observed in heavy fermion compound YbRh$_2$Si$_2$ under the effect of magnetic field varying in the range from 9.5 to 13 T. We identify these features with a sequence of topological transformations of the sophisticated Fermi surface of this compound, namely a cascade of Lifshitz topological transitions. In order to undoubtedly attribute these anomalies to the specific topological changes of the Fermi surface, we employ the renormalized band method. Basing on its results we suggest a simplified model consisting of the large peripheral Fermi surface sheet and the number of continuously appearing (disappearing) small “voids” or “necks” (see Fig.1). We account for the multiple electron scattering processes between various components of the Fermi surface, calculate the corresponding scattering times, and, finally, find the magnetic field dependence of the Seebeck coefficient. The obtained analytical expression reproduces reasonably the observed positions of the maxima and minima as well as the overall line shapes and allows us to identify the character of corresponding topological transformations (see Fig.2).

Fig. 1 The scenario of the multiple Lifshitz transitions evolution: at $H_1$ the pockets $Z_1$ appears, at $H_2$ a neck breaking occurs in the pocket $Z_2$, finally at $H_3$ the pocket $Z_1$ disappears.

Fig. 2 Magnetic field dependence of the Seebeck coefficient through a cascade of Lifshitz transitions obtained at 110mK compared with the theoretical prediction based on multi-sheet FS scattering processes. (b) Theoretical modelling of the contributions corresponding to quasiparticle scatterings from the different sheets of the FS to the Seebeck coefficient.
Fermi Surface Instabilities in the Strongly Correlated Superconductor UTe$_2$

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We present thermoelectric power ($S$) and Hall effect ($R_H$) measurements up to fields of 60 T in the recently discovered heavy-fermion superconductor UTe$_2$ with magnetic field $H$ applied along the easy magnetization $a$-axis and the hard magnetization axis $b$-axis (at low temperature) of the body-centered orthorhombic structure. For $H//a$, $S(T)$ varies linearly with temperature above the superconducting transition, $T_{SC}$ = 1.5 K, indicating that superconductivity develops in a Fermi liquid regime [1]. As a function of field, $S(H)$ shows successive anomalies which appear at critical values of the magnetic polarization, see Fig. 1(a). Remarkably, the lowest magnetic field instability for $H//a$ occurs for the same critical value of the magnetization ($0.4 \mu$B) than the first order metamagnetic transition at $H_m$ = 34.6 T for field applied along the $b$ axis. It can be clearly identified as a Lifshitz transition. For $H//b$, $S(H)$ shows only a weak field dependence in the normal state up to the first order metamagnetic transition at $H_m$ = 35 T. The discontinuous field dependence of both, $S(H)$, see Fig. 1(b-c), and the ordinary Hall coefficient $R_0(H)$, at $H_m$ for temperatures below the critical end point of the first order transition $T < T_{CEP}$, provides clear evidence of a change in the band structure at the Fermi level [2]. The Hall effect $R_H$ is very well described by incoherent skew scattering above the coherence temperature corresponding roughly to the temperature of the maximum in the susceptibility and coherent skew scattering at lower temperatures.

References

![Image](image_url)
Catastrophe theory classification of Fermi surface topological transitions in two dimensions

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We classify singularities in the electronic dispersion of two-dimensional systems that occur when the Fermi surface changes topology, using catastrophe theory. For systems with up to seven control parameters (i.e., pressure, strain, bias voltage, etc), the theory guarantees that the singularity belongs to one of seventeen standard types known as catastrophes. We show that at each of these singularities the density of states diverges as a power law, with a universal exponent characteristic of the particular catastrophe, and we provide its universal ratio of amplitudes of the prefactors for energies above and below the singularity. We further show that crystal symmetry restricts which types of catastrophes can occur at the points of high symmetry in the Brillouin zone. For each of the seventeen wallpaper groups in two-dimensions, we list which catastrophes are possible at each high symmetry point.

References

The cusp catastrophe:

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{cusp_catastrophe.png}
\caption{Energy contours of the cusp catastrophe showing the singular point at the origin.}
\end{figure}
Electron-phonon coupling in superconducting 1T-PdTe2

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We have determined the electron-phonon interaction in type II Dirac semimetallic 1T-PdTe2 by means of helium atom scattering. While 1T-PdTe2 is isostructural with 1T-PtTe2, only the former is superconductor. The origin of this difference has not been fully clarified yet. Whereas some authors have proposed that the main role is played by the topological states of a Dirac cone, a more recent theoretical study has suggested that superconductivity in 1T-PdTe2 is triggered by an increase of the electron-phonon coupling constant $\lambda$, which is consequence of the presence of a van Hove singularity at the Fermi level [1]. We show that the difference between these two isostructural materials can be traced to the substantially larger value of the electron-phonon coupling in 1T-PdTe2, experimentally determined by recording the thermal attenuation of the elastic diffraction peaks of PtTe2 and PdTe2. Based on a recently developed quantum theoretical method adapted to layered degenerate semiconductors we find that $\lambda$ in PtTe2 lies between 0.38–0.42 [1], whereas in the case of PdTe2 $\lambda$ has a value of 0.58 [2]. With this value and the surface Debye temperature, $\Theta_D = 106.2$ K, we have figured out the superconducting critical temperature, $T_c = 1.83$ K, given by the BCS theory, which is in excellent agreement with $T_c = (1.95\pm0.03)$ K obtained with low-temperature scanning tunneling microscopy. The value of the effective mass related to $\Theta_D$ indicates that the large electron-phonon coupling in 1T-PdTe2 is due to coupling, not only with the zone-center optical mode $O_2$ at 9.2 meV, as proposed in a recent theoretical study [1], but also with the zone-boundary acoustic mode LA. Our results suggest that the topological states of a Dirac cone play a negligible role on the onset of superconductivity.

References
Nematic phase in a two-dimensional Hubbard model at weak coupling and finite temperature

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We apply the self-consistent renormalized perturbation theory to the Hubbard model on the square lattice at finite temperatures to study the evolution of the Fermi surface as a function of the temperature and doping. Previously, a nematic phase for the same model has been reported to appear at weak coupling near a Lifshitz transition from closed to open Fermi surface at zero temperature where the self-consistent renormalized perturbation theory was shown to be sensitive to small deformations of the Fermi surface. We find that the competition with the superconducting order leads to a maximal nematic order appearing at zero temperature. We observe the two competing phases near the onset of nematic instability, and by comparing the grand canonical potentials, we find that the transitions are of first order\cite{1}.

References
Uniaxial pressure induces Lifshitz phase transition in BaSn$_2$. A route to increase the number of topological nodal lines in semimetals

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Highly correlated states have been proposed to be present in the surface states of topological nodal-line semimetals (NLSMs). Apart from that, pressure has been identified as a mechanism to induce transitions in the Fermi surface of NLSMs. In this talk, we analyze the effect of uniaxial pressure in the topological properties of BaSn$_2$, a NLSM in the absence of spin-orbit coupling. A combination of Density Functional Theory calculations and a modeled tight-binding Hamiltonian show that BaSn$_2$ undergoes a topological to topological phase transition. The emergence of a second nodal line for pressures higher than 4 GPa is found, thus increasing the number of edge states (see Fig. 1). The application of a magnetic field provides a topological relation between the zero-energy modes of each phase, prompting a clear signature of a topological-to-topological phase transition. Multiorbital character and crystal symmetry preservation are key factors to produce this kind of phase transition.

![Image](image.png)

Figure 1. Top view of the first Brillouin zone for both topological phases. (a) Low pressure phase, a topological nodal line is present; (b) High pressure phase, new topological nodal lines emerge.
Classification of composite Weyl nodes according to its Fermi surface geometry and Lifshitz transitions

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Weyl nodes with chiral charge $\pm 1$ are classified as types I and type II according to the tilting of the conical band dispersion at the band degeneracy. Their Fermi surface, described by a quadratic form, is different for these two types. We extend this classification to the case of composite Weyl nodes with chiral charge larger than one. When the $C_4$ and $C_6$ rotation symmetries forbid the linear band dispersion on the plane perpendicular to the symmetry axis, new terms with quadratic and cubic momentum dependence must be included. Consequently, the Fermi surfaces produced by these band degeneracies are described by a 4 or 6 order algebraic surfaces. In this more complex situation, instead of classifying Fermi surfaces, we study numerically the possible Lifshitz transitions of the Fermi surface produced by a composite Weyl node as the chemical potential is varied. We use this methodology to classify the different types the composite Weyl fermions. In particular, for the case of quadratic Weyl nodes generated by the $C_4$ rotation symmetry. We find four different types band dispersion morphologies, two analogous to the type-I and type-II case of the conical Weyl nodes, and two new distinct morphologies within the type-II class. We illustrate the existence of these new types of band degeneracies in real materials such as ferromagnetic iron.
Cascade of Lifshitz transitions in surface states of graphite aligned with hBN.

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Graphite is a semimetal allowing for unprecedented electrostatic control of its surface states via hBN encapsulation and gating. Ordinary graphite with Bernal (ABA) is a semimetal with small electron and hole Fermi surfaces and no surface states.

With self-consistent Hartree calculation we show that surface states appear at the surface of Bernal graphite upon gating (electrostatic doping) [1], Fig.1a. The size of surface state Fermi-contour grows with gate voltage, leading to growing surface quantum capacitance, confirmed experimentally.

When hBN is aligned with the top layer of graphite, a moirè pattern with a period of approx. 13 nm is formed. The reciprocal vectors of moirè pattern generate new Bragg scattering processes that are efficient if they connect points on the Fermi surface. The latter condition is achieved for Fermi contours of the surface states at certain critical doping. Moirè Bragg processes then result in a Lifshitz transition, where the reconstructed Fermi contour changes its nature from electron to hole type and vice versa. As the doping grows, further Lifshitz transitions are observed, related to Bragg scattering between the first and the second band of surface states.

References

Figure 1. (a) Dispersion branches of gated Bernal graphite film. Red color indicates surface states.
(b),(c) Surface states Fermi contours at dopings $1.8 \times 10^{12}$ cm$^{-2}$ (b) and $2.0 \times 10^{12}$ cm$^{-2}$ (c), showing the evolution from electron-like to hole-like Fermi contour. Black dotted lines illustrate the moirè mini-Brillouin zone, blue/red lines are electron/hole like Fermi contours.
Direct observation of 1D-Moiré charge density wave and heavy fermion quantization in URu$_2$Si$_2$.

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URu$_2$Si$_2$ is one of the few systems where the formation of heavy quasiparticles has been directly observed thanks to surface interference experiments using Scanning Tunneling Microscopy (STM). In addition, previous experiments have shown that the hidden order phase is characterized by a gap and dynamical spin modes at $q_0=(0 0 1)$ and $q_1=(0.6 0 0)$ that quench into an antiferromagnetic order under pressure and at high magnetic fields, respectively. Here, using Scanning Tunneling Microscopy-Spectroscopy (STM-S) at very low temperatures (0.1 K), I will report on the discovery of a one-dimensional charge modulation with a wavevector that is a moiré combination of the atomic lattice periodicity and a hot spot for electronic scattering in the bandstructure of the hidden order (HO) state of URu$_2$Si$_2$ at $q_1$. I will show that the moiré pattern is produced by fracturing the crystal in presence of a dynamical spin mode at low temperatures and how its presence suggests that charge interactions are among the most relevant features competing with hidden order in URu$_2$Si$_2$ [1]. Finally, I will show that band hybridization in URu$_2$Si$_2$ modifies the local density of states resulting in heavy fermion quantization which can be directly visualized on small-sized atomically flat areas.

References
LiCoO$_2$ (LCO) is extensively used as a cathode in Li-ion batteries due to its high-energy capacity and long cycle life [1]. Stoichiometric LCO is an insulator but upon Li removal of only 0.5% (x=0.95) it undergoes a transition to a metallic state, which is interpreted as a Mott or Anderson type transition [2]. The understanding of the electronic behavior of LCO with hole doping (x<1) is important, both for Li-ion battery applications [1] and for its potential use in neuromorphic computing [3].

The changes in the band structure close to the Fermi level as a function of hole doping (x) are crucial to determine the nature of the metal-insulator transition. Fermi surface and band mapping using high resolution ARPES and synchrotron radiation have been applied in the hole doping range 0.24<x<1 to investigate these changes. The samples are epitaxial thin films of LCO of high structural quality, grown on Nb-doped SrTiO3(111) by pulsed laser deposition. The valence band of LCO is dominated by Co states. Co changes upon delithiation from Co$^{3+}$ to Co$^{4+}$. While the Co$^{3+}$ band is split in three t$_{2g}$ (full) and two e$_g$ (empty) bands, the Co$^{4+}$ valence band accommodates an additional hole in the t$_{2g}$ band [4]. This simple description is verified by XPS measurements of Co 3p and 2p core levels and by X-ray Absorption Spectroscopy (XAS) results. The hole doping induces a rigid shift of the band structure towards the Fermi level for small doping levels. The metallization is observed as the appearance of a hole-like band. A change of band shape is detected for larger doping levels, followed by a band splitting and a reorganization of the spectral distribution in the Fermi surface. These results are discussed in view of the different models proposed to understand the metallization of LCO and are compared to the case of the related cobaltate compound Na$_x$CoO$_2$.

References
Piezoelectric-driven uniaxial pressure cell for muon spin relaxation experiments
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We present a piezoelectric-driven uniaxial pressure cell operable at cryogenic temperatures, and optimized for muon spin relaxation and neutron scattering experiments. These methods often require larger sample sizes, and so the cell is designed to generate a force of up to ~1000 N. It incorporates calibrated displacement and force sensors, the combined knowledge of which can determine quickly whether the sample and its mounts remain within their elastic limits. An earlier version of this cell was presented in [1] and cells of the current design have accumulated use in multiple beamtimes [2], demonstrating its practicality. Data on Sr₂RuO₄ will be presented, showing achievement of a uniaxial stress of ~1.05 GPa within an active sample volume of 5 mm³. We anticipate this cell will be useful for a range of other materials, in which the Fermi surface or magnetic interaction strengths can be tuned leading to strong modifications of the electronic state.

References:
Ab-initio studies on NbO$_2$

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Niobium dioxide NbO$_2$ is a 4d transition metal oxide which exhibits two structural phases with different electronic properties. At ambient temperature NbO$_2$ is insulating with a body centered tetragonal (bct) crystal structure and a semi-conducting band gap, which amounts to 0.7 eV (indirect) and to at least 1 eV (direct). Upon heating NbO$_2$ transforms into the more symmetric rutile phase and becomes electrically conductive [1, 2]. Its metal-insulator transition can be excited both thermally and optically. While in the latter case the bct structure is conserved, the thermal phase transition is accompanied by a change of the crystal structure. Unlike its lower homologue, VO$_2$, NbO$_2$ exhibits this thermally induced metal-insulator transition not around room temperature, but at a considerably elevated value of $T_c = 1080$ K. This opens up the possibility to separate electronic and structural degrees of freedom and trigger the conductivity change also at a considerably lower temperature than $T_c$ by the optical excitation of only the electronic system, as observed experimentally in ref. [3].

We study the phases involved in this transition in detail by all-electron first-principles calculations with the programme code Questaal [4]. In particular, we investigate the ground-state properties by gradient-corrected density-functional calculations; upon excitation we include screening effects by quasi-particle self-consistent GW and excitonic effects with the Bethe-Salpeter equation on the RPA level.

As discussed on the basis of both experiments [1] and theoretical studies [2], NbO$_2$ behaves like a one-dimensional conductor in its metallic phase. We can confirm that result and find the conducting state to be composed of Nb 4d$_{xy}$-orbitals. We further observe one-dimensional Fermi-surface nesting in the rutile phase and conclude that NbO$_2$ is a Peierls-type material [4]. Regarding excitonic effects, we analysed the dielectric function, and the partial density of states.

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References
The role of the d_{xy} orbital in the nematic and superconducting state of FeSe

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The nematic state of the iron-based superconductors is associated with pronounced anisotropic electronic and magnetic properties, however its origin, mechanism and relationship to superconductivity are still subject of debate, both from the experimental and the theoretical point of view. Hitherto, nematic order in iron-based superconductors was thought to involve mainly d_{zx} and d_{yz} orbitals of the Fe atoms, arising either due to frustration of various magnetic instabilities (Ising nematic order) or due to a purely electronic (Pomeranchuk-like) instability, with the more strongly correlated d_{xy} orbitals assumed to play rather a secondary role. Here we propose a new scenario in which nematic order appears predominantly in the d_{xy}-orbitals. We show that, for the case of FeSe, this scenario solves several puzzles arising in recent experiments, such as the previously unexplained Fermi surface topological transition that occurs upon entering the nematic state. We find that this scenario can also describe both the ARPES and Quantum oscillation measurements of FeSe and the FeSe_{1-x}S_x systems and, furthermore, can account for the highly anisotropic momentum dependence of the superconducting gap. We then predict how the momentum dependence and size of this superconducting gap will evolve as nematicity is suppressed, e.g. via Sulphur doping, and suggest experiments which could detect the predicted Lifshitz transition. This result provides a quantitatively accurate model to study the tetragonal to nematic transition of FeSe and the FeSe_{1-x}S_x series and poses strong constraints on the possible mechanisms associated with the nematic instability.

References

Figure 1. Model of the Fermi surface of FeSe in (a) the tetragonal state, (b) the nematic state.
Quantum phase formation driven by multicritical Lifshitz transitions

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The role of van Hove singularities in the physics of strongly correlated materials has long been recognised as a key driver in stabilising new quantum phases. One of the most well-known basic mechanisms is encapsulated in the physics of Stoner ferromagnetism where a peak in the density of states combined with strong electronic correlations is critically driving phase formation. Early on, Rhodes and Wohlfarth realised that a key criterion for phase formation does not only depend on the magnitude but also shape of the singularity.

In my talk I will discuss how this insight can be utilised to control the impact of van Hove singularities on phase formation through controlled symmetry breaking via the concept of multicritical Lifshitz transitions [1]. In particular, I will demonstrate how through this mechanism one can strongly enhance the divergence of a van Hove singularity from e.g. a logarithm to effectively a power law divergence in the relevant energy regime. In the first part of the talk I will focus on the unique insights these concepts provide into the phase formation occurring in the vicinity of the metamagnetic quantum critical end point of Sr$_3$Ru$_2$O$_7$. In the second part of the talk I will give an outlook on how multicritical Lifshitz transitions potentially play a role in related ruthenates [2] and an overview of a range of other material classes in which they occur naturally, warranting further investigation.

References
Direct observation of a uniaxial stress-driven Lifshitz transition in Sr$_2$RuO$_4$

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Application of uniaxial pressure has recently been shown to more than double the transition temperature of the unconventional superconductor Sr$_2$RuO$_4$, leading to a peak in $T_c$ versus strain whose origin is still under debate. Here we develop a simple and compact method to apply large uniaxial pressures in a way compatible with angle-resolved photoemission. We directly visualize how uniaxial stress drives a Lifshitz transition of the $\gamma$-band Fermi surface, pointing to the key role of strain-tuning its associated van Hove singularity to the Fermi level in mediating the peak in $T_c$. Our measurements provide stringent constraints for theoretical models of the strain-tuned electronic structure evolution of Sr$_2$RuO$_4$. Furthermore, our experimental approach opens the door to future studies of strain-tuned phase transitions where large pressure cells or piezoelectric-based devices may be difficult to implement.