

3rd QMA retreat

Book of abstracts

12th - 14th October 2022

Friedrichroda



ct.qmat

**Complexity and Topology
in Quantum Matter**

Session 1

Nonlinear dynamics of Dirac fermions in topological HgTe structures

Tatiana Aureliia Uaman Svetikova

Helmholtz-Zentrum Dresden-Rossendorf

High harmonic generation (HHG) has applications in various fields, including ultrashort pulse measurements, material characterization and imaging microscopy. Strong THz nonlinearity and efficient third harmonic generation (THG) were demonstrated in graphene [1], therefore it is natural to assume the presence of the same effect in other Dirac materials, such as topological insulators (TI). Topological states can be found in HgTe quantum wells with a thickness of more than 6.3 nm [2], and strained 3D Hg_{1-x}Cd_xTe thin films with cadmium fraction $x < 0.16$ [3].

We used a series of HgTe samples corresponding to three qualitatively different cases: 2D trivial and topological structures and 3D topological insulators. By using moderate THz fields, the presence of highly efficient THG was measured in these samples at different temperatures and THz powers. This provides insight into physical mechanisms leading to THG in TIs. For in-depth understanding of Dirac fermions dynamics and dominating scattering mechanisms in HgTe TI, we conducted THz pump-probe experiments that reveal several relaxation time scales.

[1] Hafez, H. A. et al., Nature 561, 507 (2018).

[2] Bernevig, B. et al. Science 314, 5806 (2006): 1757-1761.

[3] Brüne, C., et al. Phys. Rev. Lett. 106, 12 (2011): 126803.

Nontrivial gapless electronic states at the stacking faults of weak topological insulators

Gabriele Naselli

IFW Dresden

Lattice defects such as stacking faults may obscure electronic topological features of real materials.

Motivated by recent experiments on three-dimensional (3D) topological systems, we examine the effect of stacking faults on the electronic properties of weak topological insulators (WTIs).

Working with a simple model consisting of a 3D WTI formed by weakly-coupled two-dimensional (2D) topological layers separated by trivial spacers, we find that 2D stacking faults can carry their own, topologically nontrivial gapless

states.

Depending on the WTI properties, as well as the way in which the stacking fault is realized, the latter can form a topologically protected 2D semimetal, but also a 2D topological insulator which is embedded in the higher-dimensional WTI bulk.

This suggests the possibility of using stacking faults in real materials as a source of topologically nontrivial, symmetry-protected conducting states.

Investigating the transition from 2D to 3D topological insulators in magneto-optics

Leonid Bovkun

JMU Würzburg

Topological properties of (Hg,Cd)Te material systems are directly connected to edge or surface states. It is essential to understand the band structure of the bulk material to be able to clearly assign the regime in which the topological phase occurs. Magneto-optical transmission experiments provide information on transitions between Landau levels across the electrochemical potential, allowing accurate reconstruction of the energy spectrum calculated theoretically in the $k \cdot p$ model.

While the observed experimental features qualitatively match axial calculations, particular features require further improvement in the model. The magneto-optical response and the energy spectrum for thicknesses near 30 nm shed more light on (the physics at) the crossover between 2D and 3D topological insulators.

Obstruction on the triangular lattice

Philipp Eck

JMU Würzburg

Stimulated by the discovery of the triangular Quantum Spin-Hall Insulator (QSHI) indenene on SiC, I will discuss a variety of topological phases on the triangular lattice ranging from non-trivial \mathbb{Z}_2 over higher-order topology to obstructed QSHI-phases. They are stabilized by the interplay of symmetry breaking and local Spin-Orbit Coupling (SOC). In the presence of strong reflection symmetry breaking, the localization of the Wannier centers detaches from the atomic lattice resulting in an obstructed atomic limit with higher-order topology. Further, I will establish one-to-one correspondence between the valley Dirac fermions of the triangular lattice and Kane-Mele-type honeycomb systems, albeit being gapped with atomic SOC, a key ingredient towards large-gap QSHIs and room temperature applications.

Session 2

Magnetocaloric effect in $(\text{La,Ce})(\text{Fe,Si,Mn})_{13}$ with tunable, low transition temperature

Marc Straßheim

Helmholtz-Zentrum Dresden-Rossendorf

Lattice defects such as stacking faults may obscure electronic topological features of real materials.

Motivated by recent experiments on three-dimensional (3D) topological systems, we examine the effect of stacking faults on the electronic properties of weak topological insulators (WTIs).

Working with a simple model consisting of a 3D WTI formed by weakly-coupled two-dimensional (2D) topological layers separated by trivial spacers, we find that 2D stacking faults can carry their own, topologically nontrivial gapless states.

Depending on the WTI properties, as well as the way in which the stacking fault is realized, the latter can form a topologically protected 2D semimetal, but also a 2D topological insulator which is embedded in the higher-dimensional WTI bulk.

This suggests the possibility of using stacking faults in real materials as a source of topologically nontrivial, symmetry-protected conducting states.

Frequency-resolved functional renormalization group for quantum magnetic systems

Janik Potten

JMU Würzburg

Strongly correlated materials are one of the most prolific topics of contemporary condensed matter physics. Within this field, the functional renormalization group (FRG) approach for spin models relying on a pseudo-fermionic description has proven to be a very powerful technique in simulating ground state properties of strongly frustrated magnetic lattices. However, the FRG as well as many other theoretical models, suffer from the fact that they are formulated in the imaginary-time Matsubara formalism and thus are only able to predict static correlations directly. Nevertheless, describing the dynamical properties, especially of magnetic systems is one of the fundamental theoretical challenges, as they are the key to bridging the gap to experimental data from neutron scattering experiments.

For the pseudo-fermion FRG (pf-FRG), we remedy this shortcoming by establishing a methodical approach based on the Keldysh formalism, originally developed to handle non-equilibrium physics. It directly formulates the problem using real time arguments or frequencies by introducing a time contour that allows for both forward and backward evolving particles and thus the calculation of retarded correlation functions.

This novel approach, combining pf-FRG and Keldysh formalism, allows for calculating the dynamic properties of spin systems on arbitrary lattices. We can identify the correct low-energy behavior of the dynamic spin structure factors for exemplary nearest neighbor Heisenberg systems. These first results are promising and extensions of this work might allow for an easy calculation of dynamic properties even for non-equilibrium magnetic systems in the future.

Triple-Q order in $\text{Na}_2\text{Co}_2\text{TeO}_6$ from proximity to hidden-SU(2)-symmetric point

Wilhelm Krüger

TU Dresden

The frustrated honeycomb material $\text{Na}_2\text{Co}_2\text{TeO}_6$ is proposed as an approximate Kitaev magnet. The spin-wave spectrum obtained by inelastic neutron scattering shows characteristic low-energy branches which indicate triple-Q magnetic order in this material. We argue that the underlying microscopic model is close to a hidden SU(2)-symmetric point. By using linear spin-wave theory, we demonstrate the evidence of ring exchange in order to reproduce the qualitative features of the experiment, including its surprisingly-high symmetry and the dispersive low-energy and flat high-energy bands. Our result demonstrates the importance of bond-dependent interactions in cobaltates.

Session 3

Phase diagram of a Kondo heterostructure

Zihong Liu

JMU Würzburg

We consider a two-dimensional quantum spin system described by a Heisenberg model embedded in a three dimensional metal. The two systems couple via an antiferromagnetic Kondo coupling. In such a setup, the ground state generically remains metallic down to the lowest temperatures and allows us to study magnetic quantum phase transitions in metallic environments. From the symmetry point of view translation symmetry is present in two out of three lattice directions such that crystal momentum is only partially conserved. Importantly, the construction provides a route to study, with negative sign free auxiliary field quantum Monte Carlo methods, the physics of local moments in metallic environments. Our large scale numerical simulations show that as a function of the Kondo coupling, the system has two metallic phases. In the strong coupling limit, a heavy fermion phases emerges. Here the spin degree of freedom is screened by means of the formation of a composite quasiparticle that participates in the Luttinger count. At weak coupling magnetic order is present. This phase is characterized by Landau damped Goldstone modes. Furthermore, the aforementioned composite quasiparticle remains intact across the quantum phase transition.

Marginal Fermi Liquid in Kondo heterostructures

Bernhard Frank

TU Dresden

We study a Kondo heterostructure created by embedding a layer of magnetic moments into a three dimensional metal. Using Quantum Monte Carlo simulations we identify a novel metallic quantum critical point which separates an antiferromagnetic phase from a nonmagnetic phase. Moreover, the Fermions form a marginal Fermi liquid without typical Landau quasiparticles. These result in an anomalous temperature dependence of the electric resistance of the sample.

Kondo interaction of quantum spin Hall edge channels with charge puddles

Christopher Fuchs

JMU Würzburg

Under time reversal symmetry, quantum spin Hall edge channels are protected against elastic backscattering. However, even for samples which exhibit conductance quantization due to the quantum spin Hall effect, reproducible fluctuations shape the quantization plateau when the chemical potential is tuned through the bulk gap. Here, we examine those fluctuations in micron-sized HgTe quantum well devices. By performing temperature and gate-dependent measurements, we conclude that "charge puddles" in the narrow gap material have a Kondo-type interaction with the edge channels resulting in the observed conductance fluctuations. Our results provide insight into the underlying mechanisms of scattering in quantum spin Hall edge channels.

An intermediate-scale theory for electrons coupled to frustrated

local-moments

Adam McRoberts

MPI-PKS Dresden

A classic route for destroying long-lived electronic quasiparticles in a weakly interacting Fermi liquid is to couple them to other low-energy degrees of freedom that effectively act as a bath. We consider here the problem of electrons scattering off the spin fluctuations of a geometrically frustrated antiferromagnet, whose non-linear Landau-Lifshitz dynamics, which remains non-trivial at all temperatures, we model in detail. At intermediate temperatures and in the absence of any magnetic ordering, the fluctuating local-moments lead to a non-trivial angular anisotropy of the scattering-rate along the Fermi surface, which disappears with increasing temperature, elucidating the role of "hot-spots". Over a remarkably broad window of intermediate and high temperatures, the electronic properties can be described by employing a local approximation for the dynamical spin-response. This we contrast with the more familiar setup of electrons scattering off classical phonons, whose high-temperature limit differs fundamentally on account of their unbounded Hilbert space. We place our results in the context of layered magnetic delafossite compounds.

Session 4

Spin polarized ballistic transport: MONA on the Rashba-split BiAg₂ surface alloy

Markus Leisegang
JMU Würzburg

Transport measurements that are sensitive to the band structure of a material require techniques that operate on the length scale of the charge carriers mean free path. A novel method that fulfills this requirement is the molecular nanoprobe (MONA), which uses a single molecule to detect charge carriers [1]. In this study, we utilize the accompanied rotation and tautomerization of phthalocyanine on the ($\sqrt{3} \times \sqrt{3}$)Bi/Ag(111)R30° surface to investigate transport in a Rashba-split surface state. We find that both processes are driven by the N-H stretching mode, which can be triggered by a single-electron excitation [2]. Our transport measurements prove the sensitivity to hot charge carriers which propagate preferably in the Rashba-split surface state of the BiAg₂ alloy. Comparison of the tautomerization rates observed for the different rotational states of the molecule reveals that the phthalocyanine molecule exhibits two different faces with distinct excitation probabilities. Measurements with a spin-polarized tip predict the detection of spin-momentum locked transport in the surface state of the Rashba alloy.

[1] M. Leisegang et al., *Nano Lett.* 18, 2165–2171 (2018)

[2] J. Kügel et al., *Journ. Phys. Chem. C* 121, 28204–28210 (2017)

Interference of superconducting quasiparticles observed by STM with extra- spatial and energy resolution

Artem Odobesko
JMU Würzburg

In this work, we attach CO molecule to the superconducting STM tip apex to maximize the spatial resolution and keep at the same time high energy resolution. With such multi-functionalized STM tip we probe the spatial LDOS distribution of YSR bound states around the magnetic dimer, consisting of the two coupled Fe atoms placed on Nb(110) surface. The last results into hybridization of YSR bound states, that can be treated as symmetric and antisymmetric combinations of the YSR excitation at the single magnetic impurity. Using new multi-functionalized probe we are able to map both the

symmetric and antisymmetric interference pattern of hybridized YSR wave functions in vicinity of Fe dimer, that in turn carries information about the structure of the Nb(110) Fermi surface. By comparison with measurements of the same magnetic dimer using common superconducting probe, we demonstrate an extraordinary spatial sensitivity combined with high energy resolution with new multi-functionalized probes.

**Magnetization of the Exact Dimer Ground State in the Maple Leaf Model:
interactions, correlated hopping, and bound states**

Pratyay Ghosh

JMU Würzburg

We present here the exact dimer ground state of a quantum antiferromagnet on the maple-leaf lattice [1]. A coupling anisotropy for one of the three inequivalent nearest-neighbor bonds is sufficient to stabilize the dimer state. Together with the Shastry-Sutherland Hamiltonian [2], we show that this is the only other model with an exact dimer ground state for all two-dimensional lattices with uniform tilings.

We construct an effective Hamiltonian for the magnetic particles by treating magnetic excitations generated by an external magnetic field as bosons. Magnetization plateaus are created when anisotropic repulsions between the bose particles produce "insulating" spin density wave (SDW) states with particular structures. Altering the magnetic field causes supersolid phases to form around insulating SDW phases. The characteristics of these supersolid phases are thoroughly addressed. We also show the dynamics of magnetic excitations and the lattice geometry plays a crucial role and novel multi-particle bound states condense at very low magnetization.

[1] P. Ghosh, T. Mueller, R. Thomale, Phys. Rev. B 105, L180412 (2022)

[2] B. S. Shastry and B. Sutherland, Physica B+C 108, 1069 (1981)

Session 5

On the emergence of geometry in a quantum system

Moritz Dorband

JMU Würzburg

Recently, a new approach to understand aspects of the AdS/CFT duality in terms of von Neumann algebras has been discussed, in particular explaining the notion of time as an emergent quantity. Starting from these field theoretic analyses, we aim to obtain a better understanding of the holographic duality, in particular its applicability to quantum mechanical systems. As a first step toward this long-term goal, we study the entanglement properties associated with the geometry of the phase space of an N -component quantum system. We discuss thermodynamic limits, namely the large N limits of these models and determine to what extent the entanglement structure of these quantum mechanical systems bears similarities with that of a black hole spacetime, purely in terms of the aforementioned algebraic properties. By this geometric characterisation, we also find a clear distinction between the algebras at large N and at finite N . This distinction between the algebras can explain nicely the fundamental difference between classical and quantum gravity.

Horizon physics of quasi-one- dimensional tilted Weyl cones on a lattice

Viktor Könye

IFW Dresden

To simulate the dynamics of massless Dirac fermions in curved spacetimes with one, two, and three spatial dimensions we construct tight-binding Hamiltonians with spatially varying hoppings. These models represent tilted Weyl semimetals where the tilting varies with position, in a manner similar to the light cones near the horizon of a black hole. We illustrate the gravitational analogies in these models by numerically evaluating the propagation of wave packets on the lattice and then comparing them to the geodesics of the corresponding curved spacetime. We also show that the motion of electrons in these spatially varying systems can be understood through the conservation of energy and the quasi-conservation of quasimomentum. This picture is confirmed by calculations of the scattering matrix, which indicate an exponential suppression of any noncontinuous change in the quasimomentum. Finally, we show that horizons in the lattice models can be constructed also at finite energies using specially designed tilting profiles.

Thermalization by a synthetic horizon

Lotte Mertens

IFW Dresden

Synthetic horizons in models for quantum matter provide an alternative route to explore fundamental questions of modern gravitational theory.

Here, we apply these concepts to the problem of emergence of thermal quantum states in the presence of a horizon, by studying ground-state thermalization due to instantaneous horizon creation in a gravitational setting and its condensed matter analogue.

By a sudden quench to position-dependent hopping amplitudes in a one-dimensional lattice model, we establish the emergence of a thermal state accompanying the formation of a synthetic horizon. The resulting temperature for long chains is shown to be identical to the corresponding Unruh temperature, provided that the post-quench Hamiltonian matches the entanglement Hamiltonian of the pre-quench system.

Based on detailed analysis of the outgoing radiation we formulate the conditions required for the synthetic horizon to behave as a purely thermal source, paving a way to explore this interplay of quantum-mechanical and gravitational aspects experimentally.

Session 6

Disentangling the Emerging Physics in Topological van-der-Waals Heterostructures

Philipp Kagerer

JMU Würzburg

Starting with Graphene as the first 2D-material suitable for electronic applications [1] it has always been the longstanding vision to stack multiple 2D materials in order to enable new emerging physics from their interaction. With the discovery of topological insulators, often realized in van-der-Waals crystals [2] and 2D-magnets the variety of available materials for this approach has increased significantly.

By using MBE, we have grown heterostructures [3,4], consisting of the prototypical TI Bi₂Te₃, its intrinsic magnetic counterpart MnBi₂Te₄ and the novel high T_c 2D magnet Fe₃GeTe₂. Using both angle-resolved photoemission spectroscopy (ARPES) and x-ray magnetic circular dichroism (XMCD), we investigate the interplay of topology and magnetism as well as the coupling of multiple magnetic layers along the stacking direction of our van-der-Waals planes. Helping to understand the interplay of the components, our results pave the way towards a more complex device design in magnetic topological structures, potentially spanning the entire phase diagram of topology, superconductivity and magnetism.

[1] Novoselov, K.S. et al., Science 306, 5696 (2004)

[2] Zhang, H.J. et al., Nat. Phys. 5, 6 438-442 (2009)

[3] Kagerer et al., J. Appl. Phys. 128, 135303 (2020)

[4] Kagerer et al., arXiv 2207.14421 (2022)

Observation of cnoidal wave localization in non-linear topoelectric circuits

Hendrik Hohmann

JMU Würzburg

Topological phases have been realized in a variety of classical metamaterials providing easily accessible platforms to study topology in regimes beyond experimental limitations imposed by quantum mechanical systems.

As of yet, the majority of investigated models are of linear nature — introducing non-linear effects promises new intriguing phenomena, such as solitons and chaos.

To study the intertwining of topology and non-linearity we engineered a

topoelectrical circuit reminiscent of the SSH-model, supplemented by variacap diodes with voltage dependent capacitances inducing on-site non-linearity. We observe the localized cnoidal (LCn) state by feeding a sinusoidal voltage excitation around midgap frequencies into the end of the the circuit. This state maintains the spatial exponential localization of the SSH edge mode while distorting the sinusoidal input into eccentric waves in time domain.

This novel phenomenon is described theoretically within a joined formalism of the non-linear Korteweg-de Vries equation sustaining soliton and cnoidal wave solutions, and SSH-type localization.

Mott insulators with boundary zeros

Niklas Wagner

JMU Würzburg

In the recent literature, the concept of topological Mott insulators has been spelled out in quite different ways. Most of the proposed realizations rely either on Hartree-Fock approximations or on appropriately defined auxiliary degrees of freedom. I will present a novel, remarkably simple way of describing a topological Mott insulator without long-range order based on the topological properties of their Green's function zeros in momentum space. After discussing the fate of the bulk-boundary correspondence in these systems, I will show how the zeros can be seen as a form of "topological antimatter" with distinctive features associated to the annihilation with conventional topologically protected edge modes.

Posters

P01: NMR investigations of the 2D Heisenberg system CuPOF under pressure

Florian Bärtl

Helmholtz-Zentrum Dresden-Rossendorf

The molecular-based material $(\text{Cu}(\text{pz})_2(2\text{-OHpy})_2)(\text{PF}_6)_2$ (CuPOF) is an excellent realization of a two-dimensional square-lattice $S=1/2$ Heisenberg antiferromagnet, with intralayer and interlayer exchange-coupling constants of $J/k_B = 6.8$ K and $J' \sim 10^{-4}J$, respectively. Previously reported NMR data revealed a low-temperature transition to commensurate antiferromagnetic (AFM) quasistatic long-range order (LRO), with a preceding crossover from Heisenberg to anisotropic XY behavior. We present further NMR studies of the low-temperature correlations in magnetic fields up to 7T and temperatures down to 0.3K. The application of hydrostatic pressure up to 10kbar changes the interlayer coupling and, therefore, the magnetic correlations in the critical regime. The transition regime is probed by ^1H and ^{31}P spectroscopy and relaxometry, revealing a monotonic change of T_N with increasing pressure. The AFM LRO below T_N persists at high pressures, as revealed by a splitting of the ^1H NMR lines, stemming from the broken symmetry of the local spin polarization in the LRO regime.

P02: Quench-Probe Setup as an Analyzer of Fractionalized Entanglement Spreading

Nicolas Bauer

JMU Würzburg

We propose a novel spatially inhomogeneous setup for revealing quench-induced fractionalized excitations in entanglement dynamics. In this quench-probe setting, the region undergoing a quantum quench is tunnel-coupled to a static region, the probe. Subsequently, the time-dependent entanglement signatures of a tunable subset of excitations propagating to the probe are monitored. We exemplify the power of this generic approach by identifying a unique dynamical signature associated with the presence of an isolated Majorana zero mode in the post-quench Hamiltonian. In this case excitations emitted from the topological part of the system give rise to a fractionalized jump of $\log(2)/2$ in the entanglement entropy of the probe. This dynamical effect is highly sensitive to the localized nature of the Majorana zero mode, but does not require the preparation of a topological initial state.

P03: Symmetry, Structural and Electronic Correlations in a Family of Bismuth-based Layered Materials

Eduardo Carrillo-Aravena

TU Dresden

Topological insulators (TIs) are semiconductors with protected electronic surface states that allow dissipation-free transport. They are proposed as ideal materials for spintronics and quantum computing.

The first verified 3D weak TI, Bi₁₂Rh₃I₉, consists of two types of alternating charged layers. The anionic layer of edge-sharing [Bi₂I₈]²⁻ octahedra and the topological non-trivial layer [Bi₁₂Rh₃I]²⁺. The latter determines the electronic states with inverted parity around the Fermi level and consists of a net of edge-sharing Rh-centered Bi cubes forming a prismatic rhombitrihexagonal honeycomb lattice, with an iodide ion at the center of each hexagonal prism.

The TI layer has been observed in the structurally similar, but topologically trivial compounds Bi₁₃Pt₃I₇ and Bi₁₂Pt₃I₅ that contain a different spacer, stacking sequence and electron count. Therefore, it was found that the anionic spacer played a decisive role in defining whether the topological properties of the material would be trivial or not.

Herewith, we present the structure and properties in a series of layered materials derived from those mentioned above: Bi₁₂Rh₃Cu₂I₅(1)[8] (Figure 2), Bi₁₂Rh₃Ag₂I₅(2), Bi₁₂Pt₃CuI₅(3), Bi₁₂Pt₃AgI(4) and Bi₁₂Rh₃Ag₆I₉(5). For those compounds, the TI layer is left unchanged, while the spacer layer is substituted for studying its impact on the topological properties. Full-relativistic DFT studies in conjunction with ARPES have shown a relationship between the size of the bulk bandgap and the thickness and chemical nature of the spacer layers. Structural characterization of these materials is challenging not only because of stacking faults – intrinsic to their layered structure – but also atomic disorder within the spacer layers. Furthermore, twinning by pseudo-merohedry is common for 1, 2, 3 and 4, all of which share highly specialized metrics close to a hexagonal cell, but orthorhombic or monoclinic space groups.

P05: Finite and Infinite Chains of an Iron Analogue of Heavy Atom Clusters

Maria Herz

TU Dresden

"During the search for new topological insulators[1] with magnetic properties, the novel subiodides Fe[PtBi₆I₁₂] and (Fe,Bi)[PtBi₆I₁₂] were discovered following the reaction of Bi with Fe, Pt and BiI₃ above 300 °C. The shiny, black, air insensitive crystals that were yielded from this reaction consist of alternating cuboctahedral [PtBi₆I₁₂]²⁻ clusters and Fe²⁺ cations in an octahedral coordination between trigonal faces of two cuboctahedra, which concatenate them into linear chains, which makes it an analogue to the

compounds $\text{Pb}[\text{PtBi}_6\text{I}_{12}]$ [2] and $\text{Sn}[\text{PtBi}_6\text{I}_{12}]$ [3]. Additionally, the crystals' cube-like morphology originates from six weaker Bi...I inter-cluster bridges per cluster connecting the chains. This, in combination with the composition of predominantly heavy elements, and hence a strong spin-orbit coupling within the compound, lead to the hope that the information obtained about the band gap could lead to this being fine-tuned and reduced in order to apply to other compounds and obtain compounds with both topological and magnetic properties."

[1] a) M. Z. Hasan, C. L. Kane, *Rev. Mod. Phys.* 2010, 82, 3045; b) Y. Ando, *J. Phys. Soc. Jpn.* 2013, 82.

[2] M. A. Herz, M. Knies, K. Finzel, M. Ruck, *Z. Anorg. Allg. Chem.* 2020, 647, 53.

[3] M.A. Herz, K. Finzel, M. Ruck, *Z. Anorg. Allg. Chem.* 2022, e202200080.

P06: Bismuth-rich Stacked Topological Insulator Candidates: Structural and Electronic Properties

Johannes Heßdörfer

JMU Würzburg

The electronic and structural properties of weak topological insulator (TI) candidates are investigated by varying techniques including angle-resolved photoelectron spectroscopy (ARPES), scanning tunneling microscopy (STM) and density functional theory calculations. The compounds consist of alternating layers of a 2D TI in a Kagome configuration, separated by insulating spacer layers. The Kagome net is formed by rhodium/platinum centered bismuth cubes, while the spacer consists of iodine and silver or copper.

P07: Band structure and effective masses of the topological semimetal PdGa

Freya Husstedt

Helmholtz-Zentrum Dresden-Rossendorf

De Haas-van Alphen (dHvA) measurements at low temperatures and fields up to 18 T provided insight into the band structure of the topological semimetal PdGa which is presented in this poster. Previous investigation of PtGa revealed the topological character [1] of this sister compound of PdGa.

Hence, angle-resolved measurements of the dHvA effect were performed on PdGa and showed a good agreement with the calculated band structure. This revealed a multitude of Fermi surfaces and eight spin-split bands crossing the Fermi energy. In particular, the calculations show a similar band structure as for PtGa, including two topologically protected multifold degenerate band-touching nodes. Furthermore, we analyzed the temperature dependence

of the dHvA oscillations to determine the effective masses for field aligned along the crystallographic [100] axis. The low masses also show a good agreement to the calculations and, therefore, indicate insignificant correlations of the electrons.

[1] M. Yao, K. Manna et al., Nat. Commun. 11, 2033 (2020).

P09: Doping of 1D topologically protected edge states on the (001) surface of the topological crystalline insulator (Pb,Sn)Se

Florian Keller

JMU Würzburg

Topological crystalline insulators (TCI) are a class of materials with topological protected surface states protected by crystalline symmetry. A particularly popular representative of this material class is (Pb,Sn)Se which exhibits four Dirac cones per Brillouin zone. It has been shown that surface step edges with a height equivalent to an odd number of atomic layers results in a topologically protected one-dimensional edge state which is characterized by a peak at the Dirac energy [1].

Theoretical analysis suggests that this state is caused by the broken translation-invariance at the step edge and originates from flat-dispersing bands which connect pairs of surface Dirac nodes [1]. Due to intrinsic doping, the energy of the edge modes of as-grown crystals is usually well separated from the Fermi level. Here we investigate the behavior of these one-dimensional edge modes during Fe surface doping. Since Fe donates charge to p-doped PbSnSe, it results in a downwards-bending of the surface band structure. We observe a peak splitting as the Dirac energy gets close to the Fermi level. We discuss the potential origins of this observation in terms of electron correlations.

[1] Sessi, Paolo, Science 354, 6317 (2016)

P12: Phase transitions in the two-dimensional Su-Schrieffer-Heeger model

Changan Li

JMU Würzburg

The two-dimensional Su-Schrieffer-Heeger model is endowed with rich topological physics. First we show that the random flux can induce a metal-insulator transition in the two-dimensional Su-Schrieffer-Heeger model, thus reporting the first example of such a transition. Remarkably, we find that the resulting insulating phase can even be a higher-order topological insulator

with zero-energy corner modes and fractional corner charges. Employing both level statistics and finite-size scaling analysis, we characterize the metal-insulator transition and numerically extract its critical exponent. By proposing another inclined two-dimensional Su-Schrieffer-Heeger, a deformed one, we show that a pair of Dirac points protected by space-time inversion symmetry appear in the semimetallic phase. Remarkably, the locations of these Dirac points are not pinned to any high-symmetry points of the Brillouin zone but highly tunable through parameter modulations. Moreover, the merging of two Dirac points undergoes a topological phase transition, which leads to either an anisotropic topological insulating phase or a nodal-line metallic phase. We provide a systematic analysis of these topological phases from both bulk and boundary perspectives combined with symmetry arguments.

P13: Bose–Einstein Condensation in non-Hermitian dilute Bose gas

Eduard Naichuk

JMU Würzburg

We study Bose-Einstein condensation in non-Hermitian dilute Bose gas. The non-Hermiticity is encoded in PT-symmetric terms. We can express particle density in terms of Green's function and separate the condensate part. This allows us to obtain an expression for the critical temperature in the ideal case and study the behaviour of the condensate density for zero temperature in the case of an interacting gas. We argue that condensation in case of interacting gas is possible only for the case of spontaneously broken PT-symmetry.

P14: Magnetocaloric effect in Tb₃Ni studied in high magnetic fields for cryogenic applications

Timo Niehoff

Helmholtz-Zentrum Dresden-Rossendorf

Tb₃Ni exhibits a large variety of temperature and magnetic field dependent phase transitions in a temperature range of 3–90 K. This gives rise to a very competitive conventional magnetocaloric effect and an inverse magnetocaloric effect at very low Temperature. These properties make this material an interesting candidate for magnetic refrigeration applications in the gas liquefaction temperature range. In this work, we present a comprehensive analysis of the magnetocaloric effect in a Tb₃Ni single crystal in pulsed magnetic fields up to 50 T and by heat capacity measurements.

P15: Landau level collapse in graphene in the presence of in-plane radial electric and perpendicular magnetic fields

Ihor Nimyi
IFW Dresden

It is known that in two-dimensional relativistic Dirac systems placed in orthogonal uniform magnetic and electric fields, the Landau levels collapse as the applied in-plane electric field reaches a critical value $\pm E_c$. We study this phenomenon for a distinct field configuration with in-plane constant radial electric field. The Dirac equation for this configuration does not allow analytical solutions in terms of known special functions. The results are obtained by using both the WKB approximation and the exact diagonalization and shooting methods. It is shown that the collapse occurs for positive values of the total angular momentum quantum number, the hole (electron)-like Landau levels collapse as the electric field reaches the value $+(-)E_c/2$. The investigation of the Landau level collapse in the case of gapped graphene shows a number of distinctive features in comparison with the gapless case.

P16: Observation of non-Hermitian topology in a multi-terminal quantum Hall device

Kyrylo Ochkan
IFW Dresden

One of the simplest examples of non-Hermitian topology is encountered in the Hatano-Nelson (HN) model, a one-dimensional chain where the hopping in one direction is larger than in the opposite direction.

Starting from this model, we present here the first experimental observation of non-Hermitian topology in a quantum condensed-matter system.

We use a multi-terminal quantum Hall device, obtained by placing a high mobility GaAs/AlGaAs two-dimensional electron gas ring under a perpendicular magnetic field. The conductance matrix that connects the currents flowing from the active contacts to the ground with the voltage of the active contacts is topologically equivalent to the HN Hamiltonian. In the limit of maximal nonreciprocity, when the hopping in one direction vanishes identically, the HN Hamiltonian effectively describes a one-dimensional, unidirectionally propagating mode, which constitutes a direct link to the edge modes of the quantum Hall effect.

In our device, we directly measure and evidence the non-Hermitian skin effect. We also compute for our experimental device two topological invariants that are related to the skin effect. These invariants are more robust than the Chern number, since they remain well-quantized also across quantum Hall plateau

transitions. We also use the unique properties of our system and realize, in a single device, both open and periodic boundary conditions, as well as smooth tuning between these two conditions, showing the high potential of this kind of device for the investigation of non-Hermitian, topological physics.

P17: 2D van-der-Waals Heterostructures

Burak Özer

IFW Dresden

Research on two-dimensional atomic crystals and especially on graphene is intense and is likely to remain one of the leading topics in condensed matter physics and materials science for many years. Looking beyond this field, materials can be reassembled into heterostructures made layer by layer with help of their van der Waals properties.

The first, already remarkably complex, heterostructures so-called van der Waals heterostructures have been developed since 2013, and it's still revealing their unusual properties.

In this poster, I will focus on 2D materials and how to produce heterostructures. In general, what I will show you is how to go from the 3D system to the 2D through exfoliation and how I can reconstruct artificial heterostructures by mechanically stamping flakes of different materials onto each other.

P18: Zoology of charge orders in the electron-doped cuprates

David Riegler

JMU Würzburg

P19: Protecting quantum spin Hall insulator (QSHI) from air via intercalation into graphene/SiC

Cedric Schmitt

JMU Würzburg

In the search for new quantum materials, ultrathin metals are interesting as they push bulk properties to the 2D limit and foster novel quantum effects. Unfortunately, these systems are prone to oxidation in air, making them useless for quantum transport devices. Metal intercalation is a relatively new capping method, that utilizes graphene, an inert quantum material that can be easily produced by heating of a SiC substrate [1,2]. Hereby, the metal is intercalated between the SiC/graphene layer, thus forming freestanding graphene, which is

believed to protect the intercalated layers against oxidation [3]. Hitherto studies focused mainly on identifying stable allotropes but lacking a detailed investigation of metal coverage and oxidation [3]. Here, we study the intercalation of indenene, a recently discovered QSHI on a triangular lattice [4]. First experiments indicate the indium layer to remain intact upon air exposure, indeed pointing to an effective protective function of the overlayer graphene.

- [1] K. S. Novoselov et. al. *Science* 306, 666 (2004)
- [2] C. Berger et. al. *J. Phys. Chem. B* 108, 19912 (2004)
- [3] N. Briggs et al. *Nat. Mater.* 19, 637-643 (2020)
- [4] M. Bauernfeind et al. *Nat. Commun.* 12, 5396 (2021)

P20: Unveiling non-trivial topology in Weyl semimetals by photoemission

Jakub Schusser

JMU Würzburg

By performing angle-resolved photoemission spectroscopy (ARPES) on the paradigmatic Weyl semimetals TaP and TaAs, we reveal spectroscopic manifestations of the Berry flux monopoles in the intensity distribution of the photoelectrons. This is confirmed over a broad range of excitation energies, ranging from the surface-sensitive vacuum ultraviolet (VUV) to the more bulk-sensitive soft X-ray (SX) regime. Our experimental observations were complemented by state-of-the-art first principle photoemission calculations based on the one-step model of photoemission and density functional theory (DFT) which allow us to clearly disentangle surface resonances from real surface states close to Fermi level. We further show the drawbacks of the existing ARPES-based criteria used to determine the surface-projected Weyl point chirality. Instead, we suggest an improved approach, namely the use of dichroic ARPES measurements. Lastly, we discuss the importance of proper final state description in the context of ARPES combined with linear and circular dichroism.

P21: Fermi-surface investigation of CaCdGe and CaCdSn

Valentin Schwarze

Helmholtz-Zentrum Dresden-Rossendorf

CaCdSn and CaCdGe are nodal-line semimetal candidate materials. Band-structure calculations [A, B] show for both systems non-topological and topological valence bands with the nodal band-crossings above the Fermi level. Previous measurements of the magnetoresistance provide some support for the topological nature of the materials. Here, we present our investigation of the

Fermi surfaces of CaCdSn and CaCdGe by use of de Haas-van Alphen measurements and band-structure calculations. Our measurements reveal many quantum-oscillation frequencies, which are not predicted by calculations. This discrepancy calls the calculated band structures [A, B] and, thus, the precise nature of the topology of these systems into question.

[A] A. Laha et al., Phys. Rev. B 102, 035164 (2020).

[B] E. Emmanouilidou et al., Phys. Rev. B 95, 245113 (2017).

P22: Quantum transport on anisotropic surfaces revealed by MONA

Manuel Seitz

JMU Würzburg

The ability to detect how charge carriers propagate in well defined bands is of great importance for the exploitation of novel materials, e.g, in the context of spintronics or topological insulators. In order to probe this quantum transport we developed the molecular nanoprobe (MONA) technique [1] which utilizes a single molecule to detect ballistic charge carriers injected by the tip of a scanning tunneling microscope (STM). In this study, we investigate charge carrier transport in the structurally anisotropic Cu(110) surface which exhibits a surface state at the Y-point of the surface Brillouin zone[2]. By performing directional- and distance-dependent measurements we are able to link the band structure with the surface transport properties of Cu(110).

[1] Leisegang, M. et. al., Nano Lett. 18, 2165 (2018)

[2] Jiang, J., et al., Phys. Rev. B 89, 085404 (2014)

P23: Frozen deconfined quantum criticality

Vira Shyta

IFW Dresden

There is a number of contradictory findings with regard to whether the theory describing easy-plane quantum antiferromagnets undergoes a second-order phase transition. The traditional Landau-Ginzburg-Wilson approach suggests a first-order phase transition, as there are two different competing order parameters. On the other hand, it is known that the theory has the property of self-duality which has been connected to the existence of a deconfined quantum critical point (DQCP). The latter regime suggests that order parameters are not the elementary building blocks of the theory, but rather consist of fractionalized particles that are confined in both phases of the transition and only appear — deconfine — at the critical point. Nevertheless, many numerical

Monte Carlo simulations disagree with the claim of a DQCP in the system, indicating instead a first-order phase transition. Here we establish from exact lattice duality transformations and renormalization group analysis that the easy-plane CP1 antiferromagnet does feature a DQCP. We uncover the criticality starting from a regime analogous to the zero temperature limit of a certain classical statistical mechanics system which we therefore dub “frozen”. At criticality our bosonic theory is dual to a fermionic one with two massless Dirac fermions, which thus undergoes a second-order phase transition as well.

P24: Dynamical correlations and domain wall relocalisation in transverse field Ising chains

Philippe Suchsland
MPI-PKS Dresden

We study order parameters and out-of-time-ordered correlators (OTOCs) for a wide variety of transverse field Ising chains: classical and quantum, clean and disordered, integrable and generic. The setting we consider is that of a quantum quench. We find a remarkably rich phenomenology, ranging from stable periodic to signals decaying with varying rates. This variety is due to a complex interplay of dynamical constraints (imposed by integrability and symmetry) which thermalisation is subject to. In particular, a process we term dynamical domain wall relocalisation provides a long-lived signal in the clean, integrable case, which can be degraded by the addition of disorder even without interactions. Our results shed light on a proposal to use an OTOC specifically as a local dynamical diagnostic of a quantum phase transition even when evaluated in a state with an energy density corresponding to the paramagnetic phase.

P26: Relative entropy in neural networks

Yanick Thurn
JMU Würzburg

Using methods from quantum field theory and quantum information theory we try to improve the training of neural networks. We introduce a new way to use the Kullback-Leibler divergence to get insight into the training of neural networks. The Kullback-Leibler divergence, also known as relative entropy, can be seen as a distance measure between probability distributions. Similar to restricted Boltzmann machines, the relative entropy is calculated between two different activations in the same layer instead of neighboring layers, whereas the second activation is determined by a new propagation method we introduce.

Intuitively, it can be seen as propagating the most important features to the next layer and, subsequently, back to the original one. This allows a comparison of the transported information between layers. We refer to this approach as reflective relative entropy (RRE). In the large- N limit, the trainability of neural networks depends on different parameters including the variance of the weights and biases while initialization. This results in a phase diagram, where the trainability of the network seems to be optimal close to the critical point. A relation between the RRE and the critical phase is observed. This indicates a phase sensitivity of the RRE, which could be used to improve the training of neural networks.

P28: Observation of YSR bound states on 4f-atoms on Clean Nb (110)

Yu Wang

JMU Würzburg

Magnetic impurities on a superconductor induce sub-gap Yu-Shiba-Rusinov (YSR) bound states, localized at the impurity site and fading away from it for distances up to several nanometers. Since YSR of 3d-atomic impurities have already been fully studied, we are interested in studying 4f-atomic impurities (Gd) on superconductivity (SC) by a low-temperature scanning tunneling microscope at 1 Kelvin. Tunneling spectra obtained on single Gd shows no sub-gap excitations. However, by artificially manipulating Gd atoms with normal W-tip, we managed to create Gd dimers. These dimers show 2 induced sub-gap YSR bound states due to the hybridization of excitations from the two Gd atoms. These excitation states are locally asymmetric with respect to the tunneling of electrons and holes. This is the first time that YSR bound states are observed on Gd, it shows high potential that we could create 1D topological insulator of Gd atomic chain on Nb(110).

P29: Wormholes from Berry phases in AdS₃/CFT₂

Anna-Lena Weigel

JMU Würzburg

The AdS/CFT correspondence states that certain CFTs admit a description in terms of a gravitational theory in asymptotically AdS geometries of one dimension more. A central question in understanding the mechanism behind the duality is how the geometry in the bulk spacetime is encoded in the dual CFT state. Berry phases present a useful tool for understanding this. In their most general form, Berry phases are geometric phases acquired by states due to the presence of holonomies when parallel transported around a closed loop in parameter space. The AdS/CFT correspondence admits the description of bulk

geometries with semi-classical spacetime wormholes in terms of two entangled CFTs. Wormholes are a topological feature of the bulk spacetime that presents as a holonomy and thus can be probed with Berry phases. The entanglement induced by the wormhole in the bulk geometry implies the dual CFTs no longer factorize. We show that non-factorization in the dual entangled CFTs is evident in Berry phases for such systems.

P30: Hall viscosity and hydrodynamic inverse Nernst effect in graphene

Zhuo-Yu Xian

JMU Würzburg

Motivated by Hall viscosity measurements in graphene sheets, we study hydrodynamic transport of electrons in a channel of finite width in external electric and magnetic fields. We consider electric charge densities varying from close to the Dirac point up to the Fermi liquid regime. We find two competing contributions to the hydrodynamic Hall and inverse Nernst signals that originate from the Hall viscous and Lorentz forces. This competition leads to a non-linear dependence of the full signals on the magnetic field and even a cancellation at different critical field values for both signals. In particular, the hydrodynamic inverse Nernst signal in the Fermi liquid regime is dominated by the Hall viscous contribution. We further show that a finite channel width leads to a suppression of the Lorenz ratio, while the magnetic field enhances this ratio. All of these effects are predicted in parameter regimes accessible in experiments.