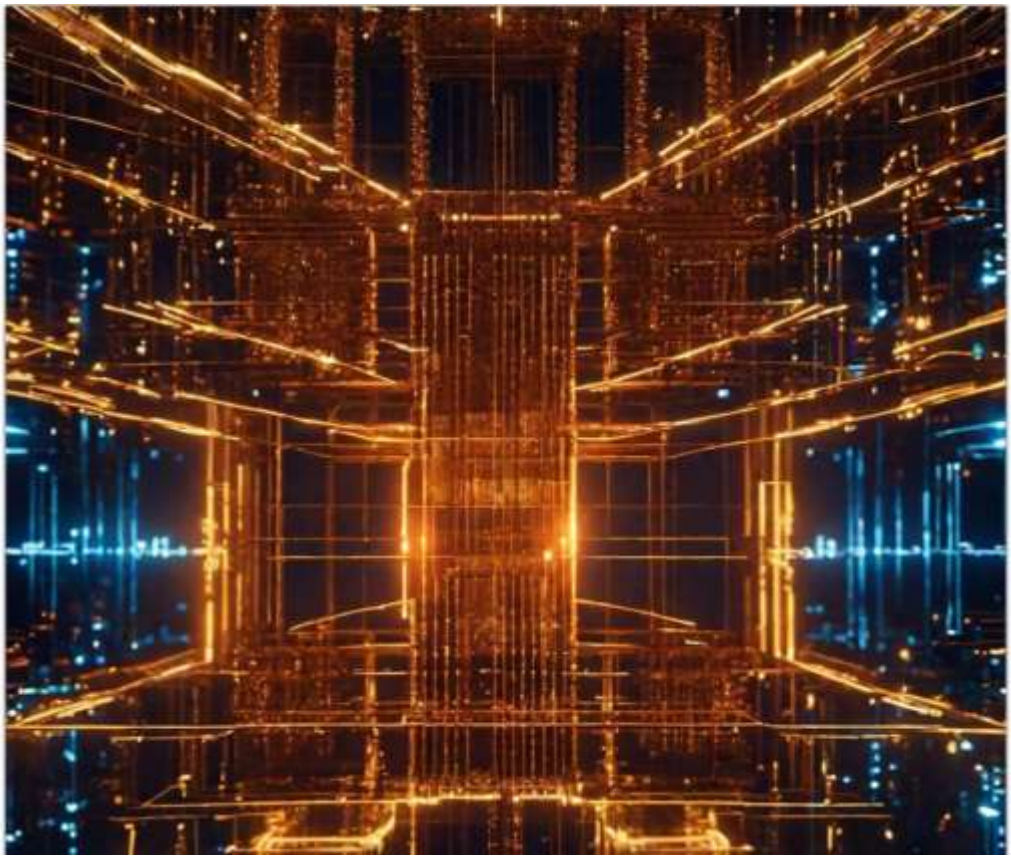
Topological Matter School

Optical and electronic responses of Topological Matter

(August 21-25 2023)



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Outline

Optical and electronic responses of topological matter are fundamental to understand topological properties in real materials. The Berry curvature is behind numerous effects such as the anomalous Hall effect, the spin Hall effect or even heat currents as observed in the anomalous Nerst effect and the thermal Hall effect. Even more interestingly, the Berry curvature has been recently shown to determine novel and sizable non-linear optical effects, non-linear Hall responses without magnetic fields and universal responses of topological metals. Lastly, magnetotransport in topological metals is an exciting frontier to uncover exotic anomalous responses rooted in concepts from high-energy physics, such as the chiral anomaly. In this edition we will tackle all these phenomena, offering a pedagogical and broad picture of the main responses of topological matter.

Topological Matter School 2023 (August 20-25): during one week we will provide extended lectures on these exciting topics by leading experts in both experiment and theory. Our program will be spread in 1 week with 6 lectures per day. Outdoors activities to get to know the city and the Basque culture will also be organized, such a surf class in our precious Zurriola beach.

List of speakers

- Philip J. W. Moll (Max Planck Institute, Hamburg, Germany)
- Phuan Ong (Princeton University, USA)
- Julen Ibañez-Azpiroz (University of the Basque Country and CSIC, Spain)
- Andrei Bernevig (Princeton University, USA)
- Stepan Tsirkin (University of the Basque Country and CSIC, Spain)
- Dmytro Pesin (University of Virginia, USA)
- Jennifer Cano (Flatiron and Stony Brook University, USA)
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- Qiong Ma (Boston College, USA)
- Prineha Narang (UCLA, USA)
- David Vanderbilt (Rutgers, USA)
- John Sipe (University of Toronto, Canada)
- David Abergel (Chief editor Nature Physics, UK)

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Multiplicative Kitaev Chain

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Abstract

Topological qubits composed of unpaired Majorana zero-modes are under intense experimental and theoretical scrutiny in efforts to realize practical quantum computation schemes. In this work, we show the minimum four unpaired Majorana zero-modes required for a topological qubit according to braiding schemes and control of entanglement for gate operations are inherent to multiplicative topological phases, which realize symmetry-protected tensor products—and maximally-entangled Bell states—of unpaired Majorana zero-modes known as multiplicative Majorana zero-modes. We introduce multiplicative Majorana zero-modes as topologically-protected boundary states of both one and two-dimensional multiplicative topological phases, using methods reliant on multiplicative topology to construct relevant Hamiltonians from the Kitaev chain model. We furthermore characterize topology in the bulk and on the boundary with established methods while also introducing techniques to overcome challenges in characterizing multiplicative topology. In the process, we explore the potential of these multiplicative topological phases for an alternative to braiding-based topological quantum computation schemes, in which gate operations are performed through topological phase transitions.

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Transport properties of magnetically doped V-Bi_4Te_3

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Bi_2Te_3 is a 3D topological insulator with a single Dirac cone on the surface [1]. This surface state can be gapped by means of magnetic doping, resulting in the quantum anomalous hall state [2]. Recently, there has been an increasing interest in natural superlattices containing Bi_2Te_3, such as Bi_4Te_3 [3]. This compound consists of alternating Bi_2 and Bi_2Te_3 layers. The exact topological nature of these compounds is still under debate. We fabricated (V-doped) Bi_4Te_3 thin films with molecular beam epitaxy and characterized the films with X-ray diffraction, transmission electron microscopy and electrical transport measurements. We show that the level of V-doping influences the dominant carrier type in transport and observed the presence of magnetism in the films with the highest level of V-doping.

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Preparation and study of potential amorphous topological superconductors of Bi-Sb

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Exotic properties of topological superconductivity are expected to pave the way towards quantum computing [1,2]. However, a stable topological superconductor has not yet been found experimentally. Good candidates have been proposed to be bismuth and its alloys (particularly, bismuth-antimony, Bi-Sb), which are among the most studied topological insulators [3,4] and which, in amorphous state, become superconductors below a critical temperature close to 6 K [5].

The aim of this work is to grow Bi_xSb_{100-x} alloys and induce, by ion beam irradiation, enough damage to their internal structure as to amorphize the material. Although amorphous Bi-Sb tends to recrystallize unless at low temperatures [5,6], our idea to overcome such difficulty is trying to amorphize only a region of the material a few μm deep from the surface. To do so, we will use ions in the MeV range, exploiting the capabilities of CMAM's 5 MV ion-beam accelerator [7]. By characterizing the morphological, structural and electrical properties of the resulting material, we will analyze its potential as an amorphous topological superconductor.

We present here preliminary experiments, including our current work focused on optimizing the sample fabrication process and testing different strategies: alternative substrates, growing techniques, ions (protons, Bi ions) and measurement setups.

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Non-Hermitian Isospectral Reductions

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In this work, we study a class of non-Hermitian Hamiltonians that host interesting boundary phenomena. By employing the isospectral reduction technique, we can determine whether these models host the non-Hermitian skin effect and/or topological edge states. Furthermore, our approach reveals that such models exhibit an energy (or frequency)-dependent non-Hermitian skin effect, where eigenstates can simultaneously localize on either ends of the systems, with different localization lengths. Additionally, we predict the existence of various topological edge states, pinned at non-zero energies, with varying exponential envelopes that depend on their energies. Overall, our work sheds new light on the nature of topological phases and non-Hermitian skin effect in one-dimensional systems, and the isospectral reduction proves to be a powerful tool for predicting and understanding these phenomena.

References: Paper soon to be uploaded to arXiv.

Transversality-Enforced Tight-Binding Model for 3D Photonic Crystals aided by Topological Quantum Chemistry

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Tight-binding (TB) models can accurately predict the band structure and topology of crystalline systems and they have been heavily used in solid-state physics due to their versatility and low computational cost. It is quite straightforward to build an accurate TB model of any crystalline system using the maximally localized Wannier functions (WF) of the crystal as a basis [1, 2]. Unfortunately, in 3D photonic crystals (PhCs) transversality condition of Maxwell's equations precludes the construction of a basis of maximally localized WF via usual techniques [2]. In this work, we show how to overcome this problem by using topological quantum chemistry which will allow us to express the band structure of the PhC as a difference of elementary band representations (EBRs). This can be achieved by the introduction of a set of auxiliary modes, as recently proposed by *Soljačić et. al.* [3], which regularize the Γ-point obstruction arising from tranversality constraint of the Maxwell equations. The decomposition into EBRs allows us to isolate a set of pseudo-orbitals that permit us to construct an accurate transversality-enforced TB model that matches the dispersion, symmetry content and topology of the 3D PhC under study. Moreover we show how to introduce the effects of a gyrotropic bias in the framework [4], modeled via non-minimal coupling to a static magnetic field. Our work provides the first systematic method to analytically model the photonic bands of the lowest transverse modes over the entire Brillouin zone via a transversality-enforced TB model.

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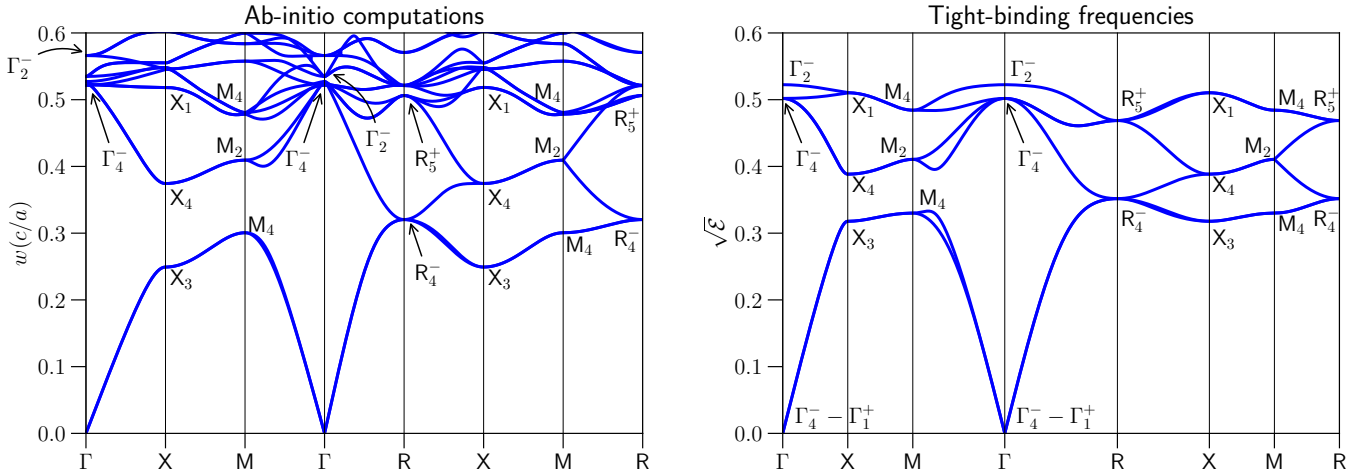

Ultraquantum Limit of Axionic Charge Density Waves

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Abstract

Magnetic Catalysis (M.C.) of Chiral Symmetry Breaking is the mechanism whereby a magnetic field induces a gap in an otherwise gapless system of weakly-interacting chiral fermions [1]. It was originally explored in the context of the QCD phase transition in high energy-physics. However, the advent 3D Dirac/Weyl semimetals has raised the possibility of observing the phenomenon in condensed matter systems as well in the form of Axionic Charge Density Waves [2,3].

Models of the phenomenon often rely on the fact that the energy scale provided by the magnetic field is lower than the UV cutoff of the theory, which in condensed matter systems is at most of the order of the inverse lattice spacing. We consider the opposite scenario where the magnetic field scale is of the order or larger than the UV cutoff, a scenario originally proposed in the context of the QCD [4]. Among other consequences, we find that in that case there is a wider parameter window for which M.C. can observably take place and that dimensional reduction from 3 to 1 spatial dimensions becomes stronger, enabling a beyond mean-field description through 1D bosonization [5].

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Acknowledgments

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Finite-depth scaling of infinite quantum circuits for quantum critical points

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The scaling of the entanglement entropy at a quantum critical point allows us to extract universal properties of the state, e.g., the central charge of a conformal field theory. With the rapid improvement of noisy intermediate-scale quantum (NISQ) devices, these quantum computers present themselves as a powerful tool to study critical many-body systems. We use finite-depth quantum circuits suitable for NISQ devices as a variational ansatz to represent ground states of critical, infinite systems. We find universal finite-depth scaling relations for these circuits and verify them numerically at two different critical points, i.e., the critical Ising model with an additional symmetry-preserving term and the critical XXZ model.

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Polarization-dependent measurements of bulk electronic structure in chiral topological semimetal CoSi

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The chiral topological semimetal CoSi has a rich electronic structure in which unconventional chiral fermions are observed near the Fermi level [1]. These quasiparticles exist at band-crossing points carrying a non-zero Chern number and lead to long surface Fermi arcs, as explored by ARPES. We studied the bulk electronic structure in CoSi using soft X-ray ARPES experiments via the ASPHERE endstation at PETRA III (DESY, Hamburg). Topological features such as the symmetry-enforced nodal plane and chiral fermions near the Fermi level are investigated with high energy-resolution. We conducted polarization-dependent measurements with the aim of addressing the orbital character of the electronic states, which previously proved useful in the study of Weyl fermions [2].

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Visualizing the localized electrons of a kagome flat band

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Kagome metals possess unique electronic properties stemming from destructive interference in their two-dimensional (2D) kagome lattice, which generates flat bands, fostering exploration of intriguing many-body quantum states. The key of the successful realization of these proposals is to demonstrate the real-space localization of electrons occupying the flat bands. However, spatial electron localization and interactions with complex lattice structures remain hitherto unknown. In this study, we synthesized CoSn films using molecular beam epitaxy (MBE) and probed the real-space localized flat bands of CoSn with scanning tunneling microscopy (STM). Our findings revealed a substantially shorter electron localization length (2-3 angstroms) than theoretical predictions and demonstrated the flat band's quasi-2D nature with a minimal quasiparticle velocity. Hence, interaction effects in the flat bands of CoSn could be much more significant than previously thought. Our study provides fundamental insight into the electronic properties of kagome metals and motivates further work on the potential emergence of many-body quantum states in the flat bands of CoSn and other kagome materials.

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Acknowledgments

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VQE algorithm for topological one-dimentional many-body systems

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In recent years, the development of noisy intermediate-scale quantum (NISQ) computers has opened up new possibilities for efficiently studying complex quantum systems. In this work, we will use a quantum minimization algorithm, the Variational Quantum Eigensolver (VQE), to investigate the ground state of systems exhibiting non-trivial topological behavior. In the field of condensed matter physics, these systems have not only theoretical interest, but also numerous potential applications in materials science and quantum technologies. We will analyze one-dimensional Su-Schrieffer-Heeger (SSH) and Kitaev models with the aim of identifying ad hoc strategies to improve VQE results by implementing appropriate cost functions based on the entanglement properties of the non-trivial topological ground state.

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Encapsulation engineering for clean air-sensitive heterostructure devices

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Since the experimental realization of graphene, 2D materials have been studied due to their exceptional quantum properties. Their reduced vertical dimensionalities (ranging from a single atomic thicknesses to ~100nm thick heterostructures) are key for the current roadmap of sample miniaturization. Nonetheless, the quality of the devices (mobility, responsivity, working temperatures…) as well as sensitivity to the environment, limits their straightforward application. In order to study said heterostructures, exceptionally clean conditions must be reached to achieve high signal-to-noise ratios. In this context, 2D hexagonal boron nitride has been used to encapsulate other 2D materials. As an insulator ($E_g \approx 6.1$ eV), it allows for electrostatic gating and conduction of optical measurements. Nonetheless, electric contact to semiconducting materials can lead to large contact resistances when patterning side contacts in typical device fabrication procedures. In this work, bottom contacts are deposited on top of graphene gated hBN heterostructures. Followed by encapsulation of transition metal dichalcogenides and thermal annealing. This fabrication method demonstrated improved contact resistances for optoelectronic measurements and allows for the study of air sensitive materials. The long term goal of the optimization of this process is to study topological phases displayed in several TMDs both optically and electrically.

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Acknowledgments

Sample fabrication was performed using NanoLabNL facilities. This work is supported by the research program “Materials for the Quantum Age” (QuMat) for financial support. This program (registration number 024.005.006) is part of the Gravitation program financed by the Dutch Ministry of Education, Culture and Science (OCW).

Electronic properties of *2D* and *3D* layered $ZeTe_5$

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Abstract

Topological insulators have been studied intensively over the last decades. Zirconium Pentatelluride ($ZrTe_5$) is one of the prominent material for the experimental study of topological phase transitions. However, physical properties depend on the synthesis method, and it is hard to explain experimental results with theories. For a monolayer of $ZrTe_5$, our experimental group has detected a conduction band with tiny effective mass. This outcome has not been reported before and may indicate a possible Dirac cone. To explain it, we use Density Functional Theory (DFT) to computationally simulate the material. Here, we present the DFT results for the 3D compound and 2D monolayer of $ZrTe_5$.

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Acknowledgments:

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Axion Topology in Photonic Crystal Domain Walls

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Axion insulators (AXI) are 3D magnetic higher-order topological insulators, protected by inversion (I)-symmetry, which support hinge-localized chiral channels and quantized topological magnetoelectric effects. Recent studies have suggested that AXI may detect dark-matter axion-like particles by coupling to their axionic excitations. Beyond its fundamental theoretical interest, designing a photonic AXI offers the potential to enable the development of magnetically-tunable photonic switch devices through magnetic manipulation of AXI modes and their chiral propagation. Motivated by this, we propose an approach to induce axionic band topology in gyrotropic 3D Weyl photonic crystals (PhC) gapped by supercell modulation (SM). To quantize an axion angle, we create domain walls in I-symmetric PhC, incorporating a phase-obstruction in the SM of their dielectric elements. This binds chiral channels on I-related hinges, leading to an axionic chiral channel of light. By controlling the gyrotropic response, we manipulate the AXI modes via a small external magnetic bias, providing a topological switch between different 1D chiral photonic fiber configurations. The unidirectional AXI hinge states in the photonic AXI are buried in a fully connected 3D dielectric structure, protected from radiation in the electromagnetic continuum, making them suitable for guided-light communication, where preservation and non-reciprocal propagation of photonic signals are crucial.

Surface and Structural Analysis of MBE grown (110)-oriented $Pb_{1-x}Sn_xTe$ Topological Crystalline Insulator

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The novel class of semiconductors namely topological crystalline insulators (TCIs) is a rapidly developing research area of modern solid state physics. $Pb_{1-x}Sn_xTe$ alloy has been experimentally discovered as a member of TCIs family in the previous decade. It exhibits topological phase transition above a critical concentration of Sn ($x \geq 0.36$ at LHe temperature) [1]. Theoretical predictions of band inversion at high symmetry L point in the Brillouin zone, and experimental evidence for topologically protected states on (001) [2] and (111) surfaces [3] of $Pb_{1-x}Sn_xTe$ alloy have already been proclaimed in literature. However, (110)-oriented $Pb_{1-x}Sn_xTe$ has not been studied experimentally in this context yet. We have grown thin layers of $Pb_{1-x}Sn_xTe$ solid solution by molecular beam epitaxy (MBE). To our knowledge the growth of $Pb_{1-x}Sn_xTe$ in the (110) orientation has not been reported so far. We have found that direct growth on epi-ready GaAs(110) substrates resulted (100) orientations. To avoid this problem we have used hybrid substrates with thick CdTe(110) buffer. The layers have been investigated by several characterization techniques such as atomic force microscope, X-ray diffraction and, high resolution transmission electron microscopy which reveals the (110)-orientation of $Pb_{1-x}Sn_xTe$. Angle-resolved photoemission experiments are underway to identify topologically protected surface states on the $Pb_{1-x}Sn_xTe$(110) surface.

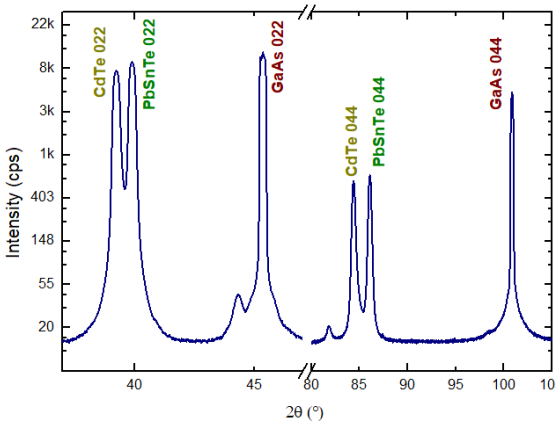

Fig. 2Θ/ω scan of (Pb,Sn)Te/CdTe//GaAs(110). Both (Pb,Sn)Te layer and CdTe buffer show same out of plane <011> growth

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Structural spillage: an efficient method to identify non-crystalline topological materials

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While topological materials are not restricted to crystals, there is no efficient method to diagnose topology in non-crystalline solids such as amorphous materials. Here we introduce the structural spillage [1], a new indicator that predicts the unknown topological phase of a non-crystalline solid, which is compatible with first-principles calculations. Building on the ideas of the spin-orbit spillage [2] and the strange correlator [3], the structural spillage compares the occupied states between the unknown non-crystalline material and its crystalline counterpart. Since the topological characterization of the latter can be can be efficiently calculated using standard symmetry-based methods [4], the structural spillage allows to determine whether the non-crystalline system retains the topological properties of its crystalline counterpart. We illustrate the potential of the structural spillage with tight-binding and first-principles calculations of amorphous bismuth, predicting a bilayer to be a new topologically nontrivial material. Our work opens up the efficient prediction of non-crystalline solids via first-principles and high-throughput searches.

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Towards a theory of surface orbital magnetization

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The theory of bulk orbital magnetization has been formulated both in reciprocal space based on Berry curvature and related quantities, and in real space in terms of the spatial average of a quantum mechanical local marker. Here we consider a three-dimensional antiferromagnetic material having a vanishing bulk but a nonzero surface orbital magnetization. We ask whether the surface-normal component of the surface magnetization is well defined, and if so, how to compute it. As the physical observable corresponding to this quantity, we identify the macroscopic current running along a hinge shared by two facets. However, the hinge current only constrains the difference of the surface magnetizations on the adjoined facets, leaving a potential ambiguity. By performing a symmetry analysis, we find that only crystals exhibiting a pseudoscalar symmetry admit well-defined magnetizations at their surfaces at the classical level. We then explore the possibility of computing surface magnetization via a coarse-graining procedure applied to a quantum local marker. We show that multiple expressions for the local marker exist, and apply constraints to filter out potentially meaningful candidates. Using several tight-binding models as our theoretical test bed and several potential markers, we compute surface magnetizations for slab geometries and compare their predictions with explicit calculations of the macroscopic hinge currents of rod geometries. We find that only a particular form of the marker consistently predicts the correct hinge currents.

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Effective models for vortex superlattices in Kitaev's honeycomb model

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Abstract

We investigate two families of triangular vortex configurations in Kitaev's honeycomb model and introduce low-energy effective models that correctly reproduce their topological phase and energy spectra. For the first family we consider "direct" superlattices in which a triangular vortex configuration is present on a vortex-free background, while for the second family we consider "dual" superlattices in which the vortex-free plaquettes of the honeycomb lattice form a triangular configuration on a vortex-full background. The topological phase of the honeycomb model is controlled by the strength of a time-reversal symmetry-breaking term called κ which we allow to be arbitrarily strong compared to the nearest neighbor interaction called J. For sufficiently dilute direct (dual) superlattices, we show that the low-energy bands of the honeycomb model can be reformulated in terms of an effective tight-binding model that describes the tunneling of Majorana (complex) fermions between superlattice sites. The parameters of the tight-binding model are found via direct comparison of the model's total integrated density of states with that of the Kitaev, and we demonstrate that the total Chern number is simply the sum of the Chern numbers of the vortex-free/vortex-full background and that of the low-energy bands of the effective model.

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Electronic structure of noncentrosymmetric B20-type compound HfSn

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We present a density functional study of HfSn, which belongs to the family of cubic B20 intermetallics. These materials are characterized by the absence of mirror and inversion symmetries of their crystal structures, leading to a chiral character that can accommodate a novel type of topological fermionic excitations and a wide range of exotic physical properties [1][2][3]. HfSn does not exist in nature and can only be synthesized at high temperatures [4]. Here, we present a detailed study of the peculiarities of the electronic band structure and Fermi surface topology, employed then to parametrize an effective tight-binding model. Additionally, we investigate the influence of the structural details on the position of the multiply degenerate band crossings pinned at high symmetry points in the vicinity of the Fermi level. This study contributes not only to a better understanding of B20 compounds containing a transition metal from the fourth group but also represents a guide to further experimental investigations, in particular those related to sample preparation.

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Topological flat bands in $d_{x^2-y^2}$-wave superconductors

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Abstract (max 200 words)

While in the past decades single-particle models have been successfully applied to describe a wide range of topological properties in weakly correlated systems, the interplay of topology and strong correlations is still not well understood.

Interestingly, in superconductors with a $d_{x^2-y^2}$-gap symmetry, the non-zero winding number of the nodes leads to the appearance of Majorana flat-bands at two-dimensional regions of the (110) surface's Brillouin zone which are bounded by the projections of the superconducting nodes. Due to the extensive degeneracy, these bands are expected to be unstable to arbitrarily small interactions, leading to a variety of time-reversal symmetry broken surface states [1].

However, the obtainment of a clean (110) surface remained a technical challenge. Here we demonstrate a new approach to cleave crystals for angle-resolved photoemission studies in which the fracture propagation is controlled by means of micro-notches. This allowed us to probe the electronic structure on the (110) surface for the first time, which we envision will give us direct access to these topological bands.

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Insulator-metal transition and weak antilocalization in ionic gated tellurium

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The ability to control the charger carrier density inside the solids is an important factor to realize different phase transitions in materials. This could not only be interesting for technological applications but also provide new insights about the fundamental properties of materials. In particular, inducing high charge carrier density into various two-dimensional materials has led to exotic phenomena such as insulator-metal phase transition and superconductivity [1, 2] . So far, different techniques have been used to achieve this. Meanwhile, electric double layer transistor (EDLT) is a highly promising platform as it can provide high charge carrier density of up to $10^{15}\mathrm{cm}^{-2}$ in its channel material. This is two orders of magnitude larger than that in the conventional transistors as a result of using ionic liquids instead of common solid dielectrics [3] . Here, I will first give a brief overview on the EDLTs, then I will present our experimental results of ionic liquid gated p-type tellurium (Te). Our results show the possibility of gate tuning insulator-metal transition and the crossover between weak localization (WL) and weak anti-localization (WAL) into the sample. The WAL becomes more pronounced as we increase the conductivity of the sample. Moreover, temperature-dependence of WAL showed e-e interaction is the main scattering mechanism of quantum decoherence in the material. More interestingly, we have shown the ability of controlling the spin-orbit interaction in Te by changing the applied gate voltage which could be interesting for spintronics application.

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First-order effect of electron-electron interactions on the anomalous Hall conductivity of massive Dirac fermions

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The influence of electron-electron interactions on the behaviour of two-dimensional Dirac fermion systems has been a subject of a longstanding debate. In this study, we investigate the first-order corrections to the anomalous Hall conductivity of massive Dirac fermions arising from contact interactions. Our calculations are performed using linear response theory at finite temperature and chemical potential using Matsubara Green's functions and diagrammatic perturbation theory. Notably, the presence of these interactions induces renormalisations of the gap, chemical potential, and Fermi velocity. In order to preserve both particle-hole symmetry and the Ward identity, we employ a non-trivial regularisation method for the contact interaction. Remarkably, in the limit of zero temperature and zero chemical potential, we find that the first-order corrections vanish, in accordance with the Coleman–Hill theorem [1], implying the absence of perturbative corrections to the topological Hall conductivity. Our findings shed light on the potentially crucial role of electron-electron interactions in shaping the transport properties of two-dimensional Dirac fermion systems.

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Topological phases in the presence of disorder and long-range couplings

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Abstract

We study the combined effects of disorder and range of the couplings on the phase diagram of one-dimensional topological superconductors. We consider an extended version of the Kitaev chain where hopping and pairing terms couple many sites. Deriving the conditions for the existence of Majorana zero modes, we show that either the range and the on-site disorder can greatly enhance the topological phases characterized by the appearance of one or many Majorana modes localized at the edges. We consider both a discrete and a continuous disorder distribution. Moreover, we discuss the role of correlated disorder which might further widen the topological regions. Finally, we show that in the purely long-range regime and in the presence of disorder, the spatial decay of the edge modes remains either algebraic or exponential, with eventually a modified localization length, as in the absence of disorder.

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Raman and photoluminescence studies on twisted bilayer CVD-grown MoS_2

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Twisting two monolayers of MoS_2 on top of each other gives a new tuning parameter to the system, namely the twist angle. Depending on the twist angle we observe characteristic optical features with Raman and photoluminescence spectroscopy such as the appearance of moiré phonon modes and energy shifts of the excitonic transitions. Chemical vapor deposition (CVD) was used to produce clearly separated, triangular shaped MoS_2 monolayers. Using such CVD-grown monolayers, twisted bilayers are manufactured with twist angles between 0° and 60°. Here the fabrication of such twisted bilayers and their optical features shall be presented.

Non-Hermitian topological modes from local loss engineering in photonic arrays

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Non-Hermitian systems have risen as a powerful strategy to engineer new forms of topological excitations [1]. A variety of non-Hermitian models displaying topological modes rely on non-reciprocity, the change in probability of left-right propagation. However, non-reciprocity has remained challenging to implement in photonic devices. In stark contrast, modulated photonic losses provide an alternative way of implementing non-Hermiticity, representing a realistic approach to non-Hermitian photonics. Here [2] we present a family of photonic models relying on the real-space modulation of photonic losses giving rise to non-Hermitian topological excitations. We demonstrate that the non-Hermitian topological modes survive spatial fluctuations in the loss and couplings of the system, and we elucidate the self-duality limit while studying the delocalization-localization transition of these models. Our results provide a realistic strategy to create topological modes in photonic systems from real- space loss engineering.

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Establishing Coherent Momentum-Space Electronics States in Locally-Ordered Materials

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Many current and future quantum technologies rely on amorphous materials, where translational symmetry is broken, but short-range order with well-defined structural length scales persists. This brings forward the fundamental question whether long range order is a necessary condition to establish coherence and structured momentum-dependent electronic state, and how to characterize it in the presence of short-range order.

By using angle resolved photoemission spectroscopy together with our simulations using amorphous Hamiltonians to directly access the electronic states in a momentum resolved manner, we reveal that, even in the absence of long-range order, a well-defined real-space length scale is sufficient to produce dispersive band structures. Moreover, we observe for the first time a repeated Fermi surface structure of duplicated annuli, reminiscent of Brillouin zone-like repetitions.

These results, not only lead the way to a new understanding of electronic coherence in solids, but also open the way to the realization of novel momentum-dependent quantum phenomena such as momentum pairing and spin-orbit coupling, in a much broader class of materials than the currently studied ones, lacking long range crystalline translational symmetry.

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Pressure-tuning the Weyl-Kondo semimetal candidate material $CeRu_4Sn_6$

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The vastly unexplored field of correlation-driven gapless topological phases was boosted by the discovery of Weyl-Kondo semimetal behavior in the heavy fermion material $Ce_3Bi_4Pd_3$ [1-3]. A cubic-in-temperature contribution to the electronic specific heat [1] and a giant spontaneous Hall effect [3] are extreme topological responses attributed to the presence of Weyl nodes in the immediate vicinity of the Fermi level. Tentative evidence for quantum criticality in $Ce_3Bi_4Pd_3$ [1] suggests that quantum critical fluctuations might play a role in stabilizing the Weyl-Kondo semimetal phase. An interesting material to test this hypothesis is the noncentrosymmetric Kondo semimetal $CeRu_4Sn_6$. It was theoretically proposed to be a correlated Weyl semimetal [4] and shows quantum critical behavior without any form of parameter tuning [5]. Here we present signatures of Weyl-Kondo physics across the phase diagram of $CeRu_4Sn_6$ in terms of hydrostatic pressure and magnetic field and discuss their implications.

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Numerical Simulation of Non-Abelian Anyons

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Abstract

Two-dimensional systems such as quantum spin liquids or fractional quantum Hall systems exhibit anyonic excitations [1,2] that possess more general statistics than bosons or fermions. This exotic statistics makes it challenging to solve even a many-body system of non-interacting anyons. In this work [3], we introduce an algorithm that allows to simulate anyonic tight-binding Hamiltonians on two-dimensional lattices. The algorithm is directly derived from the low energy topological quantum field theory and is suited for general abelian and non-abelian anyon models. As concrete examples, we apply the algorithm to study the energy level spacing statistics, which reveals level repulsion for semions, Fibonacci anyons and Ising anyons. Additionally, we simulate non-equilibrium quench dynamics, where we observe that the density distribution becomes homogeneous for large times – indicating thermalization.

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The extended Hatano-Nelson model

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Non-Hermitian systems attract a lot of attention in recent years as effective description of open quantum systems. A prominent example in this context is the Hatano-Nelson model. While historically the model has short-range non-reciprocal hoppings, long-range hopping has not been systematically studied. I will present our results on the extended Hatano-Nelson model. Using analytical techniques, we demonstrate how the underlying physics of the original Hatano-Nelson model is enriched when longer-range hoppings are also included. I will discuss how the crucial elements of the Hatano-Nelson model, namely, the non-Hermitian skin effect and the exceptional points, are modified for the generalized model.

Phenomena of Majorana Wavefunctions in chaotically shaped Topological Superconductors.

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Majorana billiards are finitely sized and arbitrarily shaped topological superconductors which feature fermion parity switches. The localization of the Majorana wavefunction is often assumed to be based purely on the pairing potential. We show that this wavefunction showcases scarring in chaotically shaped billiards. This can be understood by making a mapping between the p-wave Hamiltonian and a regular p^2/2m Hamiltonian when there is no or weak chiral symmetry breaking. In this mapping, the presence of chiral symmetry breaking results in a fictitious magnetic field term in the regular Hamiltonian. Furthermore, we show that the localization properties of the Majorana wavefunction can be controlled non-locally by an impurity in regions of negligible wavefunction amplitude. In the regime of intermediate chiral symmetry breaking, the Majorana wavefunction shows focusing effects in convex billiards. Finally, we establish a connection between the fully chiral Majorana modes and a quantum Hall edge state. Overall, our findings offer valuable insights into the properties of the Majorana wavefunctions and their relation to semiclassical physics and quantum chaos.

Shift photoconductivity in the Haldane model

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The shift current is part of the second-order optical response of materials with a close connection to topology. Here we report a sign inversion in the band-edge shift photoconductivity of the Haldane model when the system undergoes a topological phase transition. This result is obtained following two complementary schemes. On one hand, we derive an analytical expression for the band-edge shift current in a two-band tight-binding model showing that the sign reversal is driven by the mass term. On the other hand, we perform a numerical evaluation on a continuum version of the Haldane model. This approach allows us to include off-diagonal matrix elements of the position operator, which are discarded in tight-binding models but can contribute significantly to the shift current. Explicit evaluation of the shift current shows that while the model predictions remain accurate in the deep tight-binding regime, significant deviations arise for shallow potential landscapes. Notably, the sign reversal across the topological phase transition is observed in all regimes, implying it is a robust effect that could be observable in a wide range of topological insulators such as $BiTe_2$ and $CsPbI_3$ reported in [1].

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Topologically non-trivial polarization textures in moiré materials

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Abstract (max 200 words)

The modern theory of polarization provides a recipe for deducing the total polarization in a unit cell of any insulating system subject to periodic boundary conditions [1]. However, it cannot describe the local variation of polarization in a crystal supercell, which is important for understanding topologically non-trivial polarization textures observed in perovskite nanostructures [2] and moiré heterostructures formed by hexagonal boron nitride (hBN) or transition metal dichalcogenides [3]. While approximations to the local polarization in perovskite supercells have been used to successfully predict polar vortices and topological structures therein, these approximations are not valid in twisted bilayers, where the dynamical charges vary non-linearly throughout the supercell, forming polarization textures analogous to magnetic merons and skyrmions [3]. In this work, we show how the local polarization can be rigorously defined on the scale of single-layer unit cells as a gauge-invariant quantity [4]. We demonstrate how local polarization can be evaluated, circumventing the necessity of computing Berry phases for the total polarization of a supercell, using configuration space approximations. Furthermore, we illustrate the applications of the introduced definition of local polarization beyond the use of such approximations, in a continuum Bistritzer-MacDonald (BM) model [5] and effective 1D models with introduced superlattice periodicity.

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Solitons and topology: Observation of cnoidal wave localization in non-linear topolectric circuits

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Topological phases have been realized in a variety of classical metamaterials. They provide easily accessible platforms to study topology in regimes beyond experimental limitations of real materials. While most implementations are limited to the linear regime, investigating non-linear effects promises to reveal a plethora of new phenomena, such as solitons and chaos. To study the intertwining of topology and non-linearity we engineered a topolectric circuit reminiscent of the Su-Schrieffer-Heeger (SSH) model with added tunable onsite non-linearity. We observe the localized cnoidal (LCn) state which maintains the spatial exponential localization of the SSH edge mode while distorting a sinusoidal input into eccentric waves in time domain. In this talk, we complement the non-linear differential equations with the theory of topological localization and develop an analytic description of the LCn state.

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Stable Bosonic Topological Edge Modes in the Presence of Many-Body Interactions

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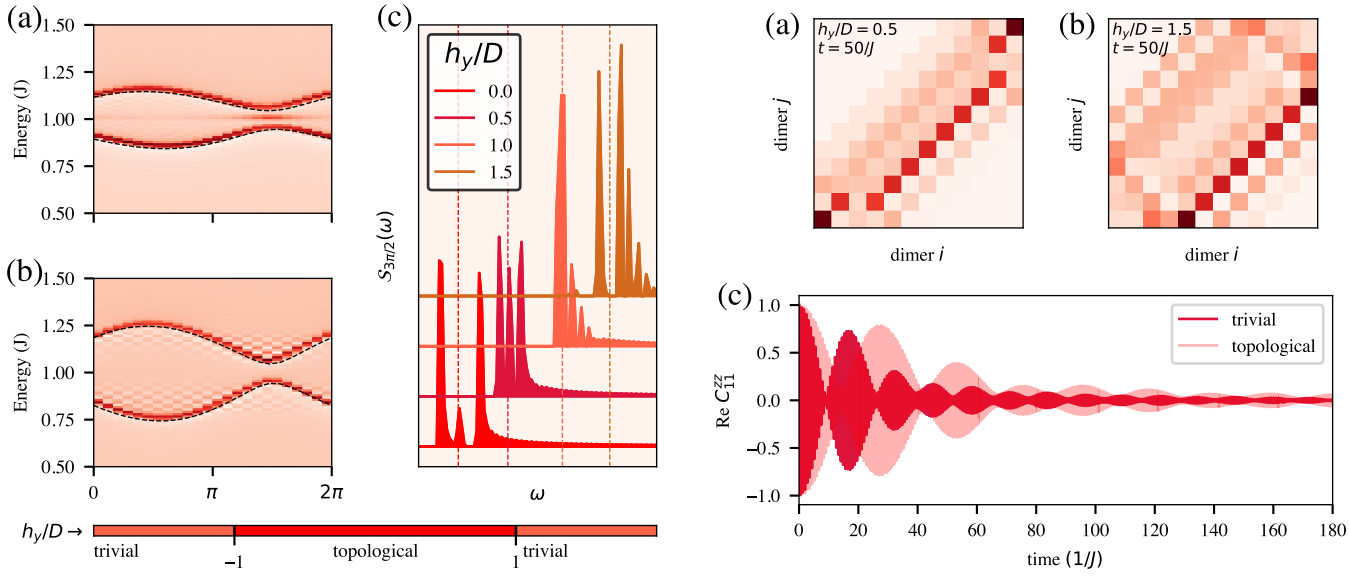
Many magnetic materials are proposed to exhibit topological thermal Hall effect. Because of the nontrivial topology of their magnon, triplon or other quasi-particle band structures, bosonic edge modes inevitably appear in their excitation spectra as dictated by the bulk-boundary correspondence. However, there is a discrepancy between theory prediction and experimental observation, which suggests some underlying mechanism that intrinsically suppresses the expected thermal Hall current. Many-body interactions and higher-order terms induced by spin-orbit coupling that are not accounted for in the non-interacting quasi-particle picture are most often identified as the reason for the absence of the topological edge modes. In this manuscript we report stable bosonic edge modes at the boundaries of a ladder quantum paramagnet in the presence of both, the full many-body interaction and spin-orbit coupling. For the first time, we use tensor networks methods to resolve topological edge modes in the time-dependent spin-spin correlations and the Dynamical Structure factor, which is directly accessible experimentally. We show that the topological edge modes have enhanced time coherence, discuss the topological phase diagram of the model, demonstrate the fractionalization of its low-lying excitations and propose potential material candidates.



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Local Topological Markers in Odd Spatial Dimensions and Their Application to Amorphous Topological Matter

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Local topological markers, topological invariants evaluated by local expectation values, are valuable for characterising topological phases in materials lacking translation invariance. The Chern marker---the Chern number expressed in terms of the Fourier transformed Chern character---is an easily applicable local marker in even dimensions, but there are no analogous expressions for odd dimensions. We provide general analytic expressions for local markers for free-fermion topological states in odd dimensions protected by local symmetries: a Chiral marker, a local $\mathbb{Z}$ marker which in case of translation invariance is equivalent to the chiral winding number, and a Chern-Simons marker, a local $\mathbb{Z}_2$ marker characterising all nonchiral phases in odd dimensions. We achieve this by introducing a one-parameter family P_ϑ of single-particle density matrices interpolating between a trivial state and the state of interest. By interpreting the parameter ϑ as an additional dimension, we calculate the Chern marker for the family P_ϑ. We demonstrate the practical use of these markers by characterising the topological phases of two amorphous Hamiltonians in three dimensions: a topological superconductor ($\mathbb{Z}$ classification) and a topological insulator ($\mathbb{Z}_2$ classification).

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Spin point groups for weak spin-orbit coupling materials

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Abstract (max 200 words)

Group and representation theory remains a central tool of condensed matter physics, constraining possible band structures, topological phases and beyond, across a wide variety of systems including electronic and magnonic degrees of freedom [1,2,3]. While the space and magnetic space groups describe systems with strong spin-orbit coupling, they are inadequate for materials with intermediate or weak spin-orbit coupling. In these cases, the spin groups are needed, but a full classification of the spin groups and their representation theory has not yet been established in the literature [4,5,6]. In this work, we lay the foundation for this classification by deriving the (co-)representation theory of spin point groups and examine some of their future applications.

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Kondo Phase in Twisted Bilayer Graphene -- A Unified Theory for Distinct Experiments

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Abstract (max 200 words)

Gapless phases in magic-angle twisted bilayer graphene (MATBG) exhibit exotic phenomena beyond naive mean-field descriptions, including (i) zero-energy peaks in spectral density at low temperatures, (ii) a quantum-dot-like cascade of transitions at higher temperatures, (iii) the Pomeranchuk effect where local moment develops upon heating, (iv) resistance peaks in gapless phases at certain integer fillings (v) an asymmetric sawtooth feature of the inverse compressibility, etc. In this work, we point out that all these result from the Kondo effect. We applied analytical and numerical RG analyses to a single-impurity version of the topological heavy fermion (THF) model of MATBG and DMFT+HF calculation to THF model, showing that the Fermi liquid ground states exhibits zero-energy peaks stabilized by Kondo screening, which develop into local moments with higher entropy when increasing temperature. The computed spectral densities, entropies, spin susceptibilities, and chemical potential are quantitatively comparable to experiments. We predict that the ground state in a wide range of fractional fillings is the heavy Fermi liquid and compute its correlated band and energy surfaces. We conjecture that the heavy Fermi liquid is the parent state of the unconventional superconductivity and the "strange metal" may relate to the competition between RKKY interaction and Kondo screening.

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Acknowledgments

Influence of the Surface States on the Nonlinear Hall Effect in Weyl Semimetals

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Nonlinear quantum transport has been a matter of great attention in recent years because it can reveal, among others, new properties of non-magnetic materials. In this work [1] we investigate the impact of the surface states on the second order Hall effect driven by the Berry curvature dipole (BCD) in time reversal Weyl semimetals (WSMs). Starting from a two band model [2] and a slab construction method, we demonstrate that in strongly tilted WSMs the BCD is sensitive to the relative number of states at the surface rather than the bulk, independently of their topological nature, enhancing the corresponding conductivity coefficient in one of the slabs under consideration. Our theoretical predictions are then corroborated by realistic simulations on WTe2 thin films. This research shows that geometry can be even more relevant than topology in nonlinear transport, and it offers an interesting avenue to explore the interfacial engineering of the nonlinear Hall effect in material interfaces and heterostructures.

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Applying uni-axial strain on Sr_2RuO_4

We look into the effects of applying uni-axial strain on the unconventional superconductor Sr_2RuO_4. A progressive strain is applied in two different directions until Van Hove singularity points are formed. Only in one of the directions, a strong enhancement of both T_c and H_{c2} are observed in experiments. The study is done using DFT (Wien2k), and then DFT+DMFT(TRIQS and w2dynamics).

Interacting Topological Phases in Commensurate Magnetic Flux

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The Hall conductivity of insulating many-body systems can be expressed as a function of the many-body Chern number, which is defined over a closed manifold of twisted boundary conditions in real space related to charge transport via flux insertion. Making use of the magnetic translation algebra for quantum Hall systems one can prove [1] similarly to the noninteracting case that the many-body Chern number C is restricted by the relation $e^{2\pi i (C p/q - \rho)} = 1$, with particle density \rho and flux quantum ratio p/q. We criticize the physical implications of this theorem by taking into account the role of spontaneous symmetry breaking for topological phase transitions and numerically investigate interacting quantum Hall phases that can realize trivial insulating phases, despite the preservation of the magnetic translation symmetry.

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Acknowledgments: This work is supported by the Deutsche Forschungsgemeinschaft (DFG) through QUAST-FOR5249 - 449872909 (project TP4)

Single-point spin Chern number for disordered two-dimensional topological insulators

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Abstract (max 200 words)

We present an approach for the calculation of the topological invariant in non-crystalline two-dimensional quantum spin Hall insulators [1]. The introduction of disorder breaks the translational symmetry and implies the use of large simulation cells, where the k-point sampling is typically reduced to the single Gamma point. We introduce a single-point formula [2] for the spin Chern number that enables to study disordered quantum spin Hall insulators within the supercell framework. Inspired by the work of Prodan [3] our approach works even when the spin operator Sz does not commute with the Hamiltonian, as in the presence of Rashba spin–orbit coupling. We validate our method on the Kane-Mele model, both pristine and in presence of Anderson disorder. Then, we investigate the disorder-driven transition from a trivial to a topological phase known as topological Anderson insulator. Finally, we leverage the Wannier-function formalism and deploy our method with ab initio tight-binding Hamiltonians.

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Effective charges in metallic systems

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The contributions of phonons to the dielectric response are quantified by the Born effective charges, describing the electrical polarization induced by the displacement of individual atomic sublattices. While in insulator the electrical polarization is a well-defined quantity and thus the Born Effective charges can be straightforwardly determined in a Berry phase formulation in the context of the modern theory of polarization [1], in metals this quantity is more challenging to deal with. Namely, the effective charges are not defined in a unique way crucially depending on the collision regime of conducting electrons ([2, 3]). In the collisionless (undamped) regime simple models for doped gapped graphene are used to obtain an insight on the nature of the static limit in comparison with the dynamical limit. Furthermore, the results of these models are compared with ab initio simulation of 2D systems ([4, 5]).

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Photo-thermoelectric effect in $MnBi_2Te_4$ devices revealed by scanning photocurrent microscopy

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$MnBi_2Te_4$ is a narrow gap semiconductor that, at low temperatures, hosts antiferromagnetic ordering and Anomalous Quantum Hall edge states. Furthermore, non-linear photocurrent responses have been predicted for this material. In this work, we study the photo-response of devices formed by $MnBi_2Te_4$ flakes with ~100nm of thickness deposited over gold electrodes by scanning photocurrent microscopy. Scanning photocurrent maps (such as the one shown in Fig. 1) at 4K show maximum current when the laser spot (λ=532nm) is placed on the $MnBi_2Te_4$/Au interface and surrounding regions. This behavior is typically associated with the photothermoelectric effect, the sample is locally heated by the light, creating a local increase of charge carriers that results in a diffusion current. This effect has been reported by other authors in MoS_2 [1] and black phosphorus [2, 3] devices. The strength of photothermoelectric effects on $MnBi_2Te_4$, could make this an interesting material for the design of thermo-electric nanodevices and photo-thermal sensors.

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Figures

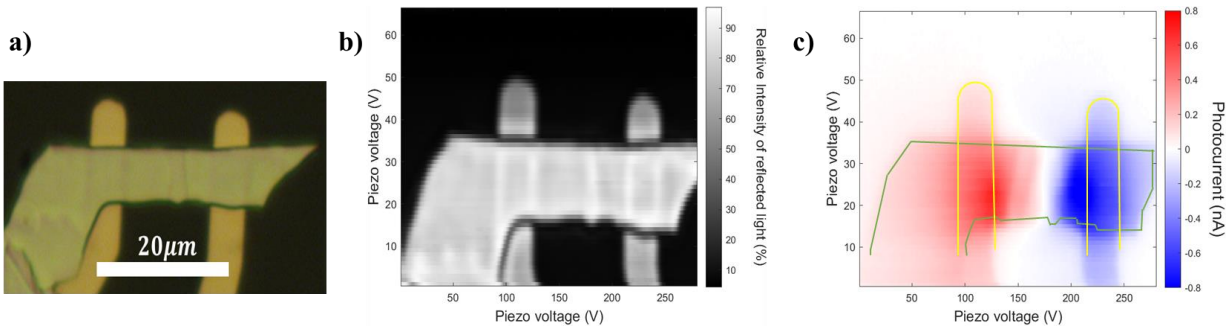

Figure 1: a) Optical microscopy image of a $MnBi_2Te_4$ device. b) Confocal microscopy map recorded simultaneously to c) Scanning photocurrent map for the device in a).

Including electron-hole interactions in non-linear optical responses: workflow to extract the DC shift current

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Optical probes are often used to extract fingerprints of materials, that later can be thought for potential device applications. In the theoretical side, first-principles DFT calculations have allowed the evaluation of macroscopic frequency-dependent responses, both in the linear and beyond-linear field regime. These response functions are found after a self-consistent calculation of the band structure, and therefore do not include many-body correlations beyond mean field. In some scenarios, as in gapped materials, including electron-hole correlations in the theory is a must to correctly match with experiments, even in a qualitative picture. While the inclusion of electron-hole interactions in linear-response calculations is being standardized nowadays, little effort has been put yet in including this theoretical ingredient in the non-linear response. Here, we show our on-going implementation of electron-hole interactions in the second-order AC response to a uniform electric field. We set a workflow to (i) set a gap-corrected band structure in the whole BZ, (ii) solve the exciton many-body states though the BSE equation and (iii) evaluate the shift-current DC response as a first calculation. Our approach is planned to work by using any Hamiltonian in a local orbital basis as the starting point; those include tight-binding models, Wannier functions-based interpolations or first-principles DFT codes using atomic orbitals basis sets.

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[Purely anharmonic charge-density wave in the 2D Dirac semimetal SnP]

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Abstract (max 200 words)

Charge density waves (CDWs) in two-dimensional (2D) materials have been a major focus of research in condensed matter physics for several decades due to their potential for quantum-based technologies. In particular, CDWs can induce a metal-insulator transition by coupling two Dirac fermions, resulting in the emergence of a topological phase. Following this idea, this study explores the behavior of three different CDWs in a new 2D van der Waals material, SnP, using both density functional theory calculations and experimental synthesis to study its stability. The layered structure of its bulk counterpart, Sn_4P_3, suggests that the structure can be synthesized down to the monolayer by exfoliation or chemical means. However, despite the stability of the bulk, the monolayer shows unstable phonons at Γ, K, and M points of the Brillouin zone, which lead to three possible charge- density-wave phases. All three CDWs lead to metastable insulating phases, and the ground-state structure is only revealed due to strong anharmonic effects. Remarkably, the metastable phase driven by the the active phonon in the K point is topologically non-trivial under strain.

Optical evidence of a charge density wave gap in the chiral superconductor TaS_2-4Hb

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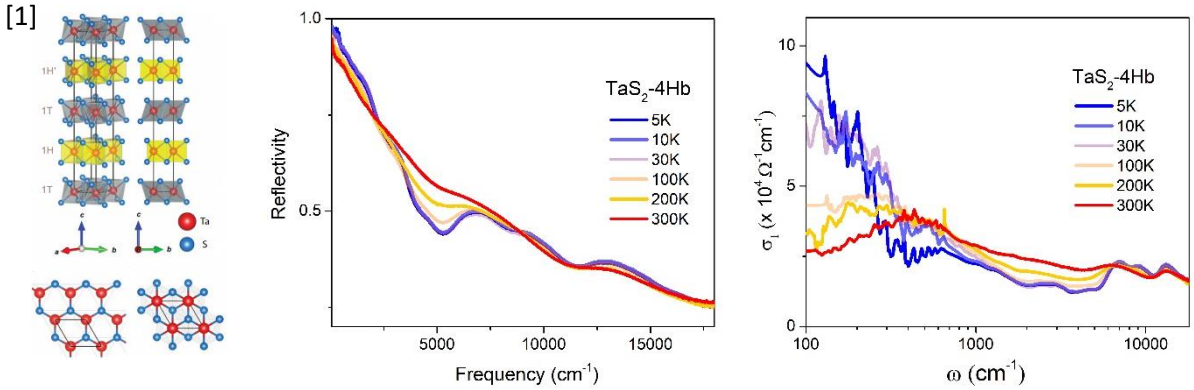
We present the temperature-dependent optical properties of TaS_2-4Hb in the infrared range from 10 meV to 2.5 eV. The 4Hb composition has properties of both, TaS_2-1T, which is a Mott insulator with a quantum spin liquid state, and the superconducting TaS_2-2H. We observe prominent features below 30K in the optical conductivity, $\sigma_1(\omega)$, corresponding to a CDW formation. With decreasing temperature, the interband transitions are reduced and shifted towards the conduction electron contributions, giving rise to an energy gap. Motivated by the recent reports of a time-reversal-symmetry broken state within the chiral superconducting region, T_C = 2.7 K [1,2], and a large magnetoresistance [3], we also look at the Kerr rotation and magnetoreflectivity of this compound in the far-infrared.



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Strain-induced topological phase transitions in kagome lattices

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We study the effects of a uniform strain on the electronic and topological properties of the 2D kagome lattice using a tight-binding formalism that includes intrinsic and Rashba spin-orbit coupling (SOC) [1]. The degeneracy at the Γ point, where a flat-band-parabolic-band touching occurs, evolves into a pair of (tilted) type-I Dirac cones owing to a uniform strain, as shown by effective Hamiltonians, where the anisotropy and tilting of the bands depend in a nontrivial way on the magnitude and direction of the strain field. Interestingly, we find that the Dirac cones become type-III (including flat dispersions) when the strain is applied along the bonds of the lattice. As expected, the inclusion of intrinsic SOC opens a gap at the emergent Dirac points, making the strained flat band to become topological, as characterized by a nontrivial Z2 index. We show that the strain drives the systems into a trivial or topological phase for strains of a few percent, allowing topological transitions via uniform deformations. Additionally, when the Rashba interaction is included, semimetallic phases appear in the topological phase diagrams. These findings suggest an alternative way of engineering anisotropic tilted Dirac bands with tunable topological properties in strained kagome lattices.

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Crossed Andreev Coupling in Parallel InAs Nanowires

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Abstract

Parallel InAs nanowires connected by an epitaxially grown superconductor (SC) shell recently became available to create hybrid nanostructures[1]. The defect-free SC-semiconductor interface and the vicinity of two quasi-one-dimensional channels can enhance the crossed Andreev reflection (CAR) between quantum dots (QD) formed in the separate wires. These properties allow high-efficient Cooper pair splitting (CPS)[2], can lead to the strong hybridization of the QDs resulting in an Andreev molecule[3], or create a SC island-semiconductor hybrid QD[4], which are milestones toward more exotic states, like Majorana or parafermions[5]. We demonstrate the experimental realization of CPS, Andreev molecule, and SC island-QD hybrid in different parallel nanowire-based nanocircuits. The CAR-mediated interaction between parallel QDs is characterized, while the electron transport in the CPS and Andreev limit is analyzed theoretically and matched to the measurements.

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A spatially resolved optical investigation on ruthenates

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Using optical methods to investigate a material is a powerful non-contact method to explore fundamental physics. In our experiment, we use optics as a versatile microscope to investigate optical birefringence as well as thermal transport with micron-scale spatial resolution [1].

We modify a pump-probe setup to measure thermal diffusivity, which is a direct ratio between thermal conductivity and heat capacity of a material. Since thermal conductivity is challenging to measure at high temperatures due to radiation losses, diffusivity is a complementary technique to understanding thermal transport and scattering mechanisms associated with heat and charge transfer.

The optical setup can also be combined with an in-situ controllable uniaxial pressure device, which has recently been shown to be a powerful tuning parameter to control lattice symmetries in quantum materials. We use optical birefringence to image the evolution of domains in Ca3Ru2O7 as a function of uniaxial pressure and temperature.

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Acknowledgments:

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Rethinking α-$RuCl_3$ again

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The honeycomb Kitaev material α-$RuCl_3$ is widely investigated due to its originally suspected proximity to a spin liquid state suggested by unusual neutron scattering results. The magnetic Hamiltonian was initially formulated as a generalized Kitaev model K_1-J_1-Γ_1-$\Gamma_1^{'}$-J_3 in a cubic spin reference orientated along the Ru-Cl bonds. Recent studies, however, suggest that a crystallographic parametrization of the Hamiltonian in a spin-ice-like language $J(XY)$-Δ-$J_{\pm\pm}$-$J_{z\pm}$-J_3 could lead to significant reduction of the parameter space, hinting towards a potential minimal model of α-$RuCl_3$. We present the classical and quantum phase diagram of this $J(XY)$-$J_{z\pm}$-J_3 minimal model candidate obtained by Luttinger-Tisza method (LT), Exact Diagonalization (ED) and Density Matrix Renormalization Group (DMRG). Further, we present the phase diagrams of three interesting parameter regions with constrained anisotropic exchanges K_1,Γ_1,$\Gamma_1^{'}$ leading to effective J_1-J_3 models which possibly capture the relevant region to describe the essential physics of α-$RuCl_3$.
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Quantum geometric photocurrents in topological matter

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A proper quantum mechanical description of condensed matter systems necessitates the inclusion of geometric properties of the wavefunction, such as the Berry curvature and quantum metric, which in turn are intimately linked to topological material properties. The light-matter-coupling can then even be dominated by such quantum geometries. These couplings can be accessed in suitable optoelectronic measurements by the corresponding symmetries and selection rules of the induced photocurrents.

Here, we present recent progress on the development of optoelectronic spectroscopy for light-matter coupling and electronic transport in quantum materials with large quantum geometry. To access the dynamics of quantum geometric interband coupling in narrow gap quantum materials, such as graphene heterostructures, we develop a mid-infrared photocurrent spectroscopy with fs-temporal resolution. Furthermore, we present a combined transport and photocurrent study on the massive Dirac semimetal $HfTe_5$. We show how an external magnetic field can be used to break the time-reversal symmetry of the Dirac Hamiltonian resulting in a net Berry curvature of the Fermi surface. In the latter case, we find that the low-temperature optoelectronic response is dominated by anomalous Hall currents induced by an interplay of the symmetry broken optical excitation and finite Berry curvature.

[Photonic band structure separation and inversion detection with use of machine learning]

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Investigating the topological characteristics of a given photonic crystal requires the precise knowledge of a photonic band structure. Band gaps and band crossings have to be identified, since photonic topological calculations are performed on a group of bands that are touching, crossing, or in other words, are not separated by a full photonic gap [1-5]. Furthermore, a specific class of systems, Z_2 topological photonic insulators, require the identification of band inversion [6]. The band inversion is defined as a change of the ordering of the symmetry eigenvectors of individual bands.

Here we present a method of connecting eigenvalues into bands based on the distance to their neighboring eigenstates in energy and in symmetry. We use an iterative algorithm similar to the k-means clustering, used in machine learning.

Additionally, we present a possibility of an alternative way of identifying the band inversion for Z_2 insulators based on the Wilson loops characteristics.

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Engineering a Skyrmion Crystal in Ferromagnetic/Antiferromagnetic Bilayers Based on Magnetic Frustration Mechanism

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A magnetic skyrmion crystal (SkX), which is a topologically nontrivial swirling spin texture, has attracted attention as the origin of the emergent electromagnetic phenomena. One of the stabilization mechanisms of the SkX is the Dzyaloshinskii-Moriya (DM) interaction. Recently, other mechanisms to stabilize the SkX have been clarified, such as short-range competing exchange interactions [1] and effective long-range exchange interactions mediated by itinerant electrons [2]. These mechanisms without the DM interaction might give a keen insight to understand the origins of the SkXs discovered in centrosymmetric magnets, such as Gd_2PdSi_3 [3] and $GdRu_2Si_2$ [4].

The present study investigates another scenario to stabilize the SkX in a bilayer system without the DM interaction. Specifically, we consider a bilayer triangular lattice system with ferromagnetic and antiferromagnetic layers. By performing the variational calculations and Monte Carlo simulations, we find that such a bilayer system can host the SkX under an external magnetic field and an easy-axis anisotropy depending on the strength of the interlayer exchange interaction. We also obtained the parameter conditions to stabilize the spiral state and the SkX with a finite-Q ordering vector in the strong coupling limit [5].

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Magnetic skyrmion resonance with density control

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Magnetic skyrmions are a candidate for next-generation spintronic devices. Their topological nature makes them robust, allowing for a non-volatile, high-speed, and low-power-consumption method of storing and processing information. In addition, recent advances in skyrmionics have demonstrated both electrical and thermal techniques for controlling skyrmion densities in thin films [1]. In this work we present measurements of magnetic resonance in ferromagnetic multilayers with interfacial Dzyaloshinskii-Moriya interaction. We have performed room temperature experiments utilizing both conventional field-driven ferromagnetic resonance and spin-torque ferromagnetic resonance. We find a difference in the resonance readout between the phases with and without skyrmions, indicating a resonance readout of skyrmions themselves. This observation is further supported by micromagnetic simulations and Lorentz transmission electron microscopy with spatial resolution on the order of a few nanometers, where we directly observe skyrmions in our thin films.

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DFT assessment of Kondo physics in the $Ce_3X_3Bi_4$ (X = Ni, Pd, Pt) family

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Abstract (max 200 words)

The $Ce_3Pd_3Bi_4$ has recently been under intense experimental investigation due to its interesting Kondo physics and to it being an example of a Kondo-Weyl semimetal. It was also found that the Kondo physics in the $Ce_3X_3Bi_4$ family heavily depends on the identity of the d-metal, as the analogues with Ni and Pt are insulators. While these features cannot be explained without taking into account correlation effects, in this work we are conducting a comprehensive DFT analysis of the materials in this family. We focus on $Ce_3Pd_3Bi_4$ and on the topology found in its DFT structure, and we then explore the effects of the d-metal (mostly due to the different spin-orbit coupling on the results of this analysis).

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Imaging electron transport and moiré structures in twisted graphene and rotatable heterostructures

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Twisting graphene-based heterostructures results in local atomic reconstructions which have large consequences in terms of local and global electronic and optical properties. At small twist angle, the moiré superstructure relaxes by forming domains with homogeneous atomic ordering, separated by domain walls (DWs), which play a major role in the observed local and global properties.

We have characterized the DWs superlattices in twisted double bilayer graphene at very small twist angle by piezoresponse force microscopy (PFM) and scattering-type scanning near-field optical microscopy (s-SNOM) in the mid-infrared range. These two techniques provide complementary information. PFM imaging (Fig. 1a) mainly reveals a contrast related to DWs, via flexoelectric effects, bond tensions and atomic orbital alterations. SNOM imaging (Fig. 1b) provides information on local optical conductivity changes within the domains and plasmons reflections at the DWs. We also develop experiments based on scanning gate microscopy (SGM – Fig. 1d), where the tip of an atomic force microscope is used to induce a moving electrostatic perturbation within an electronic device, while the changes in device conductance can simultaneously be mapped. From SGM conductance maps of graphene-based heterostructures, valuable information on charge transport at the local scale can be retrieved. We demonstrate as well how the SGM probe could be used to change in situ the crystalline orientation between two layers of 2D materials (Fig. 1c).

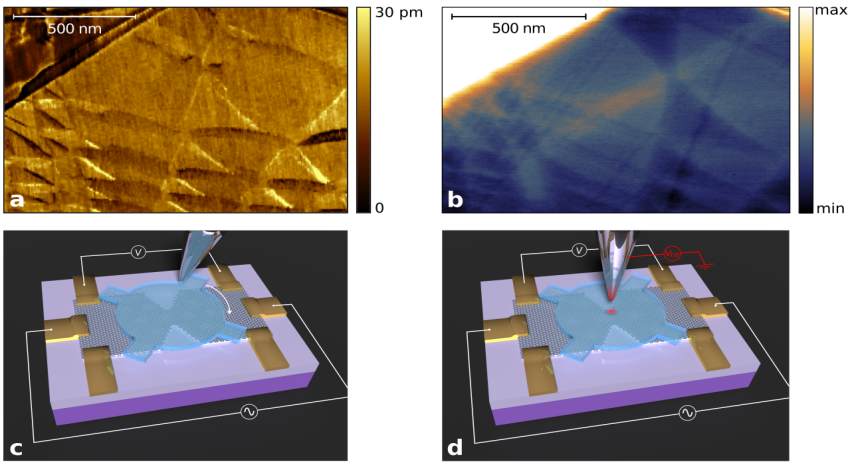

Figure 1: (a) Imaging of twisted double bilayer graphene moiré with PFM, and **(b)** with s-SNOM. **(c)** Schematic illustration of the tip-induced tuning of the twist angle between a hBN “wheel” and an electrically-contacted graphene flake. **(d)** Schematic illustration of the SGM experiment on the same rotatable heterostructure

Keldysh functional renormalization group for quantum magnetic systems

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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, we remedy this shortcoming by establishing a methodical approach based on the Keldysh formalism, originally developed to handle non-equilibrium physics. This novel approach 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.

Ab initio study of the nonlinear optical properties and dc photocurrent of the Weyl semimetal TaIrTe4

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We present a first-principles theoretical study employing nonlinear response theory to investigate the dc photocurrent generated by linearly polarized light in the type-II Weyl semimetal TaIrTe4. We report the low-energy spectrum of several nonlinear optical effects. At second order, we consider the shift and injection currents. Assuming the presence of a built-in static electric field, at third order we study the current-induced shift and injection currents, as well as the jerk current. We discuss our results in the context of a recent experiment measuring an exceptionally large photoconductivity in this material [J. Ma et al., Nat. Mater. 18, 476 (2019)]. According to our results, the jerk current is the most likely origin of the large response.

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Symmetry-based classification of higher-order topological phases of magnons

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In analogy to topology in electronic systems, magnetic excitations can exhibit band topology leading to protected boundary states. So far, mostly d-dimensional magnetic systems with (d-1)-dimensional boundary states have been investigated and classified according to the symmetries of the system. We want to extend this to systems exhibiting higher-order topological phases, which exhibit boundary states of lower dimensionality. We use the method of nested Wilson loops to calculate multipole moments for various models, which can serve as topological invariants to predict higher-order topological behavior. Connecting this to the symmetries of the systems we expect to be able to find a scheme based on symmetry-indicators to directly predict higher-order topology from the magnetic or spin-space groups.

Hall effect measurements as a probe for Weyl-Kondo semimetals

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The interplay of strong correlations and topology is expected to lead to the formation of new phases and phenomena. An example is the recently discovered Weyl-Kondo semimetal, as exemplified by the heavy fermion compound Ce3Bi4Pd3 [1-3]. This noncentrosymmetric but time-reversal invariant compound exhibits a giant spontaneous Hall effect; its characteristics indicate that, even under modest applied electric fields, the material is in a fully nonequilibrium state [2]. Here we summarize these results and report similar measurements on various other candidate materials identified within a new theory-guided selection scheme [4].

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Magnons, Magnon Bound Pairs, and Their Hybrid Spin-Multipolar Topology

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Herein [1], we consider quantum condensed matter systems without particle-number conservation. Since the particle number is not a good quantum number, states belonging to different particle-number sectors can hybridize, which causes topological anticrossings in the spectrum. The resulting spectral gaps support chiral edge excitations whose wavefunction is a superposition of states in the two hybridized sectors. This situation is realized in fully saturated spin-anisotropic quantum magnets without spin conservation, in which single magnons hybridize with magnon bound pairs, i.e., two-magnon bound states. The resulting chiral edge excitations are exotic composites that carry mixed spin-multipolar character, inheriting spin-dipolar and spin-quadrupolar character from their single-particleness and two-particleness, respectively. In contrast to established topological magnons, the topological effects discussed here are of genuine quantum mechanical origin and vanish in the classical limit. We discuss implications for intrinsic anomalous Hall-type transport and estimate that the thermal Hall conductivity brought about by the hybridization of magnons and magnon bound pairs can be as large as that of magnons with other magnons. We conclude that fully polarized quantum magnets are a promising platform for topology caused by hybridizations between particle-number sectors, complementing the field of ultracold atoms working with a conserved number of particles.

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Partition function for topologically-ordered phases

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Abstract

Topological order appears in strongly interacting systems where different phases cannot be distinguished by local symmetries. In two dimensions, it is characterized by point-like quasiparticles known as anyons that interact through self-and mutual- Aharonov-Bohm phases, and a ground-state degeneracy that depends on the surface's topology (sphere versus torus, e.g.). Only recently, experiments have brought evidence for the presence of anyons in the fractional quantum Hall effect [1,2]. Topological order is also expected to be present in spin liquids. Motivated by the dream of using topological order for quantum computation, other recent experiments have led to the observation of anyons in a quantum processor made of superconducting qubits [3,4].

On the theoretical side, one of the most studied toy models for topologically ordered phases is the string-net of Levin and Wen [5]. This model makes it possible to describe a large class of (achiral) topological quantum phases. While the determination of the energy spectrum is straightforward, determining the degeneracies of the excited states is challenging.

In this talk, after a short introduction to the string-net models, I will explain how to compute their energy-level degeneracies. Our results are valid for any achiral topological quantum phase and any surface topology. The degeneracies give access to the partition function of the string-net models, opening the door to the study of finite temperature properties.

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New magnetic topological materials from high-throughput search

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In recent years, topological magnetic materials have received significant attention in the field of condensed matter physics due to their potential for both fundamental research and technological applications. The search for new topologically non-trivial materials has been revolutionized by the formalism of topological quantum chemistry, which maps the symmetry properties of bands to topological properties. Building upon previous research, we conducted a high-throughput search for topological magnetic materials on 521 new, experimentally reported commensurate magnetic structures from MAGNDATA, doubling the number of available materials on the Topological Magnetic Materials database. For each material, we performed first-principle electronic calculations and diagnosed the topology as a function of the Hubbard U parameter. Our high-throughput calculation led us to the prediction of 244 previously overlooked experimentally relevant topologically non-trivial materials, which represent 46.83% of the newly analyzed materials. We present four examples, each showcasing a different topological phase: CaMnSi, a narrow gap axion insulator, Mn_2AlB_2, which exhibits a nodal line semimetal to topological insulator transition, $FeCr_2S_4$, a symmetry-enforced semimetal with double Weyls, and $CsMnF_4$, presenting a new type of quasi-symmetry protected closed nodal surface. Our results demonstrate the power of symmetry-based diagnosis to predict new topological phases of matter in realistic materials.

Edge states and topology in quasicrystals

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This work is based on the union of two research areas that have attracted great interest in recent decades. First, the existence of materials called quasicrystals and second, the study of phases and properties that have been widely classified and are characterized by presenting robust states called topological states. During the last years, multiple works have been devoted to intersection of both areas, pointing out that quasicrystals exhibit topological properties associated with higher dimensional systems [1], which contrasts with the previously made topological classifications.

Here, by using computational tools, the stability of these edge states is studied for systems orders of magnitude larger than those in previous studies [2]. In addition, we study the behavior of the energy gaps against small variations of the Hamiltonian parameters. Based on our results we discuss the conflicts in the available literature and the possibilities (or the lack of them) for reconciling the clash with the existing topological classification.

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Topological protection of transport in fast Thouless pumps in the presence of disorder

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Abstract

Quantized dynamics is essential for natural processes and technological applications alike. It has been shown that quantized particle transport in Thouless pumps is not restricted to the limit of slow driving in non-Hermitian Floquet systems [1]. The degree of topological protection provided by non-Hermiticity in such systems is of great interest. Here we conduct a comparative study of the robustness of directional transport in the presence of static random disorder in two periodically driven systems – quantum ratchet [2] and fast Thouless pumps [1]. In the case of the ratchet, quantized transport relies on a resonant effect that requires fine-tuning of driving parameters. On the contrary, directional transport in Thouless pumping is of a topological origin and observed for a range of driving frequencies considering the closed cycle in parameter space. Our experimental implementation of the models is realized by evanescently coupled dielectric-loaded surface-plasmon polariton waveguide arrays based on the mathematical identity between the coupled mode theory equations and the discrete Schrödinger equation in the tight-binding approximation. Thus, we analyze the effect of topological protection on directional transport by introducing identical disorder distribution to both systems.

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[Interplay between interactions and incommensurability in 1D narrow-band moiré system]

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Quasi-periodicity is a current hot topic in condensed matter systems since it drastically changes the nature of the single particle eigenstates. Even in 1D systems, the states suffer a transition from extended to critical or localized. Here we study the fate of those states in the presence of electron-electron interactions. We consider a 1D tight-binding model with sinusoidal modulated nearest-neighbours hoppings with nearest neighbour repulsion. To study those interactions, we employ a variational mean-field approach. Studying the charge distribution across the lattice we find out that the critical states generate a quasi-fractal charge density wave (CDW) for any finite interaction strength, U, in the incommensurate case, with a high number of wave vectors contributing to the charge order. Increasing U there is a transition to a CDW with much less wave vectors characterized by a peak in the localization length in the wave vector space. On the other hand, in the periodic limit at high potential strength, there is a transition between a gapless state to a Periodic-Moiré CDW with the period of the potential. At sufficiently high U, there is no major difference between the periodic and quasi-periodic cases.

Observation of Berry Curvature Quadrupole in two dimensional Kagome antiferromagnet FeSn thinfilms

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Two dimensional intermetallic Kagome lattices exhibit a topological flat band and a Dirac point in their electronic structure accompanied with long-range magnetic order. Which makes the these systems a fertile ground to investigate strongly correlation and topological band properties in intermetallic lattices. The near-ideal Kagome band structure of the intermetallic Kagome series X_1Y_1 offers opportunities to investigate the interplay among electronic correlations, topology, and magnetism.

We have fabricated epitaxial FeSn thin films using in house Molecular Beam Epitaxy and Performed Nonlinear Hall measurements up to 3rd order as a function of both in plane and out of plane B-field as a function of temperature. Where, we have observed a strong Berry Curvature Quadrupole(BCQ) response at room temperature . We will present our experimental results along with DFT calculations and Monte Carlo simulations .

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Anomalous Hall conductivity and Nernst effect of the ideal Weyl semimetallic ferromagnet $EuCd_2As_2$

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Weyl semimetal is a unique topological phase with topologically protected band crossings in the bulk and robust surface states called Fermi arcs. Weyl nodes always appear in pairs with opposite chiralities, and they need to have either time-reversal or inversion symmetry broken. When the time-reversal symmetry is broken the minimum number of Weyl points (WPs) is two. If these WPs are located at the Fermi level, they form an Ideal Weyl semimetal (WSM). In this study, we grew intrinsic ferromagnetic (FM) $EuCd_2As_2$, predicted to be an ideal WSM, and studied its electronic structure by angle-resolved photoemission spectroscopy, and scanning tunneling microscopy which agrees closely with our first principles calculations. Moreover, we observed anomalous Hall conductivity and Nernst effect, resulting from the non-zero Berry curvature, and the topological Hall effect arising from changes in the band structure caused by spin canting produced by magnetic fields. These findings can help realize several exotic quantum phenomena in inorganic topological materials that are otherwise difficult to assess because of the presence of multiple pairs of Weyl nodes.

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Electronic band structure of an intercalated Transition Metal Dichalcogenide: Co1/3TaS2

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Abstract:

Intercalating transition metal atoms into layers of transition metal dichalcogenides (I-TMDC) can induce magnetic ordering which could simultaneously lead to topological phases [1]. Within the different possible magnetic phases, non-collinear antiferromagnets are specially interesting for their several ground states. Here, we present our results of 2H-TaS2 intercalated with Co, a compound with non-collinear antiferromagnetic triangular ordering. Recently, it was reported for having a large Anomalous Hall Effect (AHE) that arises from a combination of spin-chirality and geometric frustration [2,3] Here, we combine a study of Angle-Resolved Photoemission Spectroscopy (ARPES), DFT calculations and transport measurements to solve the electronic band structure and low temperature phase of Co1/3TaS2. ARPES probes that the intercalation of cobalt atoms give rise to the characteristic Fermi Surface of a Kagome metal. We address the role of magnetism in its electronic structure and look for signals of topological band crossings as signatures of its nature as an antiferromagnetic topological system. In addition, we also explore the effects of Co on the Charge Density Wave (CDW) of 2H-TaS2. The results highlight I-TMDC as tunable systems which can host an interplay between CDW, topological properties and magnetism.

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Haldane Superfluid in the Two-Band Extended Bose-Hubbard Model

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Bosonic particles in periodic potential provide a fertile platform for studying quantum many-body systems with their unprecedented experimental controllability. The Bose-Hubbard (BH) model describes bosonic particles in lattices, and many kinds of generalized BH models have been extensively studied theoretically [1]. The most paradigmatic example is the extended BH model, which includes the nearest-neighbor interaction, and it has led to various novel phases, including the topological Haldane insulator [2]. From the experimental aspect, realizing the phenomena induced by long-range interactions is still challenging. However, a recent study [3] has reported that checkerboard, one of the translational symmetry broken phases due to the long-range interaction, can be observed with dipolar exciton in 2D lattices described in terms of the multi-band BH models. In addition, using particles with strong interactions is crucial for realizing long-range interaction, and the contributions from the higher band are not negligible. Therefore, we study the two-band extended BH model. In particular, we calculate the ground state in the 1D system using the density matrix renormalization group (DMRG) [4] method. We show that the inter-band interactions lead to the Haldane superfluid [5], which has the superfluidity and the non-zero string order.

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Acknowledgments

Fidelity and variability in the interlayer electronic structure of CsV_3Sb_5

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Materials featuring a kagome motif of corner-sharing triangles host a variety of emergent phenomena like magnetic frustration, superconductivity, charge density waves, and non-trivial electronic structure topology. A popular family of kagome materials with the formula AV_3Sb_5 (A = K, Rb, Cs) have attracted attention since these materials exhibit a combination of these phenomena [1]. Many recent studies looking at the charge density wave ordering, high pressures, and chemical doping have pointed to the critical role of interactions between kagome layers [2–4]. Given the two-dimensionality of AV_3Sb_5 single crystals, probing the electronic structure along k_z via experimental methods remains challenging and therefore, rigorous computational approaches are necessary to study these interlayer interactions. Here, we present a first-principles investigation of the electronic structure of CsV_3Sb_5 with emphasis on the k_z dispersion noting how subtleties in the band structure can have broader impacts in calculating topological invariants.

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Large positive magnetoresistance and quantum oscillations in correlated metallic oxide $BiRe_2O_6$

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Topological materials with non-trivial band structures can give rise to several exotic physical properties such as large anomalous Hall effect (AHE), anomalous Nernst effect, colossal magnetoresistance, and superconductivity, which have application potential to future spintronic devices [1,2]. Along this line, 5*d* transition metal oxides exhibit interesting topological properties due to the interplay of spin, charge, orbital, and lattice degrees of freedom [3]. In this poster, I will be presenting large positive magnetoresistance and quantum oscillations in the correlated metallic oxide $BiRe_2O_6$ (BRO). I have grown high purity single crystals of BRO using chemical vapour transport method. It crystallizes in monoclinic structure with space group *C*2/*c* (SG#15) [4]. Interestingly, it exhibits large positive magnetoresistance of 1×10^3 % at 2 K. Unlike other topological semimetals that show large MR, BRO shows high electron carrier density and mobility of 0.5×10^{22} cm^{-3} and 1×10^3 $cm^2\ V^{-1}\ s^{-1}$, respectively, as determined by Hall effect measurements. In addition, a small Fermi surface with a small effective mass was evidenced by de Haas–van Alphen oscillation measurements and band structure calculations. Our findings may trigger intensive studies on topological materials based on oxides.

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