Topological Matter School 2024

Poster abstract booklet



Analysis of the competition between the possible emerging Charge-Density-Wave phases of CsV₃Sb₅

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Since its recent discovery, many studies have tried to characterize the intriguing CDW phases of the family of kagome metals AV_3Sb_5 (A=K, Rb, Cs). Even though unveiling the crystal structure of the CDW phase is crucial to understand the exotic properties of these materials, there is still lack of consensus in the emerging topological phases below the CDW transition temperature (T_{CDW}). Previous theoretical studies showed that this kagome family has phonon instabilities at the M=(1/2, 0, 0) and L=(1/2, 0, 1/2) q-points in the Brillouin zone, what opens the door to a six dimensional CDW order. Later studies showed that the CDW melting is due to ionic entropy, finding the instability in L as triggering mechanism. Here we resolve for the first time the free-energy landscape of the low-symmetry topological phases emerging from the six-dimensional CDW, which leads to a competition of two CDW phases that correspond to the P6/mmm (No. 191) and Fmmm (No. 69) space-groups. By studying the temperature dependence of the free-energy of these phases considering fully the ionic kinetic energy and anharmonicity, we are able not only to get spot on results on the T_{CDW} , but also to understand all the stable topological phases below it.

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The Fragile Phases of Hydrogenated Bismuthene Decorated with Group 16 Adatoms

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In recent years, the field of topological materials has witnessed remarkable progress. In particular, the concept of fragile topology has gathered researchers' attention. Using density functional theory, we study the topological properties of hydrogenated bismuthene decorated with group 16 adatoms. In a structure preserving time reversal and P₆ point group symmetry, we find three bands with topologically fragile nature near the Fermi level. Notably, these bands arise from interaction of p_x and p_y orbitals of the hydrogenated bismuthene and adatoms.

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This work was supported by King Abdullah University of Science and Technology (KAUST).

Perturbative description of d-wave superconductivity in the Hubbard model via unitary transformation and classical spins

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A unitary transformation is applied to the Hubbard model, which maps the Hubbard interaction to a single particle term. The resulting Hamiltonian consists of unconstrained fermions, which is then mapped to a Hamiltonian of spinless fermions coupled to pseudospins. The fermions are integrated out using second order perturbation theory in 1/U, resulting in an effective spin Hamiltonian. An order parameter is identified, stabilizing d-wave superconductivity. The groundstate energy of classical spin configurations is minimized at a finite value of this order parameter after a critical chemical potential, resulting in d-wave superconductivity at non-zero doping. This suggests, that the onset of high-T_c superconductivity is governed by the groundstate of a classical spin system.

References

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[Structural Stability and Electronic Properties of Bi2XI2 (X= Sb, As or P)]

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Abstract (The rapid growth of topological matter research in condensed matter physics has led to the proposal of novel materials using computational methods like Density Functional Theory (DFT). This poster presents the proposal of Bi2XI2 (X = Sb, As, or P) as novel 2D metals, utilizing DFT. These systems exhibit intriguing phenomena, including dynamical stability driven by spin-orbit coupling (SOC). We demonstrate that the inclusion of SOC enhances stability, attributing it to Fermi surface nesting, which significantly influences the electronic properties of these materials.)

References

Acknowledgments

Topological Phonons in AgP2

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Abstract (max 200 words)

Due to recent developments in Topological Quantum Chemistry, the study of the topological propperties of electronic systems is well known. However, for phononic systems the implications of topological labels are not fully understood. Using the tools developed for the creation of the Topological Phonon Database, we will study the case of AgP2 (mp-ID: mp-8200): an ideal case of an Obstructed Atomic Band Representation (OABR). More precisely, we will obtain the surface states of AgP2 and see how they are influenced by the bands corresponding to OABRs. Afterwards, we will show the effect of topology on the selection rules for Raman and IR scattering of this compound.

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Acknowledgments

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Multiplicative Chern Insulators

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The tensor product of two Chern Insulator Hamiltonians yields a 'child' Hamiltonian with distinct topological characteristics separate from the two 'parent' phases. Extending on the previous work on Multiplicative Topological Phases [1], here we study in-depth the topological characterization and magnetic response of the Multiplicative Chern Insulator (MCI). Due to its multiplicative structure, the MCI has several discrete symmetries derived from its parents – however, we find that the child topological phase hosts edge modes robust against symmetry breaking disorders that also break the multiplicative structure. In light of this fact, we attempt a topological classification of the MCI based on the Topological Skyrmion Phases of Matter [2], which entails topological invariants and bulk boundary correspondences beyond the traditional ten-fold classification of topological insulators and superconductors. We also study the magnetic response of the MCI, which yields bulk spectral flow of a single charge upon insertion of two flux quanta possibly hinting at fractionalization and effective many-body physics in multicomponent, ostensibly non-interacting systems.

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Investigation electric properties of the Weyl semimetal GdPtBi under uniaxial strain

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Abstract

GdPtBi is a cubic Half-Heusler compound with antiferromagnetic ordering below 9 K, displaying topological properties at low temperatures, such as AHE and negative magnetoresistance (MR). Uniaxial strain investigation showed variation in AHE and in the negative MR curve, suggesting that compression diminishes these effects, while tension enhances them. Further analysis of the MR curve revealed that the initial drop in MR at low magnetic fields, possibly indicative of weak localization effect, diminished under compression. Examining high fields, quantum oscillations demonstrated movement in the electronic bands. Changes in resistivity below $T_{\rm N}$ also indicated a movement in the band structure, although the transition itself remained unaffected.

Dynamical correlations and order in magic-angle twisted bilayer graphene

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In magic angle twisted bilayer graphene, transport, thermodynamic and spectroscopic experiments pinpoint at a competition between distinct low-energy states with and without electronic order, as well as a competition between localized and delocalized charge carriers. We utilize Dynamical Mean Field Theory (DMFT) on the topological heavy Fermion (THF) model of twisted bilayer graphene to investigate the emergence of electronic correlations and long-range order in the absence of strain.

At integer fillings, we find that low energy spectral weight is depleted in the symmetric phase, while we find insulating states with gaps enhanced by exchange coupling in the zero-strain ordered phases. Doping away from integer filling results in distinct metallic states: a "bad metal" above the ordering temperature, where scattering off the disordered local moments suppresses electronic coherence, and a "good metal" in the ordered states with coherence of quasiparticles facilitated by isospin order. This finding reveals coherence from order as microscopic mechanism behind the Pomeranchuk effect. Upon doping, there is a periodic charge reshuffling between localized and delocalized electronic orbitals leading to cascades of doping-induced Lifshitz transitions, local spectral weight redistributions and periodic variations of the electronic compressibility ranging from nearly incompressible to negative.

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Manifestation of the quantum metric in chiral lattice systems

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The Aharonov-Bohm effect is a physical phenomenon where the vector potential induces a phase shift of electron wavepackets in regions with zero magnetic fields due to an obstruction in space associated with a magnetic flux. A similar effect can be observed in solid-state systems, where the topology of the Berry connection can influence electron dynamics. These are paradigmatic examples of how the dynamics can be affected by the system's geometry. Here, we show that in chiral-symmetric processes the quantum metric has a measurable effect on the mean chiral displacement of delocalized wavefunctions. This finding is supported by a photonic experiment realizing a topological quantum walk, and demonstrates an effect that can be attributed directly to the geometry of the state space.

Di Colandrea, F., Dehghan, N., Cardano, F., D'Errico, A. and Karimi, E., 2024. Manifestation of the Berry connection in chiral lattice systems. *arXiv preprint arXiv:2401.07946*. (Accepted in Nat Comm Phys)

Topological flat bands in d -wave superconductors

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In systems belonging to the symmetry class CI, the presence of time-reversal, particle-hole and chiral symmetry allows for the appearance of topologically non-trivial phases. In the case of dx2-y2-wave superconductors, these are characterized by a winding number defined on noncontractable closed loops with fixed k//. For non-zero values, the bulk-edge correspondence guarantees 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.

Here we show the results obtained from tight-binding models as well as our Angle-Resolved Photo-Emission Spectroscopy (ARPES) measurements, where we further demonstrate the use of a recently established approach to cleave crystals for angleresolved photoemission studies in which the fracture propagation is controlled by means of micro-notches.

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Topological Phase Transitions of Interacting Fermions in the Presence of a Commensurate Magnetic Flux

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Motivated by recently reported magnetic-field induced topological phases in ultracold atoms and correlated Moiré materials, we investigate topological phase transitions in a minimal model consisting of interacting spinless fermions described by the Hofstadter model on a square lattice. For interacting lattice Hamiltonians in the presence of a commensurate magnetic flux it has been demonstrated that the quantized Hall conductivity is constrained by a Lieb-Schultz-Mattis (LSM)-type theorem due to magnetic translation symmetry. In this work, we revisit the validity of the theorem for such models and establish that a topological phase transition from a topological to a trivial insulating phase can be realized but must be accompanied by spontaneous magnetic translation symmetry breaking caused by charge ordering of the spinless fermions. To support our findings, the topological phase diagram for varying interaction strength is mapped out numerically with exact diagonalization for different flux quantum ratios and band fillings using symmetry indicators. We discuss our results in the context of the LSM-type theorem.

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Noncollinear textures in moiré magnets

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Abstract

Two-dimensional magnetism and moiré physics are two very rapidly growing fields due to recent experimental advances. In this work, we demonstrate how noncollinear magnetic textures may arise in a bilayer of two-dimensional ferromagnets when the interlayer Heisenberg coupling is stacking dependent. In particular, we focus on the chromium halides CrX3 and study theoretically how the magnetic textures can be controlled through a twist, strain, or an external magnetic field. We find that ferromagnetic and antiferromagnetic regions can coexist by forming noncollinear textures in two dimensions. These can be controlled and forced to undergo spin-flip or spin-flop transitions through the external parameters.

Long Range Interactions in Synthetic Dimensions

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In recent cold atom experiments, the utilization of internal degrees of freedom as synthetic dimensions has enabled the simulation of higher-dimensional systems. Specifically, magnetic quantum numbers have been employed to transform a 1D chain of atoms into a synthetic 2D lattice, resulting in the realization of an integer quantum Hall state. However, this configuration introduces highly anisotropic and long-range particle interactions. To facilitate theoretical analysis, we use finite size Tree Tensor Networks to simulate truly 2D physics. The high connectivity of this ansatz allows us to explore the impact of long-range interactions on the phases realized in the system. Our investigation delves into the emergence of new phases, the study of phase transitions, and the stability of configurations under the influence of extreme long-range interactions. This research contributes to a deeper understanding of the intricate interplay between synthetic dimensions and particle interactions in cold atom systems.

Detecting SPT Signatures and Projective Representations in Free-Fermion Topological Crystalline Insulators

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The many-body quantum numbers of OD collective excitations bound to crystal and electromagnetic defects (such as magnetic fluxes and monopoles) provide powerful indicators of bulk topology, in that they can indicate the presence of quantized responses in the bulk that are governed by long-wavelength topological field theories that are stable to symmetric interactions. In interacting symmetry-protected topological phases (SPTs), defect quantum numbers frequently indicate nontrivial bulk topology if they transform in projective representations of the local symmetry group. We here introduce numerical methods for computing defect quantum numbers in stable and fragile free-fermion topological crystalline insulators (TCIs) via the reduced density matrix, revealing a deep connection between defect quantum numbers and the entanglement spectrum. We surprisingly find that when crystal symmetries are included in the local symmetry group, defects can appear to transform projectively even in Wannierizable (fragile) insulators. Our framework systematically characterizes stable and fragile TCIs beyond filling anomalies and higher-order topology, allowing direct connections between free-fermion TCIs and interacting SPTs.

References

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Quasiparticle Interference in Charge Density Wave Phase Of 2H-NbSe₂

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Charge density waves (CDWs) are fascinating quantum phenomena that affect various physical properties of their host. CDWs in pristine $2H - NbSe_2$ have been a topic of intense research. In the CDW phase, numerous scanning tunnelling microscopy (STM) probes¹ confirm the localization of the electron density of states (LDOS). In this work, we use an impurity scattering model to achieve similar LDOS patterns as observed in STM experiments. We further use this model to show that QPI caused by inter-K pocket transitions, led by a skew scattering mechanism, is responsible for the features seen in STM probes. We also show that acoustic phonon modes emanating from in-plane Nb orbitals and out-of-plane Nb orbitals $4d_{x^2-y^2}$, $4d_{xy}$, $4d_{z^2}$, are most likely responsible for the cocurrence of CDW features.

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Interplay of superconductivity and charge-density-wave order in kagome materials

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In several superconductors, the superconducting state emerges out of a chargedensity-wave (CDW) order. To determine the microscopic origin and structure of the ordered phases, one often studies the CDW and superconductivity independently. However, the mutual influence of the individual orders can be crucial for understanding the phase diagram. An intriguing example is the AV3Sb5 (A=K,Rb,Cs) family of superconductors, where a 2x2 in-plane CDW ordered phase, potentially breaking time-reversal symmetry, appears at a temperature of approximately 100K, followed by a transition into a superconducting phase at T_c ~1-3K.

In our work, we present a phenomenological theory of CDW and superconducting orders for the kagome lattice. In particular, we derive a Ginzburg-Landau free energy of possible superconducting and 2x2 CDW orders and explore the impact of their mutual coupling. Considering a CDW as input, we focus mainly on the coupling to s-wave and triple-Q spatially modulated superconductivity, investigating the consequences of which provides the leading instability. By considering additional spatial or time-reversal-symmetry breaking of the CDW order, we explore a rich phase diagram. We also discuss the implication of strain on our conclusions. Our results can guide future microscopic calculations as well as the experimental identification of the nature of the superconducting state.

Nanoscale patterned superlattices in topological insulator thin films

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Nanoscale patterned superlattices in topological insulators are predicted to renormalize the Dirac velocity of the surface states and correspondingly enhance electronic interactions, which may ultimately result in the emergence of correlated states, such as topological superconductivity [1]. To fabricate superlattices with the required lattice constants on the order of 10 nm, we discuss the application of He-ion beam milling. The helium ion microscope has is a versatile tool for both nanoanalytics and nanoscale fabrication with a resolution below 10 nm [2]. We characterize the transport in the superlattices by magneto-and optoelectronic transport. For the latter, we extend optoelectronic measurements from near-infrared (from 0.8 μ m) to mid-infrared wavelengths (up to 20 μ m). The latter may allow a selective excitation and read-out of the surface state and its quantum geometric properties [3] without contribution from bulk bands.

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Acknowledgments

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d-mon: Transmon with Strong Anharmonicity

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Superconducting (SC) qubits are ubiquitous in the quantum community and Transmontype devices are the industry standard for SC qubit architecture. Conventional Transmons suffer from weak anharmonicity which leads to slow qubit operation and possibility of errors due to qubits leaving the computational subspace. *d*-mon is a novel Transmon-type qubit which overcomes this problem by using s/d SC Josephson Junctions instead of s/s junctions used in Transmons. We use a simple Ginzburg-Landau argument and numerical calculations to show that such junctions can have strong tunable anharmonicity while still being insensitive to offset-charge noise as in the original Transmon. We also show that *d*mon has a gapped quasiparticle spectrum which provides advantages over other similar setups using d/d junctions which suffer from quasiparticle poisoning.

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Epitaxial two-dimensional superconductor TaC encapsulated by graphene and 2D silicon carbide

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Abstract

We demonstrate ultra-thin (3 nm) films of tantalum carbide on silicon carbide-substrates, with the entire 7 mm x 7 mm surface area encapsulated by two-dimensional SiC and graphene[1]. This is substantiated through a range of surface science techniques, including SPM, LEEM, LEED, ARPES, HR-TEM, XPS, and XRD. Our methodology combines top-down patterning of the as-deposited TaC films with bottom-up growth of graphene, facilitating self-ordered (epitaxial) formation of TaC nanowires within devices while ensuring surface protection by graphene.

The composite TaC/graphene system exhibits superconducting properties, with a transition temperature $T_c \sim 10$ K and critical magnetic fields Bc ~ 1.5 T (perpendicular) and Bc > 14 T (parallel). Transport measurements indicate characteristics of a two-dimensional superconductor, for which the Ginzburg-Landau coherence length (~ 15 nm) exceeds the film thickness (3 nm). Combined with the estimated London penetration depth (~ 60 nm), this gives an upper limit to depairing current of 2 x 10⁸ A/cm².

We further discuss quantum critical behavior recently indicated in measurements, and the potential of using TaC/graphene films in quantum information technology: The graphene encapsulation eliminates the oxide present in most superconducting films, introducing new surface chemistry to improve coherence in superconducting devices.

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Probing fusion multiplicity of non-Abelian anyons in the anyon collider

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Anyons are exotic particles characterised by non-trivial exchange properties. While Abelian anyons yield a fractional phase under exchange, the hallmark of non-Abelian anyons is the existence of an internal degeneracy or fusion multiplicity [1].

The first evidence for fractional statistics in Abelian anyons came from the "anyon collider" experiment [2]. In contrast to conventional adiabatic exchange of anyons, this experiment probes exchange of "real" anyons with "virtual" anyon-antianyon pairs created at a quantum point contact [3, 4]. Noise measurements contain fingerprints of the latter exchange process.

Here, we consider the exchange of "real" non-Abelian anyons with "virtual" non-Abelian anyon-antianyon pairs [5]. The exchange leads to a rotation of the fusion channels. We find that noise measurements akin to the Abelian case are not sensitive to the fusion multiplicity of non-Abelian anyons. We show rather that current measurements in the same geometry can access the fusion multiplicity. Our result quantitatively probes the fusion multiplicity of non-Abelian anyons, bearing implications for contemporary experiments.

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Electronic structure and charge density wave ordering in the antiferromagnetic Kagome compound FeGe

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Abstract:

Metallic Kagome systems have been raised recently as a new material hosting topological flat bands, Dirac crossings, and van Hove singularities that intertwine with charge density waves (CDW), magnetism, and superconductivity [1-3]. Topological flat bands, hosting a large electron density of states near the Fermi level, are a subject of considerable recent interest for realizing unusual forms of charge-density-wave order [4-6]. FeGe is particularly interesting since it exhibits multiple-Q CDWs that coexist with antiferromagnetic (AFM) order and populate the phase diagram [7,8]. We found a dimerization-driven 2D hexagonal chargediffuse precursor present in this system and the fraction of dimerized/undimerized phases is an important order parameter of the continuous CDW phase transition. Furthermore, we use angle-resolved photoemission spectroscopy to observe all three electronic fingerprints of the Kagome lattice in FeGe. Kagome flat bands are observed near the Fermi level. The larger agreement between the experimental and ab initio band structure, without the need for any renormalization factor, downplays the correlation effects to describe the electronic band structure of FeGe. The melting of the CDW in FeGe mediated by topological defects is found to be significantly influenced by the temperature and momentum dependency of the critical scattering parameter.



(a) Exotic Electronic orders in Kagome lattice including Superconductivity, charge density wave (CDW), and Topological state. (b) Schematic representation of the ideal band structure of Kagome lattice with Dirac cones (DC), Van Hove singularity (VHS), and flat band (FB) in momentum space. (c)-(d) Fermi surface and electronic band structure of FeGe. (blue bands from ARPES and orange bands from DFT). (e) Geometric structure of FeGe. (f)-(g) Temperature dependence diffuse scattering mapping of (h k 2) and (h k 3/2) planes, respectively.

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Raman circular dichroism of chiral Quantum spin liquids

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Abstract

We investigate the Raman circular dichroism (RCD) of chiral Quantum spin liquids as a probe of the topological properties of fractionalised spin excitations. Starting from the Loudon Fleury formalism we show that the scattering Intensity is directly related to the light matter coupling formalism of spinon bands. We reveal that the RCD signal arises as a result of the Berry curvature and Quantum geometry contributions. We show application to different model quantum spin liquids.

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Extracting Topological Information from the Interface Green's Function

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In condensed matter physics, topology is a field concerned with the inherent symmetries of a quantum many-body system unaffected by adiabatic deformations. Topological physics has gained a lot of momentum over the recent years due to the fact that the robust bound states at the boundaries of topological materials have potential applications in quantum information technology. However, it is yet to be seen how we can reliably access the topology of a quantum many-body system in an experiment.

Green's function formalism is a powerful tool for theoretical characterization of quantum many-body systems while being relatively accessible in experiments such as angle-resolved photoemission spectroscopy (ARPES) or scanning tunnelling microscope (STM) measurements. Here, we present an interface Green's function formalism [1], that we have applied to the Su-Schrieffer-Heeger (SSH) model [2]. We have found that the topologically non-trivial phases are closely related to zeros of the inverse interface Green's function.

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Orbital Competition in Bilayer Graphene's Fractional Quantum Hall Effect

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The lowest Landau level of bilayer graphene has an octet of internal degrees of freedom, composed from spin, valley and orbital two-level systems. Dominance of n = 0 orbitals over n = 1 orbitals in low energy quantum fluctuations leads to distinct fractional quantum Hall characteristics compared dominance of n = 1 over n = 0. The competition between n = 0 and n = 1 orbitals depends sensitively on particle-hole asymmetry and on Lamb shifts due to exchange interactions with the negative energy sea, which must be accounted for simultaneously in assessing the orbital competition. We identify the circumstances under which n = 1, which supports strong evendenominator FQH states with non-abelian quasiparticles, emerges robustly as the low-energy Landau level.

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Towards 2D metal-organic frameworks on weakly interacting substrates: Fe-DCA on coinage metals and Bi₂Se₃(111) surfaces

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The formation of 2D metal-organic frameworks (MOFs) featuring ferromagnetically coupled metal atoms on the surface of a topological insulator (TI) is theoretically predicted to induce an exchange gap in the surface band structure which can potentially lead to a quantum anomalous Hall effect. However, the experimental demonstration of MOFs at TI surfaces is still missing. Here, we show the first experimental realization of long-range ordered 2D MOF, Fe-dicynoanthracene (Fe-DCA), on the Bi₂Se₃(111). 2D MOFs were prepared by co-deposition of metal and organic ligands on substrate held at room temperature. Their structure and morphology were studied via scanning tunneling microscopy (STM) and low-energy electron microscopy (LEEM) and diffraction (LEED). We compare the growth of Fe-DCA on the Bi₂Se₃(111) surface with coinage metals surfaces and discuss the conditions at which we obtain closed packed (Fig. 1b) and Kagomé lattices (Fig. 1c). The demonstration of 2D MOF/TI hybrid material presents a milestone on the way towards their application in fault-tolerant spin interconnects in future quantum devices.



Fig.1: (a) DCA molecules in three-folded coordination with Fe atom, ball-and-stick model taken from [1]. (b) STM atomic resolution of Fe-DCA framework on the surface of TI Bi₂Se₃(111). The highlighted area shows the estimated hexagonal structure. (c) Model of the structure with mixed Kagome and honeycomb lattice of DCA taken from [2].

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Quantum oscillations of the quasiparticle lifetime

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Following nearly a century of research, it remains a puzzle that the low-lying excitations of metals are remarkably well explained by effective single-particle theories of non-interacting bands even though mutually interacting electronic states are a property of essentially all materials. This raises the question of direct spectroscopic signatures of phenomena beyond effective single-band behavior. Here, we report the identification of quantum oscillations (QOs) of the quasiparticle (QP) lifetime, which defy the standard description in two fundamental aspects. First, the oscillation frequency corresponds to the difference of semiclassical QP orbits of two bands, which are forbidden as half of the trajectory would oppose the Lorentz force. Second, the oscillations persist to much higher temperatures compared to the basis frequencies. The only precondition for their existence is a non-linear coupling of at least two electronic orbits, e.g., due to QP scattering on defects or collective excitations. We show that the underlying notion of QOs without corresponding Fermi surface is in excellent agreement with the three-dimensional topological semimetal CoSi and several other materials. Our theory also offers an unexpected new perspective on Fe-based superconductors, where a spontaneously emerging QO frequency has up to now been understood as Lifshitz transition, potentially leading to an incorrect assessment of the Fermi surface.

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Investigation on the electronic structures of RTi₃Bi₄ distorted kagome magnets

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Abstract

Kagome materials with van Hove singularities (VHSs), Dirac points (DPs), and flat bands serve as a versatile platform to explore electron correlation, magnetism, topological phases, and their interplay [1]. Recently, a new family of kagome magnets, RTi₃Bi₄ (R: rare-earth element) have been reported, displaying orthorhombic *Fmmm* lattice structures due to distorted Ti kagome lattices [2,3]. Unlike AMn_6Sn_6 compounds where kagome layers exhibit exchange interactions [4]. Ti kagome layers in RTi₃Bi₄ compounds remain nonmagnetic. The reduced in-plane symmetry in these compounds may lead to novel topological phases or quantum phenomena unprecedented in other kagome materials. However, both theoretical and experimental investigations on these compounds are currently insufficient. In this presentation, we unveil the electronic structures of RTi₃Bi₄ (R = Nd, Sm, Gd) investigated via angle-resolved photoemission spectroscopy (ARPES) and density functional theory (DFT). Our analysis reveals anisotropic kagome bands due to the distorted kagome lattice, and band splitting potentially indicating magnetic interactions or surface states. Our work not only elucidates the electronic structures of this new kagome family, but also provides a fresh platform to understand quantum phenomena in magnetic kagome materials.

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Majorana Fermion Mean-Field Theories

in Kitaev Quantum Spin Liquids

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We determine the phase diagrams of anisotropic Kitaev-Heisenberg models on the honeycomb lattice using parton mean-field theories based on different Majorana fermion representations of the S = 1/2 spin operators. First, we use a twodimensional Jordan-Wigner transformation (JWT) involving a semi-infinite snake string operator [1] and consider the limit of extreme Ising exchange anisotropy. Second, we use the conventional Kitaev representation in terms of four Majorana fermions [2] subject to local constraints, which we enforce through Lagrange multipliers. The interaction terms were determined self-consistently to construct the phase diagrams as a function of the anisotropy of the Kitaev couplings and the relative strength of the Ising exchange. While both mean-field theories produce identical phase boundaries for the topological phase transition between the gapless and gapped Kitaev quantum spin liquids, the JWT fails to correctly describe the magnetic instability and finite-temperature behavior. Our results show that the magnetic phase transition is first order at low temperatures but becomes continuous above a certain temperature. At this energy scale, we also observe a finite-temperature crossover on the quantum-spin-liquid side, from a fractionalized paramagnet at low temperatures, in which gapped flux excitations are frozen out, to a conventional paramagnet at high temperatures [3].

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Observation of Flat Bands in Ultrathin Kagome Lattice Nb₃X₈ by Angle-Resolved Photoemission Spectroscopy

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Abstract

Flat bands, where the energy does not depend on momentum can give rise to exotic properties, including spin-liquids [1] and high-temperature superconductivity [2]. Due to the unique geometry, the kagome lattice can naturally exhibit flat bands and host a variety of exotic states. Nb₃X₈ [3] is a recently discovered group of symmetry lowered kagome systems with triangular distortion. Materials in this family are insulating in nature, and are theorized to be obstructed atomic insulators [3], as well as nearly ideal Mott insulators in thin limit [4]. Experimental verification of their electronic structure, however, is still lacking. Here, I will present our recent experimental band structure investigation of Nb₃X₈ (X=Cl, Br, I) kagomes by means of angle-resolved photoemission spectroscopy (ARPES) in their bulk and ultrathin limit and report our findings.

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Role of quantum geometry in spin-fluctuation-mediated interaction

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The discovery of unconventional superconductivity (abbr. UcSC) in $CeCu_2Si_2$ provided the first example of superconductivity (abbr. SC) beyond the BCS paradigm. In many instances, materials exhibiting UcSC were observed to have also a magnetically ordered phase close to, or coexisting with, the SC phase(s). [1] This has led to theoretical investigations on spin-fluctuations as the common source of both [2,3].

Motivated by the work on flat-band superconductors where quantum geometry affects the transport [4], we investigate the role of quantum geometry in the strength of spin fluctuations. A recent success [5] demonstrated that in the ferromagnetic limit the quantum geometric tensor alters the shape of the free susceptibility. We pursue along these directions and extend the analysis to consider interactions [6] in an Hartree-Fock Random Phase Appoximation (abbr. HF-RPA) for ferromagnetic and antiferromagnetic cases.

Present analytical and numerical study of the RPA-renormalised susceptibilities suggests that the well-defined geometric contribution is specific to the case of non-interacting ferromagnetic susceptibility and the corrections from interactions show no explicit dependence on the quantum geometry at the RPA level.

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Topological properties of a non-Hermitian quasi-1D chain with a flat band

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The spectral properties of a non-Hermitian guasi-1D lattice in two of the possible dimerization configurations are investigated. Specifically, it focuses on a non-Hermitian diamond chain that presents a zero-energy flat band. The flat band originates from wave interference and results in eigenstates with a finite contribution only on two sites of the unit cell. To achieve the non-Hermitian characteristics, the system under study presents non-reciprocal hopping terms in the chain. This leads to the accumulation of eigenstates on the boundary of the system, known as the non-Hermitian skin effect. Despite this accumulation of eigenstates, for one of the two considered configurations, it is possible to characterize the presence of non-trivial edge states at zero energy by a real-space topological invariant known as the biorthogonal polarization. This work shows that this invariant, evaluated using the destructive interference method, characterizes the non-trivial phase of the non-Hermitian diamond chain. For the second non-Hermitian configuration, there is a finite quantum metric associated with the flat band. The two non-Hermitian diamond chains can be mapped into two models of the Su-Schrieffer-Heeger chains, either non-Hermitian, or Hermitian, both in the presence of a flat band. This mapping allows to draw valuable insights into the behaviour and properties of these systems. [1]

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Figures



Figure 1: Sketch of the non-Hermitian diamond lattice in the A and B configurations, panel (a) and (b), respectively.



Figure 2: Phase diagram of the DCA model along with the biorthogonal polarization of two cuts in this phase diagram.

Injection of vortices into a Majorana edge-mode: a time-dependent simulation

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The chiral edge modes of a topological superconductor can transport fermionic guasiparticles, with Abelian exchange statistics, but they can also transport non-Abelian anyons: Edgevortices bound to a π -phase domain wall that propagates along the boundary. A pair of such edge-vortices is injected by the application of an h/2e flux bias over a Josephson junction. Existing descriptions of the injection process rely on the instantaneous scattering approximation of the adiabatic regime [Beenakker et al. Phys.Rev.Lett. 122, (2019)], where the internal dynamics of the Josephson junction is ignored. Here we go beyond that approximation in a time-dependent many-body simulation of the injection process, followed by a braiding of mobile edge-vortices with a pair of immobile Abrikosov vortices in the bulk of the superconductor. Our simulation sheds light on the properties of the Josephson junction needed for a successful implementation of a flying topological gubit.

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Planar Hall effect in Weyl semimetals induced by pseudoelectromagnetic fields

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The planar Hall effect (PHE) is the appearance of an in-plane transverse voltage in the presence of coplanar electric and magnetic fields. In Weyl semimetals (WSM), the PHE has been ascribed to the chiral anomaly and Berry curvature effects [1]. In the presence of position- and time-dependent perturbations, such as strain, WSMs respond as if they were subjected to emergent electromagnetic fields, known as pseudofields [2]. In this work, we investigate the possibility of inducing both linear and nonlinear phenomena, including PHE, via an applied strain in a more realistic model of WSM that includes the effects of anisotropies and tilted Weyl nodes. Using the chiral kinetic theory in presence of pseudofields, we derive general expressions for the magnetoconductivity tensor by considering the simultaneous effects of the Berry curvature and orbital magnetic moment (OMM) of carriers [3]. Since pseudofields couple to the Weyl fermions of opposite chirality with opposite signs, we study chirality-dependent phenomena, including the longitudinal magnetoconductivity and the PHE, and find that the contributions stemming from the Berry curvature and OMM are of the same order of magnitude. We apply our results to real materials such as the highly anisotropic and tilted monophictide TaAs [4].

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Topological Classification of Chiral Symmetric 1D Interfaces

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Abstract (max 200 words)

A chain of magnetic impurities embedded into an s-wave superconductor bind Yu-Shiba-Rusinov states [1], creating in gap bands that can be tuned through a topological phase transition [2]. The topological classification of such an interface cannot be done through conventional methods, due to the dimensional mismatch and local nature of topological bands bound to the impurity chain. We study the topological classification of 1D chiral symmetric interfaces embedded into a 2D substrate. A proof of the validity of a topological classification based on the local Green's function [3] by explicit evaluation of the topological invariant is presented. Further, we show that due to entanglement between the in-gap modes and the substrate, the full physics of the substrate that is contained in the Green's function is required. This is done by considering a classification scheme derived from reduced ground state projector [4] which we show produces erroneous changes in the topological index due to entanglement driven gap closures.

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Hybridization and topological phase transitions in chiral twisted bilayer graphene

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Perhaps one of the most challenging novel materials due to the great plateau of phases that it exhibits is twisted bilayer graphene (TBG), and indeed this huge number of phases is the result of the interesting interplay between strong electron-electron interaction that TBG has and its intrinsic topological nature. It is well-known that the zero energy flat bands appearing in the middle of the spectrum in TBG seem to play a crucial role in strongly correlated phases, such as non-conventional superconductivity. However, understanding how the zero-energy flat band interacts with higher bands that are remote by an energy gap and what kind of hybridization process happens is still challenging. Here is presented a study that delve into these questions and explain the hybridization mechanisms between the zero energy flat bands and sub-sequence higher bands, their relationship with the Chern number (C), and berry curvature. Additionally, the orbital magnetic energy is expressed in terms of the Berry curvature. Finally, we propose some experiment setups for measuring this new wide array of phases with C= ± 2 .

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Bulk-interface correspondence from quantum distance in flat band systems

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The bulk-boundary correspondence is an integral feature of topological analysis and the existence of boundary or interface modes offers direct insight into the topological structure of the Bloch wave function. While only the topology of the wave function has been considered relevant to boundary modes, we demonstrate that another geometric quantity, the so-called quantum distance, can also host a bulk-interface correspondence. We consider a generic class of two-dimensional flat band systems, where the flat band has a parabolic band- crossing with another dispersive band. While such flat bands are known to be topologically trivial, we show that the nonzero maximum quantum distance between the eigenstates of the flat band around the touching point guarantees the existence of boundary modes at the interfaces between two domains with different chemical potentials or different maximum quantum distance. Moreover, the maximum quantum distance can predict even the explicit form of the dispersion relation and decay length of the interface modes.

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Topological responses from gapped Weyl points in 2D altermagnets

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Altermagnetism combines of both ferromagnetism aspects and antiferromagnetism, breaking spin degeneracy while possessing no net magnetization. In this work, we study the symmetry requirements for topologically protected Weyl points in 2D altermagnets, involving bands with the same spin quantum number. We classify all spin-wallpaper groups whose symmetries protect 2D Weyl points and show that their nontrivial topology is charactrized by a quantized π -Berry phase. Representative electronic tightbinding and magnonic linear spin-wave models are constructed to investigate the unusual transport characteristics of these 2D Weyl points. Different mass terms, induced for example through strain or via coupling to light or a substrate, gap out the Weyl points leading to emerging gapped topological phases. Depending on the mass terms, these phases carry finite Chern and/or spin Chern numbers and exhibit protected edge states as well as anomalous electronic and thermal Hall responses. We calculate these Hall currents for the different topological phases.

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Luttinger surface dominance and Fermi liquid behaviour of topological Kondo insulators SmB6 and YbB12

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Abstract

In the last years an increasing effort has been devoted to study the role of topology beyond the non-interacting picture. Here we first consider a model for a Quantum Spin Hall Insulator [1] (QSHI) and we add an on site Coulomb repulsion between the electrons. Using the Dynamical Cluster Approximation we investigate the role of the non-local correlations in the QSHI-MI (Mott Insulator) phase transition [2]. Between the QSHI and the MI we find a crossover to a phase where both topological poles and zeros of the Green's function coexist in a novel phase we dubbed "Topological Pseudogap Insulator".

We invoke the phenomenology of this novel phase to understand the remarkable dichotomy that has been observed in the topological Kondo insulators SmB6 and YbB12. Prompted by the peculiar mixed-valence nature of these compounds, involving f and d electrons of the lanthanide, we argue that the f and d subsystems, when considered separately, act, respectively, as electron- and hole-doped Mott insulators, featuring Fermi pockets coexisting with Luttinger surfaces responsible for the pseudogap. When the two are coupled to each other a hybridisation gap opens up and the whole turns into a topological insulator endowed with genuine chiral edge states. However, the Luttinger surfaces persist and support neutral quasiparticles.

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Witnessing environment induced topological phase transitions via quantum Monte Carlo and cluster perturbation theory studies

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Abstract

Many-body interactions play a fundamental role in quantum topological systems, being capable to alter the topological classifications of noninteracting fermion systems [1]. In open quantum systems, where interactions with the environment lead to dissipation and decoherence of the fermionic dynamics, the absence of Hermiticity in the subsystem Hamiltonian drastically reduces the stability of the topological phases of the corresponding closed systems [2,3]. Here, we explore the nonperturbative impacts of the environment on the prototype Su-Schrieffer-Heeger chain, which is connected to local harmonic oscillator baths via either intracell or intercell transfer integrals. Contrary to common belief, this form of coupling, when appropriately designed, is able to generate a transition into topological phases. Using a world-line quantum Monte Carlo technique, we establish the model's phase diagram, demonstrating that the bimodal probability distribution of polarization signifies the onset of the topological phase. Additionally, we illustrate that a qualitative description can be attained through an approach developed in cluster perturbation theory, offering an effective non-Hermitian Hamiltonian for the fermionic subsystem and insights into dissipative dynamics. Furthermore, we validate that non-Hermitian effects vanish in the presence of classical heat baths [4].

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Flat-band ratio and quantum metric in the superconductivity of modified Lieb lattices

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Flat bands may offer a route to high critical temperatures of superconductivity. It has been predicted that the quantum geometry of the bands as well as the ratio of the number of flat bands to the number of orbitals determine flat band superconductivity [1,2]. However, such results have assumed at least one of the following: an isolated flat band, zero temperature, mean-field theory, and/or uniform pairing. Here, we explore flat-band superconductivity when these assumptions are relaxed.

The superconducting order parameter, critical temperature, superfluid weight, and Berezinskii-Kosterlitz-Thouless temperature are calculated for different versions of the Lieb lattice within dynamical mean-field theory. We find that while the flat-band ratio and quantum geometry are good indicators of superconductivity near zero temperature, at finite temperatures the behavior is more complicated and the other bands near the flat band(s) are crucial. Furthermore, we find that at least in lattices with uniform pairing condition, the superfluid weight at non-zero temperatures is determined by the zero-temperature superfluid weight and order parameters at the given temperature.

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ΔT noise in multiterminal hybrid systems

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We focus on the study of the noise properties of hybrid multiterminal out-of-equilibrium normal-superconducting systems. Research has focused mainly on the transport properties of such systems; when studies of noise are made, they are usually limited to the case without temperature differences [1] [2]. Recently, intriguing results have been reported on the thermal and thermoelectric properties of nanoscale devices. However, related discussions on noise and cross correlations remain mostly limited to normal systems [3] [4], with interest in hybrid systems increasing only in recent years [5]. Here, instead, we deeply investigate the role of stationary non-equilibrium thermal conditions in the behavior of charge current noise power. By using the Landauer-Büttiker approach [6], we are able to distinguish two main contributions, called background and excess noise, highlighting differences and similarities between hybrid superconducting systems and normal ones. Namely, we notice that in hybrid systems the background noise depends on a quantity strictly related to the heat conductance, the transmission function ℓ^- . This does not appear in the noise of purely normal systems, which instead depends only on the electrical conductance-related quantity ℓ^+ . The excess noise instead shows, as expected, additional contributions due to the currents' partitioning into transport channels of particles of different types, this being caused by the presence of Andreev conversion processes in the system. After analyzing numerically the behavior of the various contributions of the excess noise by varying both the electrical and thermal boundary conditions, we resort to the study of noise in two specific physical configurations: we compare in both cases the behavior of the shot noise at thermal equilibrium and of the ΔT noise at electrical equilibrium, finally stressing the noticeable differences between electrically- and thermally-induced current fluctuations.

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RVB pairing in flat bands

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Materials with flat bands, that is, dispersionless Bloch bands, have attracted interest in reaching the high temperature superconductors. In flat bands, individual particles are localized but interacting particles can have non-zero group velocity.

The problem is that in high-temperature superconductors, the pairing interaction is often not mediated by phonons as in the BCS theory, the microscopic theory explaining superconductivity in conventional superconductors [1]. Instead, the pairing mechanism is under debate. An alternative model proposed to explain high-temperature superconductors is the resonance-valence-bond (RVB) pairing [2], where the interaction is mediated by spin fluctuations.

Within mean-field scheme, we approach the RVB model analytically and test our results numerically on various lattice models that are typically used in the flat band studies. Our aspect is to study if any properties to increase the critical temperatures can emerge.

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Broadband enhancement of second-harmonic generation at the domain walls of magnetic topological insulators

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Abstract (max 200 words)

Electromagnetic field interacting with a topologically protected one-dimensional electron helical state is shown to support a one-dimensional plasmon-polariton, which is a collective electron excitation dressed with the electromagnetic field. The electronic helical state arises at the surface of three-dimensional topological insulator in the proximity of the ferromagnet and is localized at the magnetization domain wall. This opens the possibilities to manipulate quantum optical states by altering magnetic domain configurations. An exact spectral equation for such topological plasmon-polariton is derived. We show that the second-harmonic generation (SHG) is enhanced in the chiral one-dimensional electron currents in a broad frequency range. The origin of the enhancement is twofold: first, the linear dispersion of plasmon-polariton result in the lift of the phase-matching condition. Moreover, the strong field localization leads to the further increase of the SHG in the structure. The results suggest that the chiral currents localized at the domain walls of magnetic topological insulators can be an efficient source of the second-harmonic signal in the terahertz frequency range.

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Acknowledgments

Thermal Hall transport in Semi-classical Magnets

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In recent years, the thermal Hall effect has emerged as a powerful tool for probing topological phenomena of magnetic systems. At low temperatures, the thermal Hall transport of long-range ordered magnets can be described in the framework of linear spin-wave theory (LSWT). However, how to treat regimes with increased thermal fluctuations or non-linearities beyond LSWT is an outstanding question. Therefore, within this project, we developed a novel numerical technique to extract the thermal Hall transport properties, which intrinsically includes non-linear effects. In particular, we use semi-classical spin dynamics simulations to compute topological thermal edge currents in the Kitaev honeycomb model on a cylinder geometry. The results are expected to shed new light on the topological thermal transport in Kitaev spin liquid candidate materials.

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Acknowledgments

Multifractality in fractal systems

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Abstract (max 200 words):

Eigenstate multifractality is a major characteristic of non-interacting disordered metals near the metal–insulator transition and is believed to be present in the Many-Body Localized (MBL) phase. This phenomenon holds significant promise for applications in quantum annealing, machine learning, and potentially superconductivity. In three-dimensional systems, multifractality can emerge under specific strong-disorder conditions, while in two-dimensional systems, it can appear even with weak disorder. In this work, we demonstrate that eigenstate multifractality can be induced purely through geometric manipulation by placing impurities on a lattice and reshaping it into fractal geometries. We provide a comprehensive analysis of multifractality for the Sierpinski carpet and gasket, presenting evidence for non-ergodic multifractal extended states. Potential experimental applications are also discussed.

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Relativistic Corrections to LO-TO Splitting

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A polariton is a quasiparticle resultant from the interaction between electromagnetic radiation and collective excitations within a material. Among these, the phonon polariton emerges as a hybrid mode that encompasses both phonon and photon characteristics. It describes the propagation of longwavelength light within a polar crystal. This study tackles the inherent challenges linked to investigating these modes in the mixing region. It employs the path integral formalism to derive the relative weights of the original components within the hybrid mode. To achieve a comprehensive understanding of phonon polaritons, a microscopic perspective is adopted. This approach aims at providing a more precise description of the coupling mechanisms involved, thereby enhancing our comprehension and facilitating the interpretation of experimental outcomes. A comparative analysis is conducted with the Density Functional Theory approach, which is constrained to large wavevectors due to its neglect of relativistic effects. Additionally, a comparison is made with the classical macroscopic theory, revealing its limitations in terms of predictive capabilities.

Magnetic exchange coupling to the skyrmion crystal on the electronic states of topological insulator

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The effect of magnetic exchange coupling to the spatially inhomogeneous fields of a skyrmion crystal on the electronic spectrum of the surface electronic states of topological insulator was discovered. It was shown that periodic magnetic and pseudomagnetic fields leads to a nontrivial topology of the electronic bands, namely the localized topologically protected edge states appear in the band gap of energy spectrum. It was analytically demonstrated that the magnetic field created by a skyrmion crystal can be represented as an effective vector potential, which is proportional to the topological charge.

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Quantum Theory of X-ray Photon Correlation Spectroscopy

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Abstract (max 200 words)

With the development of X-ray Free Electron Lasers (XFELs) [1], we have achieved a highly tunable coherent light source which can probe the dynamic of a system of the Angstrom in length scale and femtosecond in timescale via the X-ray Photon Correlation Spectroscopy (XPCS). However, the usual analysis of the XPCS is based on the classical dynamics of the system, i.e. Siegert relation, and usually fails to describe the quantum dynamics in the materials. Here, we propose a quantum theory to describe the g2 correlation measurement with the 4-point density correlation of the electronic system of interests. We found the Siegert relation is violated even in the non-interacting fermions due to the exchange correlation. In addition, we have calculated the 4-point density correlation in the Kitaev 1D superconducting chain which shows distinct features between topological and trivial phases, suggesting the potential of the probe to classify topological order.

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Magnon-Electron Tuned Topology in Magnetic Weyl Semimetals

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The recently identified topological materials Co₃Sn₂S₂ [1] and MnBi₂Te₄ [2], with intrinsic ferromagnetic and antiferromagnetic ordering respectively, have drawn a lot of interest in the interplay between magnetism and topology [3]. Giant anomalous electric and thermal transport has been detected in Co₃Sn₂S₂ while the manipulation of the Weyl nodes via the rotation of the magnetization has been identified as a possible source of large transport signatures [3]. Generally, in these studies, the quantum and temperature-dependent nature of magnetization is overlooked, exemplified by the interaction between electrons and magnons. Inspired by the prediction of electron-phonon interaction-driven topological phase transition predicted in Ref. [5], we examine the influence of electron-magnon interaction on the properties of electrons of selected topological magnetic materials. A model that tackles the magnon-electron interaction, for systems with multiple bands of electrons and magnons, is developed that works both for ferromagnetic and antiferromagnetic orders. Using quantum field theory techniques, we compute the band renormalization induced by this interaction in both ferromagnetic and antiferromagnetic topological models as a function of the temperature, highlighting the impact of interactions on the lifetimes of magnons and electrons, their transport properties, and topological phase transitions.

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Softening of a flat phonon mode in the kagome ScV6Sn6

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Geometrically frustrated kagome lattices are raising as novel platforms to engineer correlated topological electron flat bands that are prominent to electronic instabilities. As well as AV3Sb5 and FeGe, the kagome system ScV6Sn6 hosts a Chage Density Wave (CDW) phase. Here, we demonstrate a phonon softening at the $kz = \pi$ plane in ScV6SN6 at the temperature of the CDW transition phase [1]. Angle-Resolved Photoemission Spectroscopy (ARPES) unveils a momentum-dependent suppression of the intensity due to band folding in the low temperature phase. Inelastic X-Ray Scattering (IXS) and Diffuse Scattering show that the low energy longitudinal phonon collapses at ~98 K and $\mathbf{q} = (1/3, 1/3, 1/2)$ due to the electron-phonon interaction, without the emergence of long-range charge order which sets in at a different propagation vector $\mathbf{q}_{CDW} = (1/3, 1/3, 1/3)$. Theoretical calculations corroborate the experimental finding to indicate that the leading lattice instability is located at (1/3, 1/3, 1/2) of a rather flat mode. We relate the phonon renormalization to the orbital-resolved susceptibility of the trigonal Sn atoms and explain the approximately flat phonon dispersion. Our data report the first example of the collapse of a kagome bosonic mode and promote the 166 kagome compounds as primary candidates to explore correlated flat phonon-topological flat electron physics.

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Electronic properties of the epitaxial thin films of Fe₃Sn₂

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Quantum materials with a kagome lattice structure are a promising platform for condensed matter research due to their peculiar topological, electronic, and magnetic properties. Intermetallic compounds of tin and iron with a general formula of Fe_xSn_y are formed by stacking Fe_3Sn kagome bilayers and stannene layers along the c-axis alternatively[1]. Kagome materials host novel electronic properties such as topological flat bands, Dirac cones, and fractionalized topological phases due to spin-orbit coupling, electron correlations, and magnetism. [2][3].

We have prepared Fe_3Sn_2 epitaxial thin films on Pt(111) single crystal and Pt(111) layers deposited on Al_2O_3 (0001) substrate by using molecular beam epitaxy under ultra-high vacuum conditions. The low energy electron diffraction showed sharp diffraction spots of (2x2) periodicity with respect to the Pt(111) substrate. The scanning tunneling microscopy gives a hexagonal arrangement of atoms, characteristic of stannene and Fe_3Sn kagome layer. The samples have been transferred to the Solaris synchrotron in Krakow for further studies of the films using x-ray photoelectron spectroscopy and angle-resolved photoemission. We have observed clear electronic dispersions in the valence band with the signatures of the flat bands close to the Fermi level. Moreover, the films are characterized ex-situ using x-ray diffraction and conversion electron Mössbauer spectroscopy.

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Relative higher-order topology in Weyl materials

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The recent development of topological quantum chemistry has provided a useful framework for identifying topological crystalline insulators, offering a systematic and efficient approach to classify topological phases based on crystal symmetries [1,2]. In particular, systems with inversion symmetry are characterised by three weak \mathbb{Z}_2 indices and a strong \mathbb{Z}_4 index. The even-valued \mathbb{Z}_4 indices distinguish trivial insulators from higher-order topological insulators (HOTIs), namely 3D bulk insulators with gapped surface states that manifest gapless 1D hinge states [3]. On the other hand, the two phases with odd-valued \mathbb{Z}_4 indices exhibit similar behaviour to each other; both are Weyl semimetals, possessing Weyl points and Fermi arc surface states. This naturally raises the question regarding the distinction between them, if any exists. Here, we draw on the corner charge pump argument [4] to theoretically establish the existence of gapless hinge states between the two topological phases. We show they are robust and thereby illustrate a form of relative higher-order topology through the bulk-boundary correspondence. Finally, we construct a single-band tight-binding model as a concrete demonstration of these relative hinge states.

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Atomistic Calculations of Filling Dependent Electronic States in Magic Angle Twisted Bilayer and Trilayer Graphene

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Moiré materials offer a promising platform for designing tunable simulators of 2D strongly correlated, topological systems. In magic angle twisted bilayer graphene, the moiré lattice potential leads to the formation of flat bands at the Fermi level, which host a variety of strongly correlated phases [1]. The bands can be populated by up to eight electrons per moiré unit cell, due to four flavours (two spins and two valleys) per two energy bands. Insulating states at integer fillings, and superconductivity between them, were already observed [2-3]. Similar phenomena was seen in mirror-symmetric magic angle twisted trilayer graphene, which has better tunability of its electronic structure and superconducting properties [4].

In this work we determine the electronic properties of both platforms using an *ab initio* based, multi-million atomistic p_z tight-binding model [5]. Using Hartree-Fock methods, we determine the evolution of the ground state as a function of the filling factor, including spin occupancy. We analyze the role of the long- and short-range Coulomb interactions and their influence on the band structure of the twisted bi- and tri-layers. We also determine the topological aspects of bands, focusing on the quantum geometry and the potential in realizing integer and fractional Chern insulator states.

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Observation of Flat Bands in Ultrathin Kagome Lattice Nb3X8 by Angle Resolved Photoemission Spectroscopy

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Flat bands, where the energy does not depend on momentum can give rise to exotic properties, including spin-liquids [1] and high-temperature superconductivity [2]. Due to the unique geometry, the kagome lattice can naturally exhibit flat bands and host a variety of exotic states. Nb3X8 [3] is a recently discovered group of symmetry lowered kagome systems with triangular distortion. Materials in this family are insulating in nature, and are theorized to be obstructed atomic insulators [3], as well as nearly ideal Mott insulators in thin limit [4]. Experimental verification of their electronic structure, however, is still lacking. Here, I will present our recent experimental band structure investigation of Nb3X8 (X=Cl, Br, I) kagomes by means of angle-resolved photoemission spectroscopy (ARPES) in their bulk and ultrathin limit and report our findings.

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