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2021

Keynote talks

Parton picture of doped antiferromagnets: signatures in theory and experiment

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Recent experimental advances, both in solids as well as quantum simulators, allow unprecedented microscopic studies of the structure of strongly correlated quantum matter. In the Fermi-Hubbard model, believed to underlie high-Tc superconductivity, this allows to revisit a decades-old idea that strongly interacting electrons may fractionalize into partons — loosely speaking, the analogues of quarks in high- energy physics — called spinons and chargons. In this talk I will give an overview of recent theoretical and experimental results supporting this idea. A particular focus will be on dynamical signatures of parton formation, which also reveal their strong and non-local interactions. Moreover, I will discuss spectroscopic signatures of the parton picture, and how I envision quantum simulators will be able to probe the structure of emergent mesons in the near future.

[1] Bohrdt et al., arXiv:2101.09280
[2] Ji et al., Phys. Rev. X 11, 021022 (2021)
[3] Bohrdt et al., New J. Phys. 22, 123023 (2020)
[4] Bohrdt et al., Phys. Rev. B 102, 035139 (2020)
[5] Grusdt et al., Phys. Rev. X, 8, 011046 (2018)

From quantum many-body scars to time crystals: entanglement steering via periodic driving

Maksym Serbyn[1]

[1]*Institute of Science and Technology, Austria*

In my talk I will discuss a new mechanism of the weak ergodicity breaking relevant for the experimentally realized Rydberg-atom quantum simulators [1]. This mechanism arises from the presence of special eigenstates in the many-body spectrum that are reminiscent of quantum scars in chaotic non-interacting systems [2]. After review of different mechanisms that lead to scars, I will discuss more recent experiments [3] that demonstrated that coherent revivals associated with quantum many-body scars can be stabilized by periodic driving, generating stable subharmonic responses over a wide parameter regime. I will propose a simple model which explains experimental phenomena by spatiotemporal ordering in an effective Floquet unitary, corresponding to discrete time-crystalline (DTC) behavior in a prethermal regime. Unlike conventional DTC, the subharmonic response exists only for Neel-like initial states, associated with quantum scars. I will discuss robustness to perturbations and identify emergent timescales that could be observed in future experiments.

[1] H. Bernien, et al., Nature 551, 579–584 (2017), arXiv:1707.04344
[2] C. J. Turner et al., Nature Physics (May 2018), arXiv:1711.03528 and Phys. Rev. B 98, 155134 (2018) arXiv:1806.10933
[3] D Bluvstein, et al., arXiv:2012.12276
[4] N Maskara, A A Michailidis, WW Ho, D Bluvstein, S Choi, M D Lukin, M Serbyn, arXiv:2102.13160

Ultrafast Photocurrents in a Topological Insulator – an Inside View

Hadas Soifer[1]

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Topological insulators have been in the focus of condensed-matter research in recent years. In particular, much effort was dedicated to optically excite and control currents involving the topological surface states. We use time- and angle-resolved photoemission spectroscopy (trARPES) to image the unoccupied band structure of a topological insulator as its population evolves following an optical excitation, and observe the signature of a photo-induced current [1]. By analyzing the rise times of the population, we gain a complete view of the occupied and unoccupied electronic states, and how they are coupled by the optical excitation. This enables us to determine that photocurrents are excited only via the resonant optical transitions coupling to spin-orbital textured states. Our work provides a microscopic understanding of how to control photocurrents in materials with spin-orbit coupling and broken inversion symmetry.

[1] H. Soifer et al., Phys. Rev. Lett. 122, 167401 (2019)

Lattice, charge, orbital and spin dynamics studied with ultrashort X-ray pulses

Roman Mankowsky[1]

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Selective optical excitation of low energy degrees of freedom can manipulate the material properties of strongly correlated materials on ultrafast timescales. In this talk, I will present in two examples how the energy tunable, femtosecond x-ray pulses of Free electron lasers can be used to selectively follow the electronic, magnetic and structural degrees of freedom, shedding light on their interaction.
In the first part of the talk, we will discuss, how the resonant excitation of a substrate phonon mode can induce propagating changes of the magnetic, structural and charge order in a $NdNiO_3$ Nickelate thin film, similar to how static strain engineering is used to design materials properties. $NdNiO_3$ grown on $LaAlO_3$ shows an insulator-metal transition at 130 K, involving melting of magnetic AFM and charge order as well as a structural change. While these changes all occur at the same temperature in equilibrium, they become transiently decoupled during the optically induced phase change.
The second part of the talk concerns the frustrated $Tb_2Ti_2O_7$ pyrochlore, which exhibits an exotic spin-liquid phase. In the low temperature regime, low energy optically active excitations are observed that are related to hybrid modes of coupled magnetic, orbital and structural degrees of freedom. Here, I will present our ongoing investigation on the resonant excitation of these modes with strong field THz pulses and the induced coherent orbital and structural dyamics. Whereas the atoms simply follow the electric field of the THz pulse, the orbital order is resonantly excited, showing oscillating also after the excitation field is over.

Topological physics and strong correlations in the 2D kagome network

Riccardo Comin[1]

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The kagome network is a tiling of two-dimensional space comprised of corner-sharing triangles, and one with the same point symmetries as the hexagonal lattice of graphene. Recent theoretical developments suggest that the combination of magnetism, spin-orbit coupling, and geometric frustration in kagome metals is a promising platform to realize phenomena at the intersection of topology and strong correlations, such as the fractional quantum Hall and intrinsic anomalous Hall effect. Here, a major role is played by the three distinctive features of the kagome electronic band structure, namely the Dirac points, the van Hove singularity, and the flat bands.

In this talk, I will report on studies of the experimental band structure of various kagome compounds to highlight the rich physics arising from the combination of topology, magnetism, and correlations, and the prospects for further exploration of new phenomena in this class of materials.

In the first part, I will discuss the family of transition metal stannides (Fe_3Sn_2, FeSn, and CoSn). In these systems which intertwine robust magnetism and electronic topology, we observed various manifestations of topological physics. These include the realization of the Kane-Mele model for 2D Dirac fermions with a spin-orbit-induced topological gap, as well as the discovery of the elusive flat bands with nontrivial topology.

In the second part, I will discuss our most recent studied of the AV_3Sb_5 family of correlated kagome metals, where superconductivity and charge-density-waves have been found to coexist. Here, I will focus on the role of the van Hove singularity in creating the conditions for multiple instabilities of the Fermi surface and the emergence of collective electronic phases.

Invited talks

Moiré heterostructures: a condensed matter quantum simulator

Dante M. Kennes[1]

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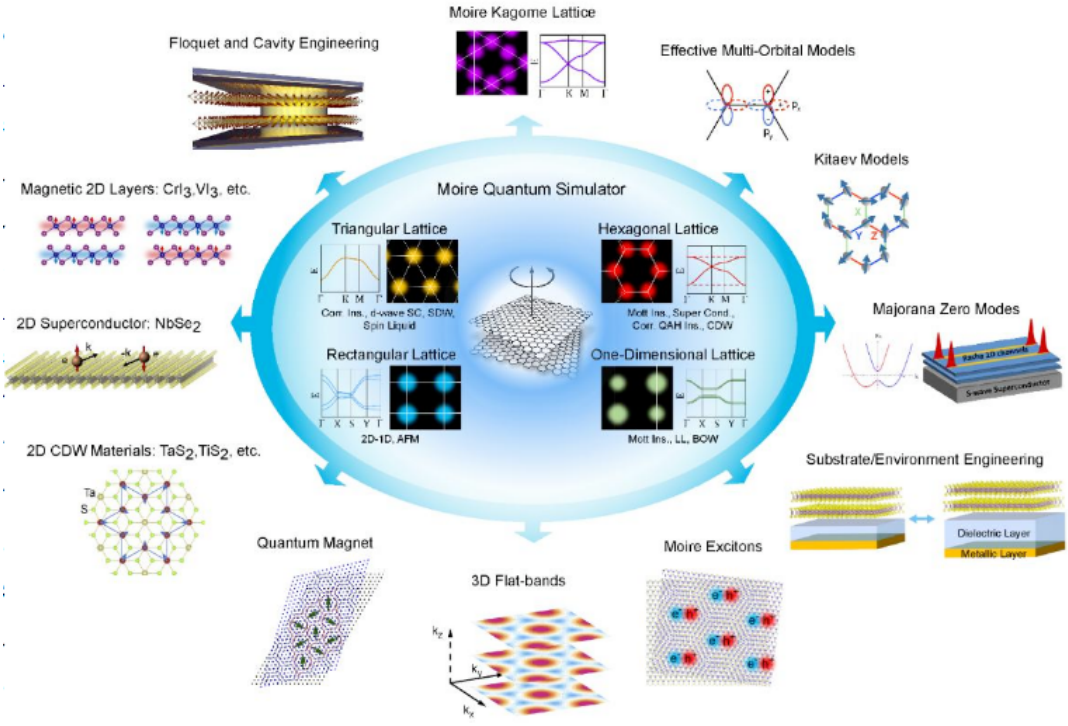
We propose twisted van der Waals heterostructures as an efficient, reliable and scalable quantum platform that enables the seamless realization and control of a plethora of interacting quantum models in a solid state framework. These new materials hold great promise to realize novel and elusive states of matter in experiment. We survey these systems as platform to study strongly correlated physics and topology that is notoriously difficult to study computationally [1]. Among the features that make these materials a versatile toolbox are (i) tunability of properties via readily accessible external parameters (such as gating, straining, packing and twist angle), (ii) ability to realize and control a large number of fundamental many-body quantum models relevant inthe field of condensed matter physics and beyond and (iii) state-of-the-art experimental readouts exist to directly map out their rich phase diagrams in and out of equilibrium. This general framework, besides unravelling new phases of matter, permits to identify their key microscopic ingredients and therefore to robustly realize and functionalize those new phases in other material systems, deepening our fundamental understanding and holding many promises for future technological applications. As examples we discuss our recent findings in twisted bilayer graphene, bilayer BN, double bilayer graphene, bilayer WSe_2, bilayer MoS_2, bilayer GeSe and generalizations to three dimensions [2].



[1] Nature Physics 17, 155 (2021)
[2] Nature 572, 95-100 (2019), Nature Communications 11, 1124 (2020), Nature Materials 19, 861 (2020), Phys. Rev. B 102, 085109 (2020), Phys. Rev. B 103, 041103 (2021), PNAS January 26, 2021 118 (4), Nat. Comm. 12, 242 (2021), arXiv:2004.02964, arXiv:2012.09649

Quantum Impurity Physics in Circuit Quantum Electrodynamics

Roman Kuzmin[1], Nicholas Grabon[1], Nitish Mehta[1], Amir Burshtein[2], Moshe Goldstein[2], Vladimir Manucharyan[1]

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We present a new approach to analog simulations of quantum impurity problems in circuit quantum electrodynamics. Our approach relies on the phenomenon of single photon decay, which is the decay of a microwave photon into lower energy photons driven by a local quantum non-linearity (impurity) [1, 2]. Although there is no practical analog for a single photon decay in traditional quantum optics, this phenomenon is ubiquitous in the bosonic description of strongly correlated 1D systems, which is at the heart of the modern understanding of strongly correlated phenomena. We illustrate our approach with a generic quantum impurity, consisting of a weak Josephson junction galvanically embedded into a long section of a high-impedance transmission line. Using the photon lifetime data, we successfully verified the outcome of the simulation in the parameter regime available to analytical calculations. With minor modifications of the impurity circuit, the technique can easily be applied to many other quantum impurity models relevant in the description of electron tunneling in Luttinger liquids, dissipative phase transitions, and Kondo impurities.

[1] R. Kuzmin et al., PRL 126, 197701 (2021)
[2] A. Burshtein et al., PRL 126, 137701 (2021)

Simulation of quantum chemistry with quantum computers and neural networks

Antonio Mezzacapo[1]

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We present two novel approaches for the electronic structure problem. First, we review the recent efforts at IBM to simulate quantum chemistry using quantum computers, which exploit the exponential memory advantage of qubits to encode many-body systems. Then, we will show a new approach to classical numerical computation of electronic structure that relies on neural network quantum states, which may help in capturing quantum correlations beyond existing numerical methods.

High-harmonic generation in strongly correlated systems

Yuta Murakami[1]

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High-harmonic generation (HHG) is an intriguing nonlinear phenomenon indued by a strong electric field. It has been originally observed and studied in atomic and molecular gases, and is used in attosecond laser sources as well as spectroscopies. An observation of HHG in semiconductors expanded the scope of this field to condensed matters [1]. The HHG in condensed matters is attracting interests since it may be used as new laser sources and/or as powerful tools to detect band information such as the Berry curvatures.
Recently, further exploration of the HHG in condensed matters are carried out in various other systems than semiconductors.
In this talk, we introduce our recent theoretical efforts on the HHG in strongly correlated systems [2,3,4]. In contract to semiconductors, the charge carriers are not normal fermions, which makes HHG in strongly correlated systems unclear. Using the dynamical-mean field theory and the infinite time-evolving block decimation for the Hubbard model, we reveal the HHG features in the Mott insulators. Firstly, we reveal that the origin of the HHG in the Mott insulator is the recombination of doublons (doubly occupied sites) and holons (no electron site). Then, we show that the HHG feature qualitatively changes depending on the field strength due to the change of mobility of charge carriers, and discuss that the HHG directly reflects the dynamics of many body elemental excitations, which the single particle spectrum may miss. These results indicate that the HHG in Mott systems may be used as a spectroscopic tool for many body excitations. We also discuss the effects of spin dynamics on the HHG, which is a unique feature in strongly correlated systems.

[1] S. Ghimire, A. D. DiChiara, E. Sistrunk, P. Agostini, L. F. DiMauro, and D. A. Reis, Nat. Phys. 7, 138 (2011).
[2] Y. Murakami, M. Eckstein, and P. Werner, Phys. Rev. Lett. 121, 057405 (2018).
[3] M. Lysne, Y. Murakami, M. Schuler, and P. Werner, Phys. Rev. B 102, 081121 (2020).
[4] Y. Murakami, S. Takayoshi, A. Koga, and P. Werner, Phys. Rev. B 103, 035110 (2021).

An alternative route out of equilibrium: probing uniaxial strain effects with ARPES

Christopher W. Nicholson[1]

[1]*Department of Physics and Fribourg Centre for Nanomaterials, University of Fribourg, Switzerland*

The fascinating properties of emergent phases in condensed matter systems can give us considerable insight into the physical mechanisms underpinning them. A central scientific goal of recent decades has been to employ external perturbations such as doping, pressure, magnetic fields and intense laser pulses in order to push materials away from their equilibrium configurations, revealing further insights into the mechanisms relevant to stabilising these phases. Within this context uniaxial strain has recently emerged as a powerful approach to influence the properties of solids [1] and offers a path to tailor both physical properties and device functionalities from the nano to the macro scale. However, there are significant challenges when combining strain with powerful probes of the electronic structure, such as angle-resolved photoemission spectroscopy (ARPES).In this seminar, I will present our recent work combining uniaxial strain with ARPES, with a particular focus on the transition metal dichalcogenide $IrTe_2$. This quasi-2D material is predicted as a type-II bulk Dirac semimetal with a Dirac point slightly above the Fermi level. It displays a number of coexisting structural phases below 180 K, severely hindering spectroscopic access to the ground state. By applying a modest uniaxial strain ($\varepsilon \sim 0.1\%$), we demonstrate the selective stabilization of a single structural phase with domain sizes four orders of magnitude larger than in unstrained samples [2]. We find that strain initiates a charge transfer into Te anti-bonding states already at room temperature, thereby removing the phase degeneracy in favour of a single phase at low temperatures. This energetic bias allows unprecedented spectroscopic access both to the previously unobserved bulk Dirac-like states –which become the dominant inter-layer transport channel –and to new quasi one-dimensional states that appear to be intermediate between Mott insulator and Luttinger liquid phases [3]. Time allowing I will briefly discuss our ongoing work and give an outlook for using strain to influence phase transitions, bonding and topology in 2D materials.

[1] Hicks, C. W., et al. Science 344, 283–285 (2014); Kim, H. H. et al. Science 362, 1040–1044 (2018); Riccò, S. et al. Nat. Commun. 9, 4535 (2018)
[2] Nicholson, C.W., et al. Commun. Mater. 2, 25 (2021)
[3] Nicholson, C.W., et al. in preparation

From Random Regular Graphs to Many-Body Localization

Konstantin Tikhonov[1]

[1]*Landau Institute for Theoretical Physics RAS, 119334 Moscow, Russia*

We will discuss Anderson (de-)localization on random regular graphs (RRG), which have locally the structure of a tree but do not have boundary (and thus possess large-scale loops). We will discuss connections between the ergodicity-to-localization transition on RRG and the many-body localization. We study dynamical and spatial correlations of exact eigenstates in the Anderson hopping on random regular graph (RRG) and near the many-body localization transition (XXZ spin chain in random field). We explore correlations of eigenstates in their dependence on the energy difference (frequency). We find the results for the many-body localization transition to be qualitative similar to the ones for the RRG with important difference showing up in the fractal scaling of exact many body eigenstates at the critical point -- contrary to localized character of critical eigenstates on the RRG.

Chern bands of twisted bilayer graphene: fractional Chern insulators and spin phase transition

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When one of the graphene layers of Magic Angle Twisted Bilayer Graphene is nearly aligned with its hexagonal boron nitride substrate (a configuration dubbed TBG/hBN), the active electronic bands are nearly flat, and have a Chern number C=±1. Recent experiments demonstrated a quantum anomalous Hall effect and spontaneous valley polarization at integer filling νT=3 of the conduction band in this system. Motivated by this discovery, we ask whether fractional quantum anomalous Hall states (FQAH) could also emerge in TBG/hBN. We focus on the range of filling fractions where valley ferromagnetism was observed experimentally. Using exact diagonalization, we find that the ground states at νT=10/3 and νT=17/5 are fractional Chern insulator states in the flat band limit (in the hole picture, these are the fractional quantum Hall fractions 2/3 and 3/5). The ground state is either spin polarized or a spin singlet depending sensitively on band parameters. For nominally realistic band parameters, spin polarization is favored. Flattening the Berry curvature by changing a band parameter gives way to the spin singlet phase. Our estimation of the charge gap in the flat band limit shows that the FQAH state may be seen at accessible temperatures in experiments. We also study the effect of a non-zero bandwidth and show that there is a reasonable range of parameters in which the FQAH state is the ground state.

Enhancing Quantum Simulations with Data-Driven Models

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In this talk, I will present some data-driven techniques inspired by machine learning for enhancing the capabilities of quantum simulations platforms. The overreaching idea is to off-load some of the most strenuous experimental tasks to classical algorithms running on conventional hardware. These consists of parametric quantum states (such as neural networks or tensor networks) which are approximately learned from measurement data generated by quantum hardware. I will focus on quantum chemistry simulations on near-term hardware, and show how to leverage this hybrid quantum-classical approach to significantly lower the sample complexity and to perform error mitigation.

THz driven dynamics in Mott insulator $GaTa_4Se_8$

Elsa Abreu[1], Danylo Babich[2], Etienne Janod[2], Sarah Houver[1,3], Benoît Corraze[2], Laurent Cario[2], Steven Johnson[1,4]

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[2]*Institut des Matériaux Jean Rouxel, Université de Nantes, France*
[3]*Laboratoire Matériaux et Phénomènes Quantiques, Université de Paris, France*
[4]*SwissFEL, Paul Scherrer Institut, Switzerland*

Mott insulators are archetypal examples of quantum materials. Strong interest in these systems has arisen due in part to the insulator-to-metal transition that some exhibit when the balance between on-site Coulomb repulsion and hopping is overturned via temperature, doping or, as more recently demonstrated, photoexcitation or the application of short electric field pulses. Driving the transition using short electric field pulses is of particular interest for technological applications. Some Mott insulators exhibit an abrupt drop in resistivity under the application of electric fields with durations of a few tens of microseconds, with typical threshold fields on the order of 1-10 kV/cm[1]. These electrical Mott transitions are volatile for fields just above threshold, but persistent switching into a metallic phase can be achieved for sufficiently high amplitude electric fields[2], making these materials promising for e.g. memory devices. Quasi-dc electric fields well in excess of 1 –10 kV/cm can currently be generated with ultrashort pulses in the low frequency or THz range, which enables the investigation of the sub-picosecond dynamics of the electric field driven Mott transition. THz pulses can also be used to track the Drude conductivity response of the material directly, without the need to deposit any electrical contacts on the sample. We will present our results on THz driven dynamics in GaTa4Se8, a Mott insulator which exhibits clear electrical Mott transitions.

[1]. P. Diener et al., Physical Review Letters 121016601 (2018).
[2] E. Janod et al., Advanced Functional Materials 256287 (2015).

Superconductivity in the locally non-centrosymmetric heavy fermion $CeRh_2As_2$

Aline Ramires[1] and David Möckli[2]

[1]*Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland*
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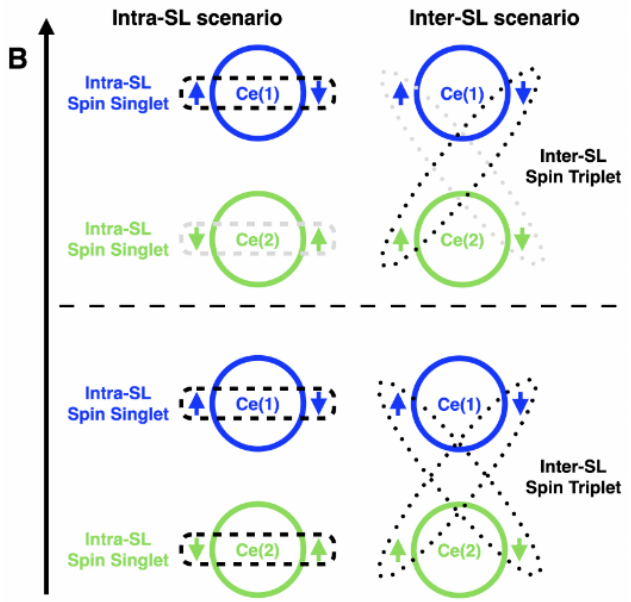

$CeRh_2As_2$, a non-symmorphic heavy fermion material, was recently reported to host a remarkable magnetic field versus temperature phase diagram with two superconducting phases. In this material, the two inequivalent Ce sites per unit cell, related by inversion symmetry, introduce a sub-lattice structure corresponding to an extra internal degree of freedom. Here we propose a classification of the possible superconducting states in $CeRh_2As_2$ from the two Ce-sites perspective. Based on the superconducting fitness analysis, we discuss two limits: a two-dimensional, Rashba spin-orbit coupling dominated normal state; and a three-dimensional, inter-layer hopping dominated normal state. In both limits, we are able find scenarios that generate phase diagrams in qualitative agreement with experiments. Figure: Pictorial view of the two scenarios accounting for a phase diagram with two superconducting phases in $CeRh_2As_2$. Left: the originally proposed "BCS-PDW" scenario, here referred to as intra-sublattice scenario. At low magnetic fields the order parameters in both sublattices have the same magnitude and sign, while at high fields they have opposite sign, depicted here by the different colours Right: novel inter-sublattice scenario. At low fields, a spin-triplet sublattice-symmetric phase is present, while at high fields a spin-triplet sublattice-anti-symmetric develops.

[1] David Möckli and Aline Ramires, "Two scenarios for superconductivity in CeRh2As2", arXiv:2102.09425 (2021)

Fingerprints of unconventional magnetism in ruthenates

H. Gretarsson[1,2], J. Bertinshaw[2], H. Suzuki[2], and B. Keimer[2]

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[2]*Max Planck Institute for Solid State Research, Heisenbergstrasse 1, D-70569 Stuttgart, Germany*

In this talk I will introduce the excitonic and Kitaev-model and show how they are applicable to two different families of Ru-based materials –square lattice Ca_2RuO_4[1] and honeycomb lattice $RuCl_3$[2]. In these compounds comparable energy scales, namely spin-orbit coupling (SOC), on-site Coulomb repulsion (U), and the crystal electric field (CEF) gives rise to non-trivial magnetism. I will demonstrate that by utilizing the well-known technique Resonant Inelastic X-Ray Scattering (RIXS) in the tender x-ray range [3] one can probe directly the key parameters and their interplay in those materials. More specifically, I'll show how Ru L_3-edge RIXS reveals a rich set of orbital excitations in Ca_2RuO_4while showing peculiar momentum dependence of quasi-elastic scattering in $RuCl_3$, both providing strong evidence for unconventional magnetism.

[1] H. Gretarsson et al., Phys. Rev. B 100, 045123 (2019)
[2] H. Suzuki et al., arXiv:2008.02037 (2020)[3] H. Gretarsson et al., J. Synchrotron Rad. 27 538-544 (2020)

Contributed oral talks

Skyrmion and Tetarton Lattices in Twisted Bilayer Graphene

Thomas Bömerich[1], Lukas Heinen[1], and Achim Rosch[1]

[1]*Institute for Theoretical Physics, University of Cologne, Germany*

Recent experiments on twisted bilayer graphene show an anomalous quantum Hall (AQH) effect at filling of three electrons per moiré unit cell. The AQH effect arises in an insulating state with both valley and ferromagnetic order. We argue that weak doping of such a system leads to the formation of a novel topological spin texture, a "double-tetarton lattice". The building block of this lattice, the "double-tetarton", is a spin configuration which covers ¼ of the unit sphere twice. In contrast to skyrmion lattices, the net magnetization of this magnetic texture vanishes. Only at large magnetic fields are more conventional skyrmion lattices recovered. But even for large fields the addition of a single charge to the ferromagnetic AQH state flips hundreds of spins. Our analysis is based on the investigation of an effective nonlinear sigma model which includes the effects of long-ranged Coulomb interactions.[1]

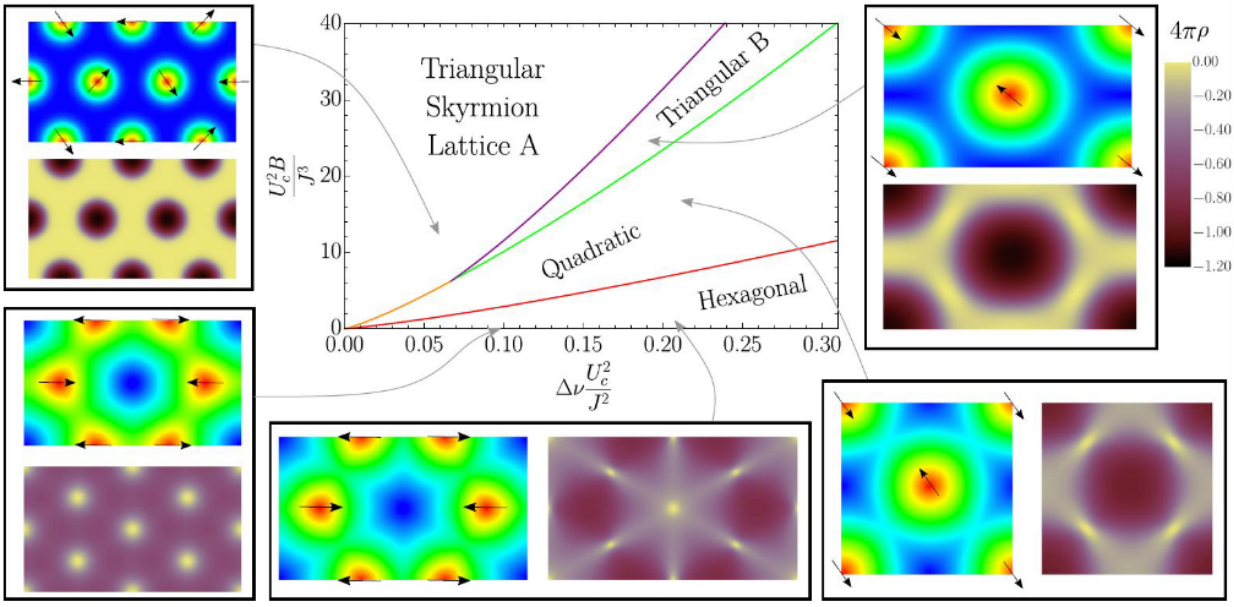

Figure 1: Phase diagram for magnetic textures with Coulomb interactions. One representative spin configuration (z-component of the spin with blue for up and red for downspins, arrows indicate the helicity) and the corresponding charge density for each phase is shown. In the case of B=0 the double-tetarton lattice (lower left corner) is the ground state. For small magnetic fields a hexagonal lattice has the lowest energy (lower middle picture), while at low density and large magnetic field the ground state is a triangular lattice of skyrmions with 120° helicity order (upper left corner). At intermediate fields, we obtain a triangular lattice with striped helicity order as well as a square lattice with an "antiferromagnetic" helicity order.

[1] Physical Review B 102, 100408(R)

Quantum transport of strongly correlated electrons through GeV complexes in silicon: a combined ab-inito and Hubbard model approach

Simona Achilli[1, 2], Nguyen H Le[3], Guido Fratesi[2, 4], Nicola Manini[2, 4], Giovanni Onida[2, 4], Marco Turchetti[5], Giorgio Ferrari[6], Takahiro Shinada[7], Takashi Tanii[8], Enrico Prati[9]

[1]*Department of Physics, University of Milan*
[2]*European Theoretical Spectroscopy Facility*
[3]*Advanced Technology Institute and Department of Physics, University of Surrey*
[4]*Department of Physics, University of Milan*
[5]*Research Laboratory - Massachusetts Institute of Technology*
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[7]*Center for Innovative Integrated Electronic Systems (CIES), Tohoku Universit*
[8]*Faculty of Science and Engineering, Waseda University*
[9]*Istituto di Fotonica e Nanotecnologie, Consiglio Nazionale delle Ricerch*

We exploit a multiscale approach that combines ab initio calculation and Hubbard model to characterize electronic properties and quantum transport in an array of Ge-vacancy complexes in silicon. These defects, obtained experimentally through high precision Ge single-ion implantation followed by thermal annealing, are promising systems for the realization of quantum Hubbard simulators working at room temperature.

On the basis of Density Functional Theory calculations performed with hybrid screened- exchange functionals we demonstrate that the Ge-vacancy is characterized by deep states in the gap, preventing thermal ionization, and high electronic correlation [1]. By exploiting the ab initio waves functions we determine the hopping term and long- range Coulomb interaction that enters as parameters in the extended Hubbard Hamiltonian while the on-site correlation is obtained as the energy required for charged excitation. We demonstrate that this approach is extremely more effective in describing the properties of such complexes with respect to the use of an hydrogenic wave functions, usually adopted for conventional dopants (P, As) in silicon [2].

We have a direct feedback of the efficiency of the theoretical model by the comparison of the theoretical conductance, obtained through a rate-equation based on the Fermi golden rule, with the measured one. By including the effect of positional disorder we are able to reproduce the temperature-activation of the quantum transport observed in the experiments. We show the establishment of different regimes corresponding to different filling of the many body states in the array, as consequence of the balancing between localization due to disorder, Coulomb repulsion and delocalization of excited states. [3]

This joint theoretical and experimental characterization, which is funded by the Horizon 2020 European Funding Programme (Project ID 188 and 517) [Nanoscale Foundries and Fine Analysis projects (nffa.eu)], represents an initial stage for the definition of a protocol for the integration of such defects in quantum technologies applications.

[1] S. Achilli, N. Manini, G. Onida, T. Shinada, T. Tanii, E. Prati, GeVn complexes for silicon-based room- temperature single-atom nanoelectronics, Sci. Rep. 8, 18054 (2018).
[2] C. J. Wellard and L. C. L. Hollenberg, Donor electron wave functions for phosphorus in silicon: Beyond effective-mass theory, Phys. Rev B 75, 085202 (2005).
[3] S. Achilli, N. H. Le, G. Fratesi, N. Manini, G. Onida, M. Turchetti, G. Ferrari, T. Shinada, T. Tanii, E. Prati, Position-controlled functionalization of vacancies in silicon by single- ion implanted germanium atoms, Adv. Funct. Mater. https://doi.org/10.1002/adfm.202011175.

Electronic structure and magnetism in UGa2: DFT+DMFT approach

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The debate whether uranium 5f electrons are closer to being localized or itinerant in the ferromagnetic compound UGa_2 is not yet fully settled. The experimentally determined magnetic moments are large, approximately 3 μB, suggesting the localized character of the 5f electrons [1,2]. In the same time, one can identify signs of itinerant as well as localized behavior in various spectroscopic observations [3-5]. The band theory, employing local exchange-correlation functionals (LSDA), is biased toward itinerant 5f states and severely underestimates the moments. The correlated band-theory (LSDA+U) enhances the magnetic moments but the spectroscopic observations are not reproduced very well [6]. Using the dynamical mean-field theory (DMFT), we probe how a less approximate description of electron-electron correlations improves the picture. We present two variants of the theory: starting either from spin-restricted (LDA) or spin-polarized (LSDA) band structure. We show that the DMFT method can accurately describe the magnetic moments in UGa_2, as long as the exchange interaction between the uranium 6d and 5f electrons is preserved by a judicious choice of spin-polarized double-counting correction. We discuss how the computed electronic structure reconciles the large magnetic moments and a small Sommerfeld coefficient with 5f spectral density found in a close vicinity of the Fermi level [7].

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Strongly correlated materials via embedding methods: solving impurity models with a noisy quantum computer

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A promising path to go beyond current algorithms for strongly-correlated materials is to leverage the quantum computer, a computation device whose quantum features are associated with an exponential speedup. Yet we are still in the so-called Noisy Intermediate-Scale Quantum (NISQ) era, with quantum computers only comprising a few tens of faulty qubits. In this work, we propose a hybrid quantum classical method to solve the two-dimensional Hubbard model using NISQ processors. We show that, by combining an advanced many-body embedding method, the Rotationally Invariant Slave Boson (RISB [1], equivalent to the Gutzwiller method [2] at the saddle-point level), and a variational algorithm, the Variational Quantum Eigensolver (VQE [3]), one can compute, even in the presence of quantum noise, and beyond a single impurity, the evolution of the quasiparticle weight as a function of the interaction strength. We go beyond previous works in this direction [4–6] by optimizing the use of quantum resources through the design of advanced variational states and an optimized orbital representation. This allows us to double the size of the impurity problem, reaching two impurities or equivalently eight qubits, while previous works were limited to two or four qubits. We carry out noisy simulations of the behavior of our hybrid method and show that it is robust to the noise levels that are reported on today's quantum processors. Finally, we argue that the method paves the way to larger impurity sizes and thus a controllable approximation of the solution to the Hubbard model.

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Improving the grasp of harmonically trapped fermions in low dimensions

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Experiments with only a few atoms shed light on the crossover from few-to many-body physics. Theoretical treatment of these experiments is challenging because the underlying Hilbert space grows rapidly with particle number. The standard effective treatment for short-ranged interactions relies on the δ-potential, for which the exact diagonalization in a truncated Hilbert space converges slowly. Moreover, in spatial dimensions larger than one, the δ-potential requires careful renormalization to converge at all. Here we exploit a particularly effective renormalization procedure adapted from nuclear physics: We fix the lowest part of the two-body spectrum using the exact solution. This provides us with an efficient tool to obtain physical observables free from a cutoff dependence at significantly reduced computational cost.

To demonstrate our approach, we show results for a few harmonically trapped fermions in 1D interacting with a static magnetic impurity at the center of the trap. By gradually increasing the particle number in the trap, a quantum phase transition is approached, manifesting itself in a level crossing between two ground states with vanishing spin and non-zero spin, respectively. Moreover, we address low-energy physics of harmonically trapped 2D Fermi gases allowing us to study the nature of particle pairing in this regime.

Toward Coherent Optical Control of the Insulator-to-Metal Transition in V_2O_3

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Multi-band correlated materials represent a class of solid-state systems which recently experienced an increasing scientific and technological interest due to their outstanding properties such as insulator-to-metal transition (IMT) or superconductivity. Prototypical correlated materials, such as vanadium sesquioxide (V_2O_3), has been intensively studied due to the possibility of controlling the Mott transition by means of small variations of chemical doping, temperature, and pressure [1]. Recently, a new excitation pathway to induce the transition has been proposed [2]. Indeed, upon photoexcitation, the resulting orbital population imbalance leads to a modification of the band structure of the material, which undergoes a transition from the insulating to a metallic (metastable) phase [3]. In this direction, we investigated the IMT in V_2O_3 thanks to an interferometric experiment, in which the orbital population is optically manipulated by two coherent pump pulses. This experimental protocol represents a potential method to investigate coherence effects of the electronic degrees of freedom on the phase transition of correlated materials.

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Tracking the ultrafast non-thermal demagnetization of $Sr_3Ir_2O_7$

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In quantum materials, antiferromagnetic order often can be suppressed to give rise to technologically-relevant phases such as high-temperature superconductivity. Typically, this is achieved through chemical doping, however, optical control of the magnetic order allows us to stabilize those phases on demand [1]. To date, most research on the interaction between optical excitation and magnetic order has focused on ferromagnetism and the mechanism of laser-induced demagnetization in antiferromagnetic compounds are less explored. In this talk, I will discuss the ultrafast dynamics of the spin subsystem in $Sr_3Ir_2O_7$, a spin-orbit Mott Insulator that exhibits a phase transition from paramagnetic to antiferromagnetic at $T_N \approx 280$ K. I will demonstrate that it is possible to track ultrafast changes in magnetic order via changes in the reflectivity of the sample in the visible region and that the optical data is comparable to that measured at XFEL sources in terms of magnetic dynamics [2]. Using a 4D dataset as a function of temperature, probe wavelength, delay time and excitation fluence I will provide evidences that in this material, above band gap excitation induces a large (>50%) and prompt suppression of magnetic order. Critically I will show that the lattice temperature remains below the equilibrium temperature thus demonstrating the non-thermal character of the phase change. Furthermore, I will discuss the mechanism of re-magnetization, which we measure to be fluence dependent exhibiting two distingue regimes: fast (< 5ps) and slow (>5ps) recovery. Our experiments and simulations suggest that the formation of photo-induced spin defects dictates the stability of the demagnetized state and the recovery of magnetic order [3].

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Optical momentum-resolved spectroscopy based on time-reversal dynamics in correlated insulators

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Intense terahertz lasers drive quasiparticle dynamics in the reciprocal space. One of the important examples is high harmonic generation (HHG) in attosecond science, which has recently been studied in strongly correlated electron systems (SCESs) [1]. In semiconductors, several methods for obtaining the energy dispersion from the HHG signals have been discussed [2]. Such an all-optical momentum-resolved spectroscopy provides an opportunity to measure the energy dispersion even in a bulk sample or in a magnetic field, although it requires the detailed analysis based on numerical simulations.

In this study, we theoretically propose a more direct protocol to visualize the dispersion relations of quasiparticles in SCESs as well as band insulators. In this protocol the quasiparticles are excited by a resonant pulse and then accelerated in the reciprocal space by an off-resonant strong electric field pulse. We mainly consider the one-dimensional Fermi-Hubbard model $\mathcal{H} = -t_h \sum_{i=0,\sigma}^{N-1}(c_{i,\sigma}^{\dagger} c_{i+1,\sigma} + h.c.) + U \sum_{i=0}^{N-1} n_{i\uparrow} n_{i\downarrow}$. This model can be solved by the Bethe ansatz. The ground state is a Mott insulator at half filling. The doublon-holon pairs are created in the optically excited states. A vector potential of light is introduced through the Peierls substitution. We simulate the real-time evolution of a matrix product state by using the infinite time-evolving block decimation method.

By calculating the electric current, we observe an echo of the resonant excitation pulse. Figure 1 shows the Fourier spectra of the electric current as a function of a vector potential shift caused by the driving pulse; the peak corresponds to the central frequency of the echo signal. The echo frequency is in good agreement with the exact doublon and holon dispersion relations derived by the Bethe ansatz. We confirmed that the echoes are generated not only in the one-dimensional systems but in a two-dimensional band insulator. Furthermore, the echo signal survives even when a long-range Coulomb interaction is introduced, which indicates that the integrability is not necessary for the generation of the echoes. These findings strongly imply that the present echoes are generated in a wide class of insulating systems including SCESs. We will discuss the mechanism of the echo generation by using an improved semiclassical treatment of the wave packet dynamics.

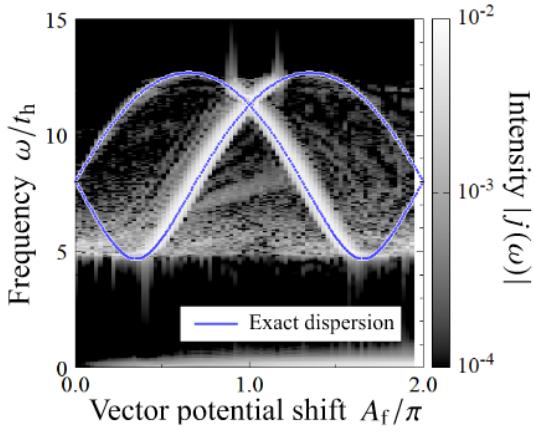

Figure 1: Fourier spectra of the echo and the exact dispersion obtained by the Bethe ansatz.

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π-ton contributions to optical conductivity in correlated electron systems

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The interaction of light with solids gives rise to new bosonic quasiparticles, with the exciton being the most famous one. While excitons are the generic excitations of semiconductors, we show that for strongly correlated systems another type of bosonic excitation is present. It originates from the dominant antiferromagnetic or charge density wave fluctuations in these systems. As these are usually associated with a wave vector (π,...) or close to it, we call these excitations π-tons [1]. Theseπ-tons yield the leading vertex correction to the optical conductivity in several correlated models studied: the Hubbard, the extended Hubbard model [2], the Falicov-Kimball [3], and the Pariser-Parr-Pople model [4], both in the insulating and in the metallic phase. The vertex corrections to the Drude peak in a 2D metal show a non-monotonous temperature dependence [5]. In insulators, the pitons lead to a gap reduction [3][4][6]. The π-ton consists of two electron-hole pairs coupled via antiferromagnetic or charge-density-wave fluctuations as illustrated in Fig. 1.

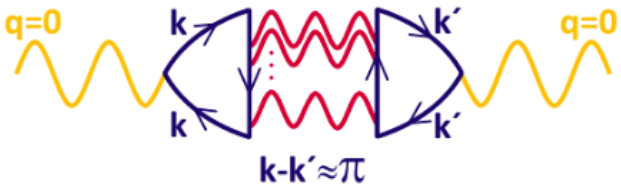

Figure 1: Feynman diagram depicting π-ton contribution to optical conductivity.

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Quadratic optical responses in a chiral magnet

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Chiral magnets breaking both spatial inversion and time reversal symmetries carry a potential for novel quadratic optical responses, for instance, photovoltaic effect (PVE) and second harmonic generation(SHG)[1]. Such nonlinear optical responses have attracted much attention in the aspect of an application for the next-generation optical electronic devices, such as unconventional solar cells and optical sensors.

In this study, we theoretically investigate quadratic optical responses in electrons coupled with a one-dimensional chiral magnet, as a prototypical example. The magnetic texture changes from a chiral helimagnetic state [Fig. 1(a)]to a chiral conical magnetic state with spin canting [Fig. 1(b)], and to a forced ferromagnetic state [Fig. 1(c)] with increasing magnetic field along the helical axis. By using the second-order response theory [2], we show that the chiral conical magnetic state exhibits the PVE [Fig. 1(d)]and SHG [Fig. 1(e)]. In particular, we find that the coefficient of the PVE changes in not only the magnitude but also the sign depending on the magnetization and the frequency of lights [3]. Our results suggest that chiral magnetic textures provide a new platform for nonlinear optical responses with flexible controllability.

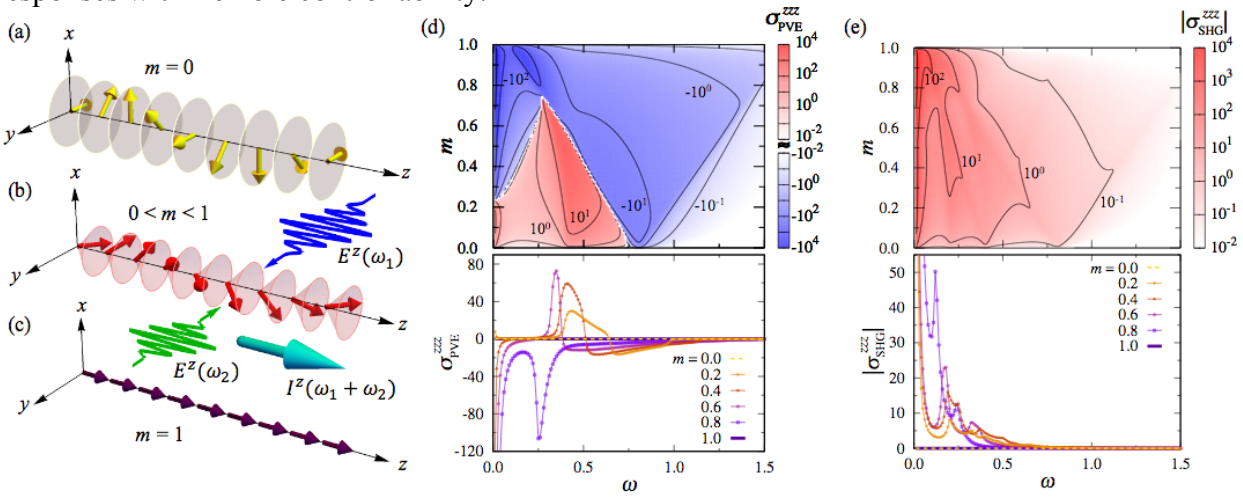

Fig. 1 Schematic pictures of (a) a chiral helimagnetic state, (b) a chiral conical magnetic state, and (c) a forced ferromagnetic state. m is the magnetization. The blue and green arrows represent incoming linearly polarized lights with frequency $\omega_1$and ω_2, respectively. The cyan arrow isa nonlinear electric current with frequency$\omega_1 + \omega_2$. Contour plots of (d) the photovoltaic coefficient $\sigma_{PVE}^{ZZZ}$with $\omega_1 = -\omega_2 = \omega$and (e) the intensity of the second harmonic generation σ_{SHG}^{ZZZ} with $\omega_1 = \omega_2 = \omega$as functions of m and ω. The lower panels show ω dependences for several m.

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Ultrafast anomalous thermal expansion in superconducting YBCO

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Ultrafast spectroscopy experiments are a formidable tool to investigate the fundamental mechanisms in complex materials at their typical femtosecond timescale. We upgrade the standard optical pump&probe approach and access new insight on the non-equilibrium dynamics of optimally doped YBCO. While the vast majority of spectroscopies rely on detecting the probe intensity, we exploret he full optical field developing a multimode heterodyne detection setup [1] which enables us to resolve amplitude and phase of the probe spectral components. We reveal that amplitude and phase dynamics are in general different and representative respectively of the dissipative and inductive response of the examined material. We focus our discussion on the phase dynamics. The typical response resulting from a photoinduced thermal excitation is a positive shift of the field phase. This describes an increased propagation time through the material, which results from the thermal expansion of the sample structure. In comparison with such a positive phase dynamics observed in transparent materials (quartz) and absorptive transition metal oxides (TiOCl), we reveal that the YBCO phase modulation presents at low temperature an anomalous negative ultrafast response. This feature signals a non-equilibrium reduction of the probe propagation time compatible with a contracting sample length or decreasing refractive index. We connect this behaviour to the anomalous thermal expansion properties of superconducting materials, which in turn establish a link with the charge order dynamics [2]. Our approach can thus represent a novel way to access unique information about charge density waves and help in understanding their debated interplay with superconductivity [3].

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Time-and Angle-Resolved Photoemission Study on Bulk VSe_2

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By means of time-and angle-resolved photoemission spectroscopy (tr-ARPES), we investigate the effect of the phase transition into the charge density wave (CDW) phase on the equilibrium and out-of-equilibrium electronic band structure of the transition metal dichalcogenide VSe_2. The electronic band structure of VSe_2 has recently been subject of investigation ranging from the bulk to the monolayer regime, in search for the manifestation of the opening of the band gap in its CDW phase [1,2]. At present, few time-resolved studies on the effect of optical excitation are available on the ultrafast timescales [1,3]. In our contribution we present a study on the bulk material. By changing the polarization of the probe pulses, tr-ARPES allows us to disentangle the d-like and p-like states from the V and Se valence bands respectively. When moving across the critical temperature of the CDW phase transition, our tr-ARPES data show indication for a change in the fast relaxation dynamics and for a different relative filling among the states near the Fermi level, which lasts for several picoseconds after photoexcitation.

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Microscopic study of the spin Seebeck effect in YIG with resonant inelastic x-ray scattering

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The SSE in insulating $Y_3Fe_5O_{12}$ (YIG) was discovered in 2010, defining it as a spin-wave-based transport effect generated by applying a temperature gradient [1]. Since then a multitude of transport studies have been reported indicating the temperature and thickness dependence, and the effect of magnetic field on SSE [2-3]. From a theoretical perspective, many models have been built to explain the experimental results [4-6]. However, no consensus has been reached on the mechanism behind the SSE in YIG; this is due to the lack of a suitable microscopic probe compatible with temperature gradient conditions and sensitive to the elementary excitations leading the transport. Here, we present state-of-the-art resonant inelastic x-ray scattering (RIXS) results on a YIG device operating in presence of spin Seebeck effect (SSE). The study uniquely reveals a momentum-and energy-resolved picture of the excitations involved in the SSE, providing key information on the microscopic mechanism behind this transport phenomenon. By controlling the applied temperature gradient across the YIG device, our RIXS data display a clear spectral weight enhancement in the anti-Stokes channel up to 100 meV. This result on one hand uncovers for the first time that the high energy magnons (up to 100meV) are involved in the SSE. On the other hand, the fine details of the spectral weight variation versus energy and momentum point to a crucial role of the magnon-polaron (the hybridization between the magnon and the phonon) mode in the SSE.

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Insensitivity of the striped charge-orders in $IrTe_2$ to alkali surface doping implies their structural origin

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We investigate the electronic structure of potassium (K)-doped $IrTe_2$ to elucidate the origin of its charge-ordered phase transitions. Upon cooling, pristine IrTe2 undergoes a first-order phase transition at about 280 K from a (1 × 1 × 1) phase into a (5 × 1 × 5) phase. At about 180 K, another first-order phase transition occurs changing the periodicity to a (8 × 1 × 8) [1,2,3]. We investigate the effect of in-situ K deposited at room temperature (RT) on the electronic structure of $IrTe_2$ by means of surface sensitive ARPES measurements. According to our density functional theory (DFT) calculations, we reveal that the K atoms give most of their electronic charge to the surface layer. Although the K atoms modify the surface electronic structure, temperature dependent ARPES shows that the critical temperatures of the phase transitions remain unaffected, while low energy electron diffraction (LEED) measurements of the low-temperature charge-ordered phases confirm that the striped periodicities remain unchanged. This demonstrates that alkali doping, within low coverages, is not sufficient to destabilze with the bonding-antibonding molecular states relevant for the phase transition. Despite the fact that alkali doping affects mainly the surface, we observe that the surface reconstruction is similarly unchanged. This suggests that local lattice effects are central to understand the formation of charge-ordered phase transitions in $IrTe_2$.

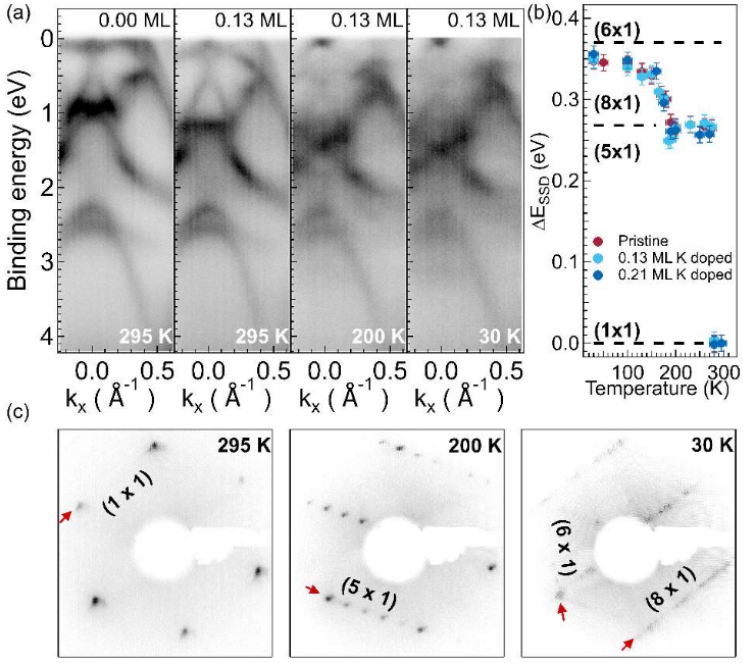

Figure: (a) ARPES spectra of a pristine and K-doped $IrTe_2$ along the HA direction in the bulk Brillouin zone at several temperatures taken with hν = 21.2 eV. (b) RT relative binding energy shift of the surface state SSD measured in ARPES as function of temperature for a pristine crystal, 0.13 ML and 0.21 ML K-doped crystals. (c) Raw LEED images of a 0.13 ML K doped IrTe2 crystal at several temperatures.

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Influence matrix approach to quantum many-body dynamics

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I will introduce an approach to study quantum many-body dynamics, inspired by the Feynman-Vernon influence functional. Its central object is the influence matrix (IM), which describes the effect of a Floquet many-body system on the dynamics of local subsystems. For translationally invariant systems, the IM obeys a self-consistency equation. For certain fine-tuned models, remarkably simple exact solutions appear, which represent perfect dephasers (PD), i.e., many-body systems acting as perfectly Markovian baths on their parts. Such PDs include dual-unitary quantum circuits investigated in recent works. In the vicinity of PD points, the system is not perfectly Markovian, but rather acts as a quantum bath with a short memory time. In this case, we demonstrate that the self-consistency equation can be solved using matrix- product states (MPS) methods, as the IM temporal entanglement is low. Using a combination of analytical insights and MPS computations, we characterize the structure of the IM in terms of an effective "statistical-mechanics" description for interfering intervals of local quantum trajectories and illustrate its predictive power by analytically deriving the relaxation rate of an impurity embedded in the system. In the last part of the talk, I will describe how to use these ideas to study the many-body localized (MBL) phase of strongly disordered interacting spin systems subject to periodic kicks. This approach allows to study exact disorder-averaged time evolution in the thermodynamic limit. MBL systems fail to act as efficient baths, and this property is encoded in their IM. I will discuss the structure of an MBL IM and link it to the onset of temporal long-range order.
Based on [1-4].

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A Quantum Boltzmann Equation for Strongly Correlated Electrons

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Collective orders and photo-induced phase transitions in quantum matter can evolve on timescales which are orders of magnitude slower than the femtosecond processes related to electronic motion in the solid. Quantum Boltzmann equations can potentially resolve this separation of timescales, but are often constructed by assuming the existence of quasiparticles. Here we derive a quantum Boltzmann equation which only assumes a separation of timescales (taken into account through the gradient approximation for convolutions in time), but is based on a non-perturbative scattering integral, and makes no assumption on the spectral function such as the quasiparticle approximation. In particular, a scattering integral corresponding to non-equilibrium dynamical mean-field theory is evaluated in terms of an Anderson impurity model in a non-equilibrium steady state with prescribed distribution functions. This opens the possibility to investigate dynamical processes in correlated solids with quantum impurity solvers designed for the study of non-equilibrium steady states.

Higgs time crystal in a high-T_c superconductor

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We propose to induce a time crystalline state in a high-T_c superconductor, by optically driving a sum resonance of the Higgs mode and a Josephson plasma mode [1]. The generic cubic process that couples these fundamental excitations converts driving of the sum resonance into simultaneous resonant driving of both modes, resulting in an incommensurate subharmonic motion. To test the rigidity of this effect, we implement a semiclassical driven-dissipative lattice gauge theory on a three-dimensional layered lattice, which models the geometry of cuprate superconductors. We find that the subharmonic motion is robust against perturbations of the drive as well as thermal fluctuations. We demonstrate this light-induced time crystalline state for mono-and bilayer systems and show that it can be detected in pulsed operation.

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Driven Majorana Box Qubit

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A topological superconductor in one dimension can host Majorana zero modes at its edge. By driving the system periodically, so-called π modes (also named Floquet-Majoranas) can arise.[1] These are topologically protected modes with an energy at the quasi-energy π/T, where T is the period of the drive. We consider the role of π modes in the presence of long-ranged Coulomb interactions. We study a Cooper pair box made of two Josephson coupled superconducting topological quantum wires. Time-dependent gate voltages periodically drive the system. We investigate how to obtain and control π modes and study their stability in the presence of interactions.

We consider the limit where the charging energy is much larger than the Josephson energy. We find that periodic gate voltages result in a periodic phase modulation of the pairing term in the topological quantum wires. The phase modulation is by gauge transformation equivalent to a time-periodic chemical potential. In this setup all phases (trivial, Majorana zero mode, Majorana π mode, both Majorana modes) are accessible. Taking into account a second order process via the bulk superconductor, we found an effective interaction term of the Hamiltonian. This interaction is of the form of non-local four body scattering in the wires. We discuss possible heating effects of the quasi-particle scattering. The presence of total two zero modes and two π modes in the Floquet box qubit allows for topologically and parity protected single- and two qubit operations within one single box. [2]

For a proper operation of the qubit, a protected adiabatic preparation scheme is crucial. We show when the adiabatic preparation of the Floquet groundstate generically fails and the system is inherently unstable against quasi-particle creation. Finally, we found a stable protocol to initialize the driven Majorana box qubit.

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Spin-orbital entanglement in magnetic quantum materials

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Strong relativistic spin–orbit coupling (SOC) in 4d and 5d materials leads to novel phenomena such as the complex phase behaviour observed in the extended Kitaev–Heisenberg model [1]. In this context we investigate spin–orbital entanglement (SOE) which plays a crucial role in the understanding of strongly correlated electrons in transition metal oxides. We study a transparent example of the intimate relation between quantum entanglement and SOC. To this end we numerically diagonalize one-dimensional spin-orbital model with the SU(2)⊗SU(2) 'Kugel – Khomskii' exchange supplemented by SOC of the Ising type for chains up to L = 20 sites [2,3]. We observe a substantial difference in the entanglement for small versus large SOC. While most of the features of the ground state with small SOC resemble the vanishing SOC limit, the phase diagram for large SOC regime is divided between the classical fluctuation—free region and surprisingly vast region where quantum fluctuations persist, including highly quantum 'stripe'—like area with maximal SOE. From a broader perspective, these results provide a basis to infer the generic properties of entanglement in transition metal oxides with finite SOC at higher dimension.

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Design and realization of a triangular QSHI: Indenene on SiC

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The key to engineer large-gap quantum spin Hall insulators is a strong spin-orbit interaction. In Kane and Mele's suggestion for honeycomb layers, SOC is promoted via a relatively weak second neighbor hopping process. Bismuthene however has impressively proven the superiority of local/atomic SOC of the in-plane p-orbitals. A new possibility arises by halving the bismuthene honeycomb lattice but enriching the orbital subspace, i. e. considering a full p-basis on a triangular lattice. Here, we conceive and realize for the first time a triangular QSHI, ''indenene'', a triangular monolayer of indium on SiC(0001) exhibiting non-trivial valley physics as a consequence of strong local spin-orbit coupling. Via tunneling microscopy of the 2D bulk we identify the quantum spin Hall phase and unveil a hidden honeycomb charge localization emerging from interference patterns in the valley Bloch wave functions.
A detailed experimental analysis on the growth and topological classification of indenene is further presented by M. Bauernfeind in a poster session at the NGSCES.

Unveiling ultrafast dynamics in quantum matter with soft x-rays: capabilities of the Furka endstation at SwissFEL

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Ultrafast spectroscopies have afforded numerous insights into understanding the fundamental properties of quantum materials and towards controlling their functionality through light-matter interaction. In this regard, the recent advent of Free-Electron Lasers (FEL) extended these techniques down to short wavelengths, reaching the VUV and x-ray range, allowing microscopic and momentum-resolved information.
In this talk, I will show some early results [1,2] of the application of time-resolved Resonant Inelastic X-ray Scattering (trRIXS), a technique capable of accessing the spin, charge, orbital, and lattice dynamics in quantum matter. I will then describe the future opportunities for ultrafast soft x-ray spectroscopy and scattering that will be available at the Furka endstation of the SwissFEL facility. The endstation will be open for user operation in 2022.

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Microscopic insight into optically induced excitations in NiO through fs time-resolved x-ray absorption spectroscopy

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X-ray absorption spectroscopy (XAS) is a mature technique for deriving element- and chemically sensitive information on solids, in particular complex materials and heterostructures. It is therefore highly desirable to bring this powerful technique to the femto- to picosecond timescales of the elementary microscopic processes involving charge, spin and lattice dynamics in solids via optical pump – x-ray probe experiments at ultrashort pulse x-ray sources such as free electron lasers.
In this talk, I will discuss recent progress on implementing fs time-resolved XAS at the SCS instrument of European XFEL by means of a transmission zone plate and grating scheme. This setup allows for a simultaneous acquisition of the ground state and optically excited x-ray spectra as well as a reference signal for normalization of the data to the incident x-ray intensity, and thus provides excellent data quality in combination with kHz repetition rates.
By means of fs time-resolved XAS, we characterize the interaction of excited charge carriers and the lattice in NiO, which represents a prototypical correlated material. We directly probe the dynamics of the valence and conduction band resulting from optical excitation of charge carriers at both the Ni L and O K edges, i.e. Ni 3*d* respectively O 2*p* states. The transient spectral features derived from this comprehensive analysis of both constituents of the oxide will be discussed in the context of the evolution of the excited charge carrier populations and their relaxation, showing the potential to gain microscopic insight into these fundamental processes in complex materials.
The results discussed in this poster were achieved with the collaborators of European XFEL community proposal 2161 and proposal 2589.

Nanoscale X-ray holographic imaging of the ultrafast insulator-to-metal phase transition in vanadium dioxide

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The nature of the phase transition in VO_2 has been the subject of contention for almost 70 years. While it was originally hoped that ultrafast measurements would be able to disentangle the key contributions to transition, effects like transient phase separation have complicated the interpretation of experiments. In order to fully understand this transition and many like it, measurements that can fully resolve the dynamics in both space and time at their natural nanometer and femtosecond scales are urgently needed [1,2]. Here we present the first space and time resolved measurements of the ultrafast phase transition in VO_2. We use X-ray holography [3] to take nanometer resolution images of a 75 nm thick polycristalline sample of VO_2 at the PAL XFEL with ≈100 fs resolution (Figure 1a), with phase contrast provided by tuning to resonances in the X-ray absorption spectrum [4]. We observe nanometer scale domains forming promptly with 200 fs, followed by sub-picosecond and picosecond dynamics (Figure 1b). Furthermore, we performed real-space imaging spectroscopy measurements on the transient state at 20 ps [5], allowing us to comment on existance of the previously claimed phase-seperated monoclinic metallic precursor phase [1,2].

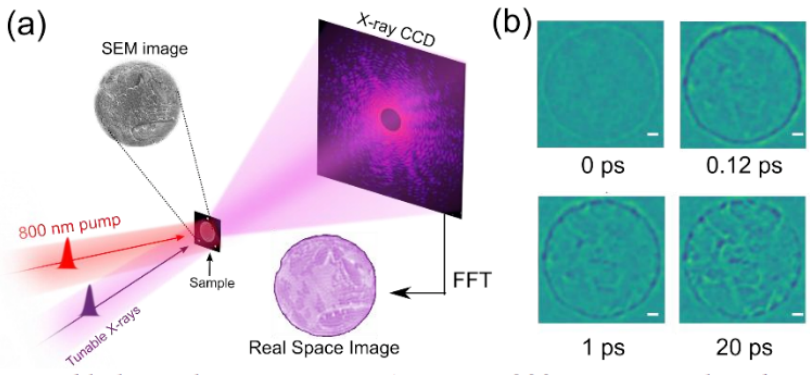

Figure 1:(a) Setup for femtosecond holographic imaging at PAL XFEL. 800 nm pump pulses drive the sample through the phase transition, while coherently scattered resonant X-ray probe pulses return real space images of the domain grown. (b) A variety of resolution-limited, sub-picosecond, and picosecond dynamics are observed in the domain growth. White scale bar, 200 nm.

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Ultrafast renormalization of the onsite Coulomb repulsion in an underdoped cuprate

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Intense ultrashort electromagnetic fields are an increasingly important tool to realize and control novel emergent phases in quantum materials. Among a variety of nonthermal excitation pathways, a particularly intriguing route is represented by the direct light-engineering of effective many-body interactions, such as electron hopping amplitudes and electron-electron repulsion. Achieving a light-induced dynamical renormalization of the screened onsite Coulomb repulsion ("Hubbard U") would have far-reaching implications for high-harmonic generation [1], attosecond spectroscopy [2] and ultrafast magnetism [3] in the solid state. However, experimental evidence for a dynamically controlled Hubbard U remains scarce [4], [5].

Here, we employ time-resolved x-ray absorption spectroscopy (trXAS) to demonstrate the ultrafast renormalization of the Hubbard U parameter in the underdoped cuprate $La_{1.905}Ba_{0.095}CuO_4$ (LBCO, x=9.5%). Our element-specific measurements reveal that intense femtosecond optical pulses (1.55 eV, 50 fs) induce a dramatic shift of the x-ray absorption maxima associated with transitions to the upper Hubbard bands (UHB), while the transition energy into Zhang-Rice singlet states near the Fermi level remains unaffected. Based on exact-diagonalization calculations of the time-dependent spectrum within the single- as well as the three-band models of cuprate superconductors, we determine a pump-induced suppression of the Hubbard U up to 10% of its equilibrium value on the Cu sites.

Our results represent a first precision measurement of dynamically-renormalized Hubbard U in strongly correlated oxides and have significant implications for the on-demand engineering of their magnetic interaction spectrum.

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Fluctuation control of non-thermal orbital orders

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Multi-minima free energy surfaces represent many physical situations [1], such as different orbital orders in transition metal compounds. In this class of systems, fluctuations of the order parameters are essential in determining the shape of the free energy. Already at equilibrium, restoring forces are of entropic origin through the order-by-disorder mechanisms [2], and fluctuations can therefore be expected to be important for the nonequilibrium dynamics. This might open non-equilibrium pathways to control the dynamics of the order parameter and even stabilize states otherwise unstable at low temperatures [3]. Here, we describe the dynamics induced by suitable time-varying protocols in the 120° compass model using time-dependent Ginzburg-Landau theory [4], and we propose to use the momentum-resolved spectrum of the fluctuations to map out the instantaneous form of the potential, what should be soon achievable in time-resolved inelastic X-ray scattering experiments. One of the protocols we analyze is a time modulation of the exchange couplings that mimics the action of oscillating electric fields that have been suggested to modify the intensity of the exchange interactions for both orbital and spin degrees of freedom. In orbital models, this can lead to a force that acts directly on the order parameter and that can be used to switch the state of the system between equivalent configurations. We particularly study the interplay between this external force and the non-thermal entropic one during an orbital switching event. In the spirit of the control of non-thermal orders by light-manipulation of the fluctuations, we analyze a similar model that, in equilibrium, has a free energy that hosts several stable solutions and, above a critical temperature Tc, several metastable states induced by the order-by-disorder mechanism. After a sudden excitation of the fluctuations, we find it is possible to transiently stabilize the metastable state even if the temperature of the order parameter is below Tc.

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Electronic Properties and Competing Zhang-Rice Singlets in a Stochastically Hole Doped Mixed Valence Cuprate with Glassy Behavior: the Case of $LiCu_3O_3$

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Fascinating phenomena may arise in Condensed Matter Physics, where a large number of components merge together in a non-trivial way leading to emerging behaviors. One example is provided by $LiCu_3O_3$ [1, 2], a mixed valence material based on 2-D square lattices of monovalent Copper atoms and 2-D CuO planes, where the stochastically introduced Lithium atoms act as charge compensator and as source of disorder. Also, these substitutional atoms are responsible for the measured 2-D Coulomb glass behavior and for the reduced quasi-particle lifetime close to the Fermi level. The divalent Copper system interacts with the monovalent one via common Oxygen ligands still forming separated subsystems, and each plane is built upon two almost electronically decoupled sublattices. Surprisingly, many-body effects appear in a counter-intuitive way with an experimental Cu(I)-based valence band [3] that turns out to be much broader compared with the Density Functional Theory expectations. Moreover stable Zhang-Rice Singlet can be found even in presence of the Lithium-induced disorder [4]. The approach used to study this intriguing physical system is both theoretical, computational and experimental, with a common interest in the underlying electronic properties of $LiCu_3O_3$.

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Unsupervised Clustering of Spatially-resolved ARPES Data

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Angle-resolved photoemission spectroscopy (ARPES) is a powerful experimental technique in modern materials science because it can directly probe electronic states, which are directly related to the physical properties of materials. Among the advanced ARPES techniques, spatially-resolved ARPES has recently attracted growing interest because of its capability to obtain local electronic information at the micro- or nano-metric length scales by utilizing a well-focused light source [1]. On the other hand, it is not trivial to analyze and understand the spatial variation of electronic states against massive datasets, typically in 4-dimensional space (energy, momentum, and two spatial axes). In this work, we present unsupervised clustering analyses based on K-means and Fuzzy-c-means methods on spatially-resolved micro-ARPES data from Y-based high-T_c cuprate superconductor $YBa_2Cu_3O_{7-x}$, which shows spatial inhomogeneity due to multiple surface terminations due to BaO or CuO layers on a cleavage (001) plane [2]. The performance of the clustering analyses will be demonstrated with the comparison of the conventional analysis method.

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High-throughput search for magnetic topological materials using spin-orbit spillage, machine-learning and experiments

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Magnetic topological insulators and semi-metals have a variety of properties that make them attractive for applications including spintronics and quantum computation, but very few high-quality candidate materials are known. In this work, we use systematic high-throughput density functional theory calculations to identify magnetic topological materials from the ≈40000 three-dimensional materials in the JARVIS-DFT database (https://jarvis.nist.gov/jarvisdft). First, we screen materials with net magnetic moment > 0.5 μB and spin-orbit spillage (SOS) > 0.25, resulting in 25 insulating and 564 metallic candidates. The SOS acts as a signature of spin-orbit induced band-inversion. Then, we carry out calculations of Wannier charge centers, Chern numbers, anomalous Hall conductivities, surface band structures, and Fermi-surfaces to determine interesting topological characteristics of the screened compounds. We also train machine learning models for predicting the SOS, bandgaps, and magnetic moments of new compounds, to further accelerate the screening process. We experimentally synthesize and characterize a few candidate materials to support our theoretical predictions.

Nonlinear magnetophononics in a frustrated quantum antiferromagnet

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Quantum magnetic materials are valuable model systems for realizing intriguing phenomena ranging from quantum phase transitions to magnon condensation and fractionalization, topological orders, and entanglement on macroscopic length scales [1,2]. The ground state of these materials is dictated by superexchange interactions between neighboring spins, which can be controlled via the crystal lattice through external pressure [3,4]. However, possible strategies to achieve dynamical control, for example, by ultrafast light pulses, remain relatively unexplored.
Here we perform terahertz (THz) pump-probe spectroscopy on the quantum antiferromagnet $SrCu_2(BO_3)_2$ [5]. By using intense terahertz pulses [6] resonantly tuned to lattice modes, we show coherent excitation of a two-triplet bound state, which is a fundamental quantum spin mode in this material. We explain the observed spin dynamics by nonlinear magnetophononics, which arises from the dynamical modulation of the superexchange interaction at the difference frequency mixing of two primary terahertz-driven phonons that break the geometrical frustration. The observed nonlinear magnetophononic effect is analyzed through first principle calculations of the phonon modes and symmetries.
Our results demonstrate a new and attractive route for ultrafast manipulation of superexchange interactions, ground states, and elementary excitations in quantum spin systems, wherein exciting physics in out-of-equilibrium conditions has high potential for major discoveries and applications.

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Ultrafast melting of a C4-symmetry-broken phase: multi-modal and disordered

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In the phase landscape of layered quantum materials recent observations of light induced superconductivity and metallicity are believed to arise from selectively melting the competing C4-symmetry breaking phase [1,2]. Here I will present the investigation of the light induced ultrafast melting of the C4-symmetry breaking phase in the prototypical quasi-2D single layer manganite $La_{0.5}Sr_{1.5}MnO_4$ measured through optical anisotropy. Our results break with proposed models that describe the system by the evolution of the order parameter on a simple free energy potential surface and rather suggest an order-disorder transition [3].

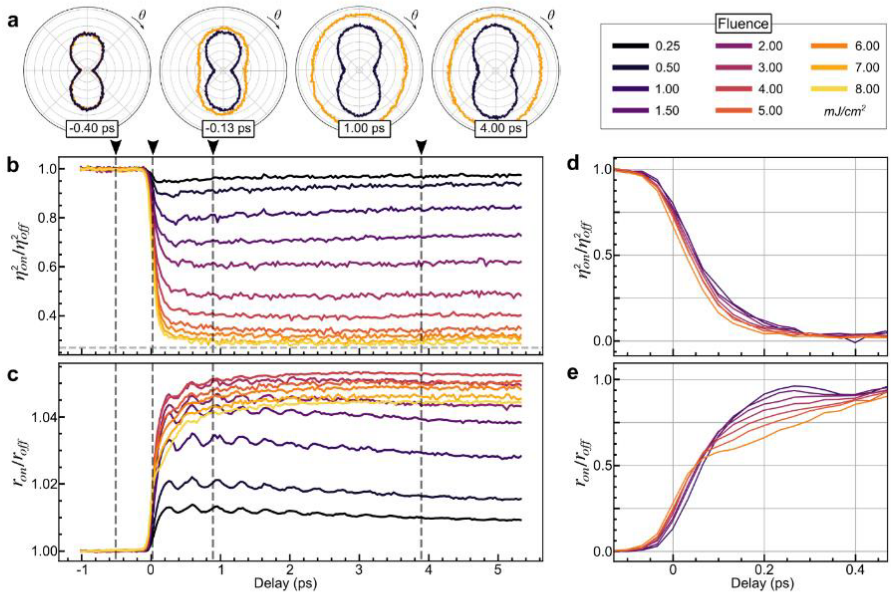

Figure: (**a**) We measure the full optical anisotropy for different pump-probe delays and fluences. (**b,c**)We extract the order parameter and isotropic reflectivity out of the anisotropy patterns. (**d,e**) Detailed analysis of the time traces shows how the order parameter follows neither the coherent evolution of electronic or lattice degrees of freedom directly but instead the C4-symmetry is promptly restored, with strongly overdamped dynamics and threshold-less behaviour.

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Photoinduced modulation of the excitonic resonance via coupling with coherent phonons in a layered semiconductor

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The coupling of excitons with atomic vibrations plays a key role on the nonequilibrium optical properties of layered semiconductors. However, addressing the dynamical interaction between excitons and phonons represents a hard task both experimentally [1] and theoretically [2]. Here, by means of time-resolved broadband optical reflectivity combined with ab-initio DFT calculations [3], we unravel the universal spectral fingerprints of exciton–phonon coupling in a representative layered semiconductor, bismuth triiodide (BiI_3). Furthermore, we resolve a periodic energy modulation of the excitonic resonance of BiI_3 that stem from the coupling to coherent optical phonons. Through a joint experimental and theoretical effort, we achieve to trace the real-space extent of the photoinduced coherent atomic displacement responsible for the exciton energy modulation. Our findings represent a step forward on the road to coherent manipulation of the excitonic properties on ultrafast timescales.

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Core-level x-ray spectroscopy of infinite-layer nickelate: DFT+DMFT analysis

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Recently superconductivity was discovered in infinite-layered nickelate ($Nd_{0.8}Sr_{0.2}NiO_2$) [1], whose microscopic origin is currently being actively studied. To understand differences and similarities with high-temperature superconducting cuprates, it is important to study the valence states of Ni ions as well as the character of the first ionization state where doped holes reside.

Motivated by recent experimental studies [2,3,4], we theoretically investigate Ni 2*p* core-level x-ray photoemission spectroscopy (XPS), Ni 2p core-level x-ray absorption spectroscopy (XAS) and Ni 2*p*-3*d* resonant inelastic x-ray scattering (RIXS). We employ density functional theory (DFT) + dynamical mean-field theory (DMFT) framework which was developed recently [5]. This method describes both realistic bands (Ni 3*d*, O 2*p* and Nd 5*d* bands) with the strong electronic correlation and a local core-valence interaction in the XPS, XAS and RIXS processes accurately. Thus, it enables us to take into account realistic hybridization effect with the valence band in these spectroscopies beyond a conventional impurity-model analysis using e.g. the cluster model or atomic model. Besides, our approach describes the reconstruction of the valence band due to hole doping and associates it with the low-energy RIXS features.

From the Ni 2*p* XPS analysis for the experimental data for $NdNiO_2$ [2], we find that Ni ion is close to the monovalent, i.e. $3d^9$ configuration in the ground state, which is reminiscent of cuprates. However, the charge-transfer energy Δ, that is the key parameter for determining the character of the doped hole, is larger (about 2~3 eV) than typical values for cuprates. Therefore, $NdNiO_2$ is more Mott-Hubbard like in the Zaanen-Sawatzky-Allen classification for transition metal oxides. The Ni 2*p* (L3-edge) XAS and RIXS analysis for the experimental data [3,4] supports the conclusion. The RIXS analysis reveals a signature of a self-doping from the Nd 5*d* bands to the NiO_2 plane, which we show in this talk is the origin for the metal-like behavior reported in the parent compound ($NdNiO_2$) of infinite-layered nickelate in contrast to the Mott-insulating ground sate in undoped cuprates.

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Calculation of collective-mode excitations in excitonic magnet Ca_2RuO_4

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Materials in which the spin-orbit coupling competes with the electron correlation have attracted much attention in recent years. A new stage for the realization of the excitonic insulator phase, where excitons are condensed in the ground state, has thus been provided. Ca_2RuO_4 is one of the candidate materials, where the singlet-triplet excitation in the system of $t2g4$ electrons is induced by the superexchange interaction, leading to the spin-triplet excitonic condensation [1]. The experimental inelastic neutron scattering (INS) and resonant inelastic X-ray scattering (RIXS) spectra are in good agreement with the results calculated for the excitonic phase of the pseudospin model [2-4]. In the *jj* coupling picture, on the other hand, the singlet-triplet excitation can be regarded as an excitation from the j=3/2 band to the j=1/2 band [5].

Here, based on the latter point of view, i.e., in the itinerant-electron approach, we investigate the collective-mode excitations of Ca_2RuO_4. The three-orbital Hubbard model with the spin-orbit coupling, which is a realistic effective model of Ca_2RuO_4, is treated in the mean-field approximation to calculate its ground state. We thus confirmed that the order parameter corresponding to the excitation from the j=3/2 band to j=1/2 band becomes dominant as the spin-orbit interaction becomes larger. Furthermore, we calculated the magnetic susceptibility of the system by applying the random phase approximation and confirmed that the transverse mode is in good agreement with the spectrum of the INS experiment [3] (see Fig. 1.). We also calculated the spectrum of the RIXS experiment using the fast collision approximation and confirmed that it agrees well with the experimental results [4].

Further details of our calculated results and their interpretation will be presented in this conference.

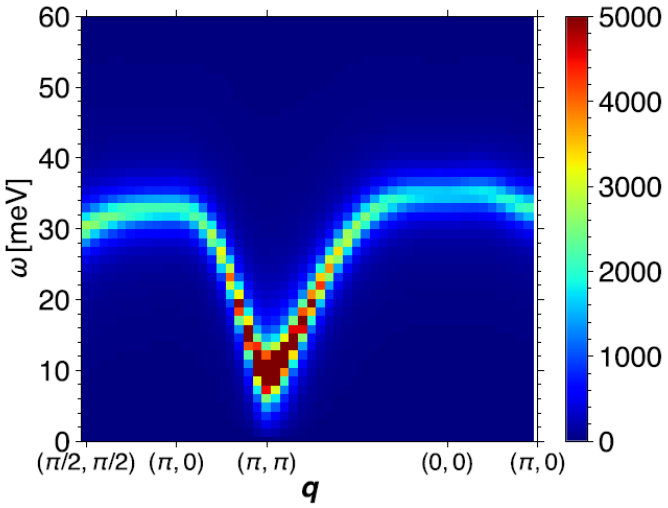

Fig. 1. Calculated dispersion of the transverse mode of the magnetic excitation of our model [6].

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Non-monotonic electron interactions in the copper oxide plane

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In strongly correlated systems the strength of Coulomb interactions between electrons plays a central role in determining their emergent quantum mechanical phases. Specifically, while electrons in free space have a Coulomb interaction energy that decays monotonically with distance, in solids, where the electrons move in a polarizable crystal, the effective Coulomb interaction may be non-monotonic, with a minimum at a finite length. This general concept of how electrons in solids interact may be key to understanding the emerging electronic phases of strongly correlated quantum materials. For instance, a non-monotonic behavior may result in an attractive interaction that could lead to superconductivity or density wave order.

We performed resonant x-ray scattering on $Bi_2Sr_2CaCuO_{8+x}$, a prototypical cuprate superconductor, to probe electronic correlations within the CuO_2 plane. We discovered a dynamic quasi-circular pattern in the *x*-*y* scattering plane with a wave vector radius that is determined by the minimum of the Coulomb potential [1], as shown in Fig. 1 panels (a) and (b), respetively. Furthermore, this radius exactly matches the wave vector magnitude of the well-known static charge order patterns. Along with a comprehensive set of doping- and temperature-dependent measurements, our experiments reveal a picture of charge order competing with superconductivity where short-range domains along *x* and *y* are allowed to dynamically rotate into any other in-plane direction [1].

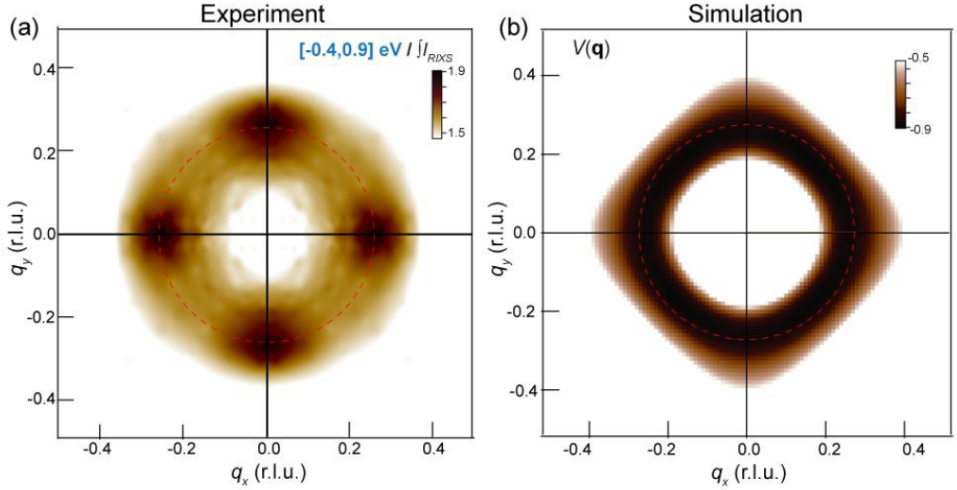

Fig. 1: (a) RIXS intensity in the *qx*-*qy* plane integrated over the [-0.4,0.9] eV range and normalized to the total fluorescence. (b) The structure of the Coulomb interaction V(**q**), calculated taking into account both short- and long-range interaction.

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Fate of charge order in overdoped La-based cuprates

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Charge order is now established in virtually all known hole underdoped cuprates. As a result, charge order is a universal property on equal footing with the pseudogap phase and superconductivity. To understand the possible relationship with the pseudogap phase, it is important to explore the evolution of charge order correlations across optimal doping and into the overdoped part of the phase diagram. In La-based cuprates, several studies on the charge and spin order have recently lead to controversial results in the overdoped regime [1-3]. At the same time, resonant inelastic x-ray scattering (RIXS) has made it possible to detect weak charge correlations above its REXS onset temperature [4]. To address the open questions on the origin of charge order, its connection to the tentative pseudogap critical point and the spin order, we performed a thorough RIXS study of charge order in $La_{2-x}Sr_xCuO_4$ and $La_{1.8-x}Eu_{0.2}Sr_xCuO_4$ samples with dopings up to $x = 0.25$. The results provide a comprehensive and a systematic overview of the charge order in La-based cuprates and sheds light on the doping evolution of the incommensurability and correlation length, as well as the temperature dependence.

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Reshaping the electronic phase diagram of a high-*T*c superconductor by strain

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The microscopic origin of the properties of high-*T*c cuprate superconductors (HTS) remains elusive after 30 years from their discovery. The high temperature normal state is a strange metal dominated by a doping dependent pseudogap regime where states are missing at the Fermi energy. Various symmetry breaking electronic ordering, such as charge density waves (CDW) and nematicity, have been revealed in the underdoped region of the phase diagram, where the pseudogap is present. One of the important issues to solve is how the different electronic ordering phenomena are related to each other and their importance for the physics of HTS, in particular their possible intertwining with superconductivity. The relation between CDW and superconductivity has been extensively studied and it is by now established that the two orders are competing. The most direct evidence of the competition is the suppression of the critical temperature *T*c below the parabolic doping dependent dome. This suppression is strongest at p=0.125 where CDW order is strongest. However, the nature of the competition is not well understood. The CDW also has implications for the normal state of HTS. In underdoped HTS the CDW causes a transformation of the Fermi surface from a large hole-like cylinder at high temperature to small electron-like pockets at low temperature. This change is seen as a change of sign of the Hall coefficient. The exact mechanism of the Fermi surface transformation is still debated, but the most straightforward theory requires a biaxial CDW to produce the electron pockets that fits to the quantum oscillation measurements of the pocket areas. The relevance of the Fermi surface transformation for superconductivity is also not clear. A possible way to study the intertwining of two orders is to tune one of them by e.g. strain or magnetic field and see how it affects the other. How would the HTS phase diagram change if the CDW was uniaxial?
To address this question we have studied the CDW order by resonant inelastic x-ray scattering (RIXS) together with measurements of the in-plane resistivity and Hall coefficient in $YBa_2Cu_3O_{7-\delta}$ (YBCO) thin films on MgO(110). The thin films are untwinned and with doping levels p covering the whole underdoped side of the phase diagram. By varying the thickness t of the films we can tune the strain that is induced by the substrate. RIXS measurements of t=50 nm films with p=0.125 show a biaxial CDW with equal amplitude along the YBCO *a*- and *b*-axis, just as found in bulk single crystals. Similar measurements of strongly strained t=10 nm films show a dramatic difference: the CDW component is completely suppressed along the YBCO *a*-axis and thus becoming uniaxial along the *b*-axis [1]. From resistivity measurements of the t=10 nm films we find that the competition between the uniaxial CDW and superconductivity is weaker; *T*c is enhanced and follows the parabolic doping dependence down to p=0.12 compared to $p\approx$0.14 in the t=50 nm films. Measurements of the Hall coefficient show no difference of the Fermi surface transformation in the t=10 nm and t=50 nm films. This finding is not compatible with mechanisms that require biaxial CDW and highlights the need of new theories to describe the Fermi surface transformation in HTS.

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Fractional magnetic excitations in a large ring-exchange cuprate observed by high resolution RIXS

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The spin ½ square-lattice antiferromagnet is one of the most studied systems in condensed matter theory, both because it is purely quantum mechanical in nature and because of its connection to the problem of High-Critical Temperatures superconductivity. After the seminal paper by Anderson, much effort has been put in the quest for exotic ground states and excitations. In particular, theoretical studies have predicted the existence of different forms of Resonating Valence Bond (RVB) states in many Heisenberg Hamiltonians with either next-nearest neighbour, frustrating couplings (e.g. J_1-J_2 model [1]) or multi-spin couplings (e.g. J-Q models [2]). These states are interesting because they cannot be described by the canonical Linear Spin Wave Theory (LSWT), and exhibit fractionalized collective excitations, each carrying spin ½, that are the 2-dimensional version of spinons in 1D spin chains. Despite many efforts, these states have so far eluded conclusive observation in the AF square lattice. Moreover, a recent exact diagonalization study [3] has shown that the ring-exchange interaction, which couples 4 spin across a square and is sizable in most layered cuprates, might drive as well quantum phase transition towards a RVB ground state. In this context, we have used Cu L_3 Resonant Inelastic X-ray Scattering (RIXS) to study the spin excitations of $CaCuO_2$, a compound where CuO_2 antiferromagnetic planes are indefinitely stacked and separated by Ca ions. This compound is special for the very large nearest neighbour AF coupling J (≈180 meV), and an exceptionally large $J_c \sim J$. At low momentum transfer in reciprocal space, we find that the magnetic spectrum is well described by a single magnon as predicted by LSWT. However, close to the magnetic zone boundary, we observe a strong decrease of the magnon spectral weight, which decays into a broad asymmetric continuum at high energies, accounting for more than 80% of the total spectral weight. Polarization analysis on the scattered beam reveals that this continuum entirely belongs to $\Delta S = 1$ excitations. All these properties are in line to what is expected for a two-spinon continuum. Therefore, we propose that this compound lies close to the quantum phase transition driven by the ring exchange predicted by the theory, and we interpret these high energy excitations as a continuum of spinons.

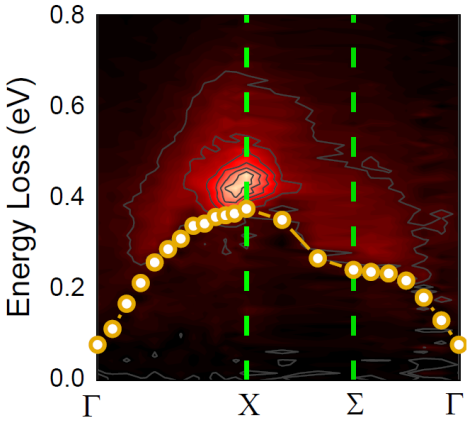

Figure 1: Momentum dependence of the continuum of excitations. Single magnon has been removed for clarity, its energy is shown in the yellow dots.

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Poster contributions

Two-fluid coexistence in a spinless fermions chain with pair hopping

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In order to enrich the understanding of pairing mechanisms in one-dimensional quantum systems, we studied the ground state properties of a spinless fermions chain with single-particle and pair hopping terms in the Hamiltonian [1,2]. We discovered an unusual behaviour of the system with regard to the transition toa pairing phase as the pair hopping parameter strength is increased. The ground state properties are incompatible with previous works on pairing transitions in one-dimensional spinless fermions systems [3,4] and demonstrate that the phenomenology of pairing transitions is even richer than expected.
By examining entanglement, correlation and local kinetic properties of the ground state computed via DMRG simulations, we show the presence of an intervening coexistence phase in which a single-particle Luttinger liquid coexists with a Luttinger liquid of pairs.
The emergence of such an intermediate phase characterized by the simultaneous presence of two gapless bosonic modes is justified by the consequences drawn from a phenomenological two-fluid model; the latter allows to interpret the transitions to/from the coexistence phase as continuous Lifschitz phase transitions associated to the appearence/disappearence of a pair of gapless points in the excitation spectrum of the system.

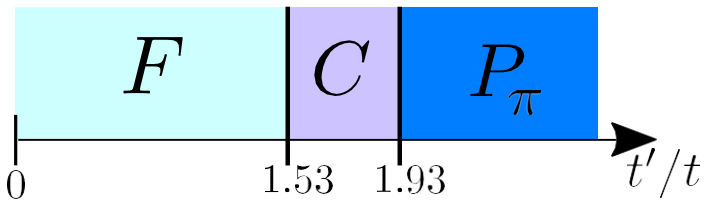

Figure: phase diagram of the model Hamiltonian as a function of the ratio between the pair hopping and the single-particle hopping amplitude in the considered parameter regime. The standard Luttinger liquid phase (F) is separated from the Luttingerliquid of pairs (P) by a coexistence phase (C) of paired and unpaired low energy degrees of freedom.

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Ultrafast dynamics of the surface photovoltage in potassium doped black phosphorus

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Black phosphorus (BP) is a quasi-two-dimensional (2D) semiconducting material with a 0.3 eV direct band gap. Its band structure is very sensitive to external perturbations such as mechanical stress or surface chemical doping, which can lead to a significant renormalization of its electronic band gap [1]. As an example, doping of BP with potassium (K) atoms can create an intense surface dipole leading to the progressive closing of its band gap and thus to a semiconductor-semimetal transition [2].

Is it possible to transiently modify and potentially control thesemimetallic/semiconducting nature of K- doped BP by means of an ultrafast external excitation? To answer to this motivating question, we excite the system with a femtosecond infrared pulse and study the response of its electronic structure by means of time- and angle- resolved photoemission spectroscopy (Tr-ARPES).

The photoexcitation of the material leads to the modification of its valence band spectral shape, resulting in a transient reopening of its electronic band gap. Nevertheless, inspired by recent work [3] and supported by our simulations/experiments, we demonstrate that this reopening is apparent and intimately linked to the creation of a large surface photovoltage (SPV) with a remarkable dynamics (see Figure). Apparent band gap reopening and SPV have the same temporal dynamics over several hundreds of picoseconds after the excitation of the system, before recovering on the nanosecond scale [4]. These results are general for 2D semiconducting materials with significant band bending and point out that care has to be taken in the interpretation of transient electronic structure modifications.

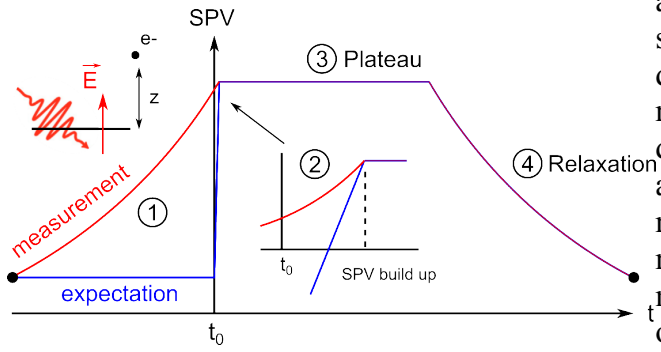

Figure. Schematic representation of the SPV dynamics of K-doped black phosphorus as measured with Tr- ARPES (red) and as expected from theory (blue).

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THz and Optical Spectroscopy Study of Magnetic Topological Materials

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Intrinsic magnetic topological materials are of interest for possible technological applications in dissipationless quantum transport[1-3], electro-optical devices, and magneto transport[4-8]. The combination of topology and magnetism permits the breaking of the time reversal symmetry, with the production of novel quasiparticles and topological phases of matter, like the magnetic topological insulators[9-11], magnetic Weyl semimetals[12-14] and axion insulators[15]. The study of these materials in the thin-film limit is recently being addressed due to the need of characterizing the interplay between the bulk and surface states, usually plagued by the presence of defects in single crystal materials, while also covering the demand of their exotic properties to produce novel electro-optical devices.
In this context, optical linear and nonlinear THz spectroscopy are key tools for the characterization of the topological features of these topological materials. In this talk, we will discuss recent experimental results for the study of two novel topological magnetic materials based on Mn atoms: Co_2MnGa, a nodal line semimetal studied at different film thicknesses, ranging from 10 nm up to 80 nm, and $MnBi_2Te_4$, a material that has been predicted to host all the magnetic topological phases[16-19]. For Co_2MnGa, we have studied its optical conductivity from THz to UV highlighting the variation of its electronic band structure at various thicknesses. Moreover, we will show how high-intensity THz transmission measurements (with a THz electric field up to 2 MV/cm) indicate an induced electromagnetic transparency, with a subtle dependence on the film thickness. For $MnBi_2Te_4$, we will present temperature dependent spectroscopic measurements from THz to UV. We highlight the weight of the surface topological states to the optical conductivity and its modification below the ferromagnetic transition at 20 K.

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Spintronics meets tDMRG: Quantum spin torque driven transmutation of an antiferromagnetic Mott insulatorand dynamical buildup of long-range entanglement within a metallic ferromagnet

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The "standard model" of magnetization dynamics driven by current via conventional (Slonczewski-Berger) spin-transfer torque (STT) is based on [1] single-particle quantum transport treatment of flowing electrons and classical treatment of localized spins within a magnetic material via the Landau-Lifshitz-Gilbert equation. In the "standard model," the transfer of spin angular momentum between flowing electronic spinsand localized spins occurs only if they are noncollinear. However, recent experiments [2] at low temperatures ~1 K suggest that fully quantum nonequilibrium many-body framework is required to describe situations where conventional STT is apparently zero, such as collinear but antiparallel electron and localized spins [3] or localized spins whose expectation value is zero [4] in equilibrium due to entanglement as in the case of quantum antiferromagnets, Mott insulators and quantum spin liquids. To solve this long-standing problem, we have recently [3] adapted time-dependent density matrixrenormalization (tDMRG) algorithms for "quantum STT," by which we term any situation where localized spins must be treated quantum-mechanically with their individual expectation values calculated only at the end. This reveals how quantum STT can generate highly entangled nonequilibrium many-body state of all flowing and localized spins, despite starting from the initially unentangled ground state of a mundane FM, with mutual information between localized spins at the FM edges remaining nonzero even at infinite separation as the signature of dynamical buildup of long-range entanglement [3]. Another prediction from tDMRG [4] shows that interaction of spin-polarized current pulses with the surface of antiferromagnetic Mott insulator (AFMI) will transmute zero expectation value of AFMI localized spins into nonzero values with such new nonequilibrium phase emerging as spatially inhomogeneous ferromagnet with zigzag profileof localized spins. The total spin absorbed by AFMI increases with electron-electron repulsion in AFMI, aswell as when no charge is allowed to penetrate into AFMI [4].

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External Electric Field Effect on Electronic Properties and Charge Transfer in CoI_2/NiI_2 Spinterface

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An important breakthrough in materials science in recent years is primarily associated with the synthesis of novel two-dimensional materials.[1] The absence of intrinsic spin polarization in graphene limits its applications as a spacer in various layered heterostructures.[2] Numerous studies demonstrated that magnetic and spin properties of low-dimensional nanomaterials fundamentally differ from those of the bulk due to the fact of magnetic moment's strong dependence upon coordination number. Bulk CoI2 and NiI2 are A-type antiferromagnets with spins aligned along the metal-iodine bonds which is confirmed by Mossbauer spectroscopy measurements.[3] Cobalt iodide possesses CdI2-type 1T structure (P-3m1 space group) while NiI2 obeys CdCl2-type structure (R-3m:H space group) with ABC-stacking of nickel and iodine ions. There are two possible configurations of TMH2 monolayers, namely, H (trigonal prismatic) and T (octahedral) which differ from each other by the orientation of second-layer ligand atoms with respect to the first-layer ligands.[4] It was estimated that atomic coordination in a monolayer stays alike to correspondent octahedral 3D analogue.[5] It was found that the single layer TMH2 keep semiconducting type of the band gaps.

Electronic structure and spin-related properties of CoI2/NiI2 heterostructure was studied by means of density functional theory. It was shown that the Density of States near the Fermi level demonstrate the antiparallel spin-polarized semiconducting nature. The effect of the external electric field on charge transfer and electronic properties of the CoI2/NiI2 interface was investigated and it was found that the band gap width depends upon the strength of the applied electric field, switching its nature from semiconducting to half-metallic one. An ease control of the electronic properties and promising spin-polarized nature of the CoI2/NiI2 spininterface allows the heterostructure to be used in spin-related applications.

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The impact of microtubule parameters on exciton-polaron energy, mobility andentropy

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We have investigated some dynamical properties of exciton-polaron in microtubule using an unitary transformation and approximate diagonalization technique. The ground state energy, the mobility, and the Tsallis entropy of the exciton-polaron are derived analytically. We found that by increasing the quantum well width, the vibrations along the protofilament increase the exciton-polaron ground state energy than vibrations along the microtubule helix. Furthermore, the high protofilament population forming MTs walls decreases both the groundstate energy and the charge-transfer of the exciton-polaron along protofilaments. We also found that the close is the protofilaments and the higher is the ground state energy of the exciton-polaron. The level of the missing information and the disorder are figured out via the behavior of the Tsallis entropy depending on the protofilament population. It is then showed that high protofilament populations on MTs enhance the disorder in the system and highlighting the dynamic instability of MT.

Vortex state in a strongly correlated d-wave superconductor

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We investigate a vortex lattice induced by the orbital magnetic field in a strongly correlated d-wave superconductor. The vortex-induced inhomogeneities, as well as effects of inherent strong electronic correlations are captured within a Hartree-Fock-Bogoliubov mean-field theory augmented with a formalismof Gutzwiller projection prohibiting all double occupancies from lattice sites. According to the conventional wisdom derived from weak-coupling descriptions, the superconducting pairing amplitude is suppressed inside vortex cores, making the regions behave locally as a normal metal. In contrast, we find that strong electronic repulsions promote formation of Mott insulating vortex cores at low doping. Our calculations indicate that strong correlations cause a non-monotonic variation of the vortex size with doping in sharp contrast with weak-coupling descriptions, leading to a large enhancement of the vortex region towards the undoped limit. The change in the nature of the normal state inside the core has prominent effects on the local density of states (LDOS), elucidating a longstanding puzzle of tunneling spectroscopic measurements in vortex cores of cuprate superconductors [1, 2, 3]. While a metallic core leads to a broad accumulation of weight at zero energy in LDOS, the approach to a Mott insulating core, suppresses this accumulation of weight resulting into subgap features within gap edges. The LDOS spectrum smoothly develops a characteristic hard gap of "Mottness" as the system approaches the undoped limit. We also study the superfluid stiffness and find that the superconducting correlations remain more robust in a vortex lattice whenstrong electronic correlations are included.

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Ensemble Green's function theory for interacting electrons withdegenerate ground states

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In nature, correlated electronic systems containing degenerate ground states are common, with the degeneracy leading to fascinating phenomena such as the quantum Hall effect and emergent magnetic monopoles. Application of the Green's function theory to degenerate systems has however not beenextensively considered, in part stemming from the adiabatic connection being ambiguous for degenerate states. Current approaches either ignore the degeneracy or incorporate it in a non-generalizable manner. In our work [1] we propose an ensemble Green's function formalism, based on the von Neumann density matrix approach, for treating the one-electron excitation spectra of a degenerate electronic system. In the spirit of Hedin, we derive a set of iterative equations for the ensemble Green's function and self-energy,and propose an 'ensemble *GW*' approximation, allowing for a well-defined treatment of degenerate electronic systems. The aim is to present the issues of degeneracy within the standard Green's function method with focus on our proposed ensemble Green's function method.

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Electronic structure of $EuNi_2(P_{1-x}Ge_x)_2$ investigated by resonant hard x-rayphotoemission spectroscopy

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$EuNi_2(P_{1-x}Ge_x)_2$ is a mixed crystal of $EuNi_2P_2$, which shows a nonmagnetic heavy fermion behavior withvalence fluctuation, and $EuNi_2Ge_2$, which is a divalent antiferromagnetic compound with T_N ~30 K [1]. Theeffective mass of conduction electrons in $EuNi_2(P_{1-x}Ge_x)_2$ increases in the vicinity of the boundary between magnetic and nonmagnetic regions, with increasing the Ge concentration x. To clarify this phenomenon, it isimportant to obtain information on not only the *c-f* hybridization but the Eu 4*f*-5*d* Coulomb repulsion U_{fd}, indispensable to understand the valence fluctuation induced quantum criticality [2]. In this study, electronicstructure of $EuNi_2(P_{1-x}Ge_x)_2$ (x = 0, 0.1, 0.2) has been investigated by resonant hard x-ray photoemission spectroscopy (rHAXPES) to understand the role of U_{fd} for the unique physical properties of this system. The rHAXPES experiments in the Eu L_3 absorption region were carried out at BL09XU of SPring-8.

Figure 1 shows the Eu 3*d* rHAXPES spectra at the Eu L_3 absorption region of $EuNi_2P_2$ (x = 0) observed at 20 K. Each of the Eu^{2+} and Eu^{3+} 3*d* components shows a clear resonance enhancement with increasing photon energy ($h\nu$). The constant initial state (CIS) spectrum, which is the $h\nu$ dependence of spectral intensity for a certain structure in the rHAXPES spectrum, for each component shows a Fano-type resonance [3]. From the fits to the CIS and rHAXPES spectra, we estimated the energy difference in thresholds of Eu^{2+} and Eu^{3+} CIS components and that in centroids of Eu^{2+} and Eu^{3+} 3*d*5/2 components, respectively. Assuming the limit of weak *c-f* hybridization, the U_{fd}-values are obtained using these energy differences, and experimentally evaluated to be 3.12, 3.18 and 3.47 eV for x = 0, 0.1 and 0.2, respectively. It is suggested that the increase in the U_{fd}-value with increasing x is attributed to the decrease of the Eu valency with increasing x, i.e., the increase of the 4*f* electrons.

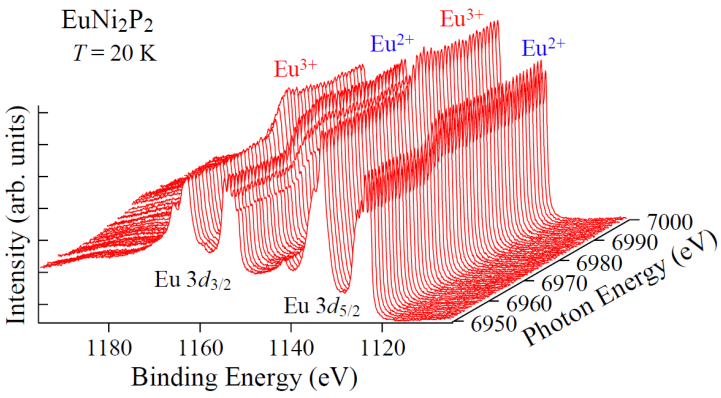

Fig. 1. Eu 3*d* rHAXPES spectra of EuNi2P2 (T = 20 K).

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Anomalous photoinduced transparency in black phosphorus driven by mid-infrared photoexcitation

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Black phosphorus (BP) is a layered semiconductor that has recently attracted increasing attention due to its widely tunable direct band gap and high carrier mobility. The band gap extends from the mid-infrared to the visible range, and can be tuned as a function of the sample thickness and external parameters, such as doping, electric fields and pressure [1]. In contrast to the vast majority of semiconductors, BP features anomalous thermoelectric properties, which lead to an increase of its gap energy with increasing temperature [2]. These peculiar electronic properties
are dictated by many-body effects, namely electron- electron and electron-hole interactions, that ultimately affect its band structure, electronic screening and optical properties [3]. Hot carrier dynamics and recombination have been studied in the near-infrared spectral range by a variety of pump- probe and time-resolved ARPES experiments, but the non-equilibrium response to gap-resonant photoexcitation remains unaddressed.Here we investigate the dynamical response of bulk BP photoexcited by mid-infrared ultrashort pulses with photon energy tunable across the equilibrium band gap. We study the transient change in the optical properties by monitoring the reflectivity of the sample over a broad visible spectral range. By comparing the ultrafast changes in reflectivity that follow photoexcitation at high photon energy with those driven by pulses resonant to the gap (Figure 1), we observe a different spectral response that we ascribe to a photoinduced modification of the screening triggered by mid-infrared pulses. Optical absorption calculations via first-principles DFT support this claim. We report a comprehensive investigation of the gap-resonantly photoexcited carrier dynamics as function of the photon energy of the mid-infrared photoexcitation and the sample temperature, revealing for the first time the temperature dependence of the non-equilibrium band gap in bulk BP. Finally, by employing a three-pulse scheme combining visible and mid-infrared photoexcitations, we could reconstructthe dynamics of the excited state-mediated screening, which is of paramount importance for both optoelectronic applications based on BP and, more generally, for undestanding the screening of excitonic resonances in quantum materials.

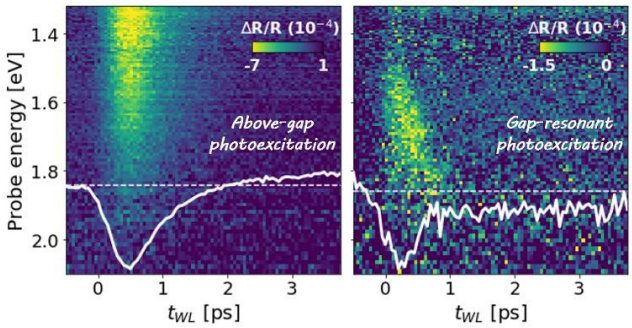

Figure 1: Time- and spectrally-resolved reflectivity induced by an above-gap (3 eV) and a gap-resonant (275 meV) photoexcitation.

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The antiferromagnetic S=1/2 Heisenberg model on the C60 fullerene geometry

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We solve the quantum-mechanical antiferromagnetic Heisenberg model with spins positioned on verticesof the truncated icosahedron using the density-matrix renormalizationgroup (DMRG). This describesmagnetic properties of the undoped C_{60} fullerene at halffilling in the limit of strong on-site interaction U. We calculate the ground state and correlation functions for all possible distances, the lowest singlet and triplet excited states, as well as thermodynamic properties, namely the specific heat and spin susceptibility. We find that unlike smaller C_{20} or C_{32} that are solvable by exact diagonalization, the lowest excited state is a triplet rather than a singlet, indicating a reduced frustration due to the presence of many hexagon faces and the separation of the pentagonal faces, similar to what is found for the truncated tetrahedron. This implies that frustration maybe tuneable within the fullerenes by changing their size. The spin-spincorrelations are much stronger along the hexagon bonds and exponentially decrease with distance, so that the molecule is large enough not to be correlated across its whole extent. The specific heat shows a high- temperature peak and a low-temperature shoulder reminiscent of the kagomé lattice, while the spin susceptibility shows a single broad peak and is veryclose to the one of C_{20}.

Dirac Fermions in a Two-Dimensional Triangular Indium Layer on SiC(0001)

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The Kane-Mele model provides an intuitive strategy to realize nontrivial topology in two-dimensional honeycomb lattices. Graphene, the most prominent representative of this class, lacks spin-orbit coupling (SOC), which prevents the formation of a sizeable bulk band gap and the utilization of the topological phase at reasonable temperatures. By enriching the orbital subspace and concomitantly switching to a triangular lattice, new possibilities arise. Here, we demonstrate by angle-resolved photoelectron spectroscopy that a triangular indium lattice grown on SiC(0001) - indenene - hosts massive, i.e., gapped Dirac Fermions at the K-point. The opening of this topologically non-trivial gap in the order of approx. 100meV relies on the strong local SOC. The in-plane inversion symmetry breaking induced by the substrate counteracts the topology but produces on the other hand a distinctive charge localization that directly reflects the non-trivial topological character of indenene, which allows us to identify this new quantum spinHall insulator by scanning tunneling microscopy.
A detailed theoretical analysis of indenene will be further presented in a talk by P. Eck at the NGSCES.

Signature of field-induced spin ice state and evolution of structural phase on La substitution in disordered pyrochlore $Dy_2Zr_2O_7$

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$Dy_2Zr_2O_7$ a disordered pyrochlore system exhibits the magnetic field induced spin freezing near ~ 10 K in ac susceptibility measurements which is akin to $Dy_2Ti_2O_7$ [1]. The magnetic heat capacity of $Dy_2Zr_2O_7$ shows a correlation peak at 2 K, but no residual entropy was observed. The low-temperature magnetic entropy at 5 kOe field is R[ln2 - 1/2ln(3/2)] which is the same as for the spin ice state. Substitution of non- magnetic, isovalent La^{3+} for Dy^{3+} gradually induces the structural change from highly disordered fluorite tostable pyrochlore phase through a biphasic mixture of both. We observed that the higher La compositions ($1.5 \leq x \leq 1.9$), show spin freezing (T ~ 17 K) similar to the field induced spin ice freezing for low La compositions ($0 \leq x \leq 0.5$), and the well-known spin ice systems $Dy_2Ti_2O_7$ and $Ho_2Ti_2O_7$. The low temperature magnetic state for higher La compositions ($1.5 \leq x \leq 1.9$) culminates into spin glass statebelow 6 K. The Cole-Cole plot and Casimir-du Pr´e fit shows narrow distribution of spin relaxation time in these compounds

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A superlattice approach to doping infinite-layer nickelates

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The recent observation of superconductivity in infinite-layer $Nd_{1-x}Sr_xNiO_2$ thin films has attracted a lot of attention, since this compound is electronically and structurally analogous to the superconducting cuprates. Because phase stabilization upon chemical doping with Sr is challenging, we synthesized artificial superlattices of $LaNiO_3$ embedded in insulating $LaGaO_3$, and used layer-selective topotactic reactions to reduce the nickelate layers to $LaNiO_2$. Hole doping is achieved via "self-doping" from the interfacial oxygen atoms and the layer thickness. We used electrical transport measurements and x-ray spectroscopy together with *ab initio* density functional theory (DFT) calculations to track changes in the local nickel electronic configuration upon reduction and found that these changes are reversible. Within DFT we find that the absence of apical oxygen sites in the inner layers of the heterostructures leads to an extension of localized orbitals into the vacancy site, while at the interface there is a strong hybridization between Ni $d_{3z^2-r^2}$ and O p_z states, favoring the formation of oxygen holes. Experimental and theoretical data indicate that the doped holes are trapped at the interfacial quadratic pyramidal Ni sites. Including local correlations in a dynamical mean-field theory (DMFT) calculation reveals that the hole formation at the interface is further supported by Hund's Coupling, which favors a high-spin state on the interfacial Ni. This behaviour persist upon introducing additional holes, whereas for electron doping we predict a different behavior, with evenly distributed electrons among the layers, thus opening up interesting perspectives for interfacial doping of transition metal oxide.

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Simulating $CaFeO_3$: charge disproportionation in the five-orbital Hubbard model

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$CaFeO_3$ (CFO) is a perovskite transition metal oxide, where the Fe^{4+} cation has a nominal d^4 electron configuration. Around room temperature, CFO exhibits a metal-insulator transition (MIT), where the degeneracy of the e_g states is lifted by a structural breathing distortion, creating alternating large and small Fe-O octahedra, and thus two inequivalent, charge-disproportionated (CD) Fe sites. To understand this coupled structural and electronic transition, we study a simplified, semi-realistic tight-binding model describing the full five-orbital d-shell with local Hubbard-type interactions using dynamical mean-field theory (DMFT). We establish the existence of a spontaneously CD-insulating phase,i.e., the low-temperature phase of CFO, within this model, and characterize this unconventional insulating state. Varying the Coulomb repulsion and Hund's interaction, we also find a metallic and a Mott-insulating state as well as high- and low-spin configurations. Based on interaction parameters we obtain for CFOwithin the constrained random-phase approximation, we expect CFO to be close to a high- to low-spin transition, which can lead to a complex interplay with the MIT. Finally, we investigate theenergetics of these transitions for CFO using fully charge-self-consistent, quantitative density-functional theory plus DMFT calculations.

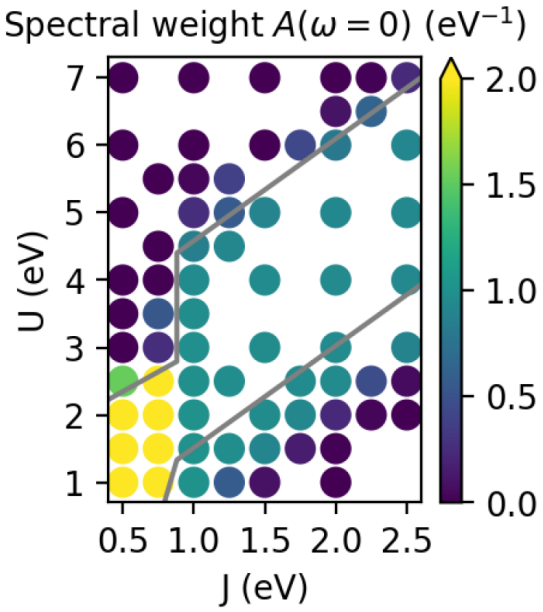

Figure: The spectral weight at the Fermi energy of the tight-binding model. Depending on the interaction parameters U and J, it shows a metallic, a Mott-insulating or a CD-insulating phase.

Comparing the generalized Kadanoff-Baym ansatz with the full Kadanoff-Baym equations for an excitonic insulator out of equilibrium

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Electron-hole pairs or excitons, bound together by the Coulomb interaction, may spontaneously form in semiconductor or semimetal systems with a narrow energy gap or a small band overlap. At sufficiently small gaps or overlaps (and low temperatures) compared to the exciton binding energy, the system can become unstable toward an excitonic insulator (EI) phase. This is conceptually very similar to BCS superconductivity but the EI is based on a purely electronic mechanism [1,2,3]. We investigate the out-of- equilibrium dynamics of an EI model perturbed by a laser pulse and a coupling to fermionic baths [4]. Our calculations, based on the full Kadanoff-Baym equations (KBE) and the generalized Kadanoff-Baym ansatz (GKBA), show that the EI system may undergo a transition toward the normal state when coupled toa bath. However, the isolated EI system perturbed by a laser pulse shows persistent oscillations in the excitonic order parameter but the excitonic order does not melt completely with the GKBA description. This anomalous behavior can be attributed to the narrow spectral features of the GKBA approach, the character of the approximation for the propagators, and correlation-induced damping in the KBE solution.

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Photoinduced *d*-wave superconducting correlation in the extended Hubbard model

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Recent development in ultrafast spectroscopy techniques has led to rapid progress in studying the nonequilibrium dynamics of quantum materials. In particular, the possibility of controlling an ordered phase of strongly correlated electron systems using pump light has attracted much attention. The realization of photo-enhanced superconductivity has been reported in several high-temperature superconductors and organic compounds [1,2]. Some theoretical studies have shown that the superconducting pair correlation in an attractive Hubbard model is enhanced under periodic external fields [3,4]. Also reported is that the pump-light irradiation enhances the *d*-wave superconducting pair fluctuation in the two-dimensional square-lattice Peierls-Hubbard model with electron-phonon couplings, which is due to the suppression of the charge-density-wave (CDW) order [5].

Here, we investigate the possible enhancement of photoinduced superconducting fluctuations by pump light irradiation. We use an extended Hubbard model at half-filling defined on a two-dimensional square lattice. Since this model includes the nearest-neighbor (NN) interaction in addition to the on-site interaction, the CDW phase competes with the spin-density-wave (SDW) phase in the ground state. We employ the time-dependent Lanczos method [6] for numerical calculations, introducing the effect of pump light irradiation via the Peierls phase. The frequency of the pump light is determined from the energy of the optical gap.

First, we consider the standard Hubbard model in which the NN interaction is absent. In this case, the ground state is in the SDW phase. After irradiating a pump light, we find that the spin correlation is suppressed while the d_{xy}-wave superconducting pair fluctuation is enhanced. Simultaneously, the double occupancy increases and the density of states at the Fermi level becomes finite. The enhancement of the d_{xy}-wave fluctuation may come from the enhancement of the charge fluctuation by suppressing the SDW order and the metallization of the system.

Next, we consider the extended Hubbard model whose ground state is in the CDW phase. After irradiating the pump light, we find that the charge correlation is suppressed while the $d_{x^2-y^2}$ wave superconducting pair fluctuation is enhanced. The density of states at the Fermi level also becomes finite. In contrast to the SDW case, the squared magnetic moment increases. The enhancement of the $d_{x^2-y^2}$ wave pair fluctuation comes from enhancing the spin fluctuation by suppressing the CDW order and themetallization of the system.

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Band Interplay and Finite-Bandwidth Effects on the Superconducting Critical Temperature of Heavily DisorderedInterfaces Hosting Multi-Gap Superconductivity

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$LaAlO_3/SrTiO_3$ interfaces are a nice example of a two-dimensional electron gas, whose carrier density can be varied by top- and back-gating techniques. Due to the electron confinement near the interface, the two- dimensional band structure is split into sub-bands, and more then one sub-band can be filled when the carrier density increases. These interfaces also host superconductivity, and the interplay of two- dimensionality, multi-band character, with the possibile occurrence of multi-gap superconductivity, and disorder calls for a better understanding of finite-bandwidth effects on the superconducting critical temperature of heavily disordered multi-gap superconductors.

Temperonic Crystal: A Superlattice for Temperature Waves in Graphene

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Coherent control of wavelike phenomena via metamaterials is driving, ever since four decades, a technological revolution in fields ranging from electronics, photonics, to phononics. Although temperature has been historically considered as the paradigmatic example of an incoherent field, undergoing diffusive as opposed to wavelike propagation, on short space and timescales Fourier law fails and the possibility for temperature wavelike propagation sets in [1]. The ultimate goal is to devise metamaterials, addressed as temperonic metamaterials, enabling coherent control of temperature oscillations arising in the hydrodynamic heat transport regime and operating at above liquid nitrogen temperature. To this end the temperonic crystal (TC), a periodic structure based on a unit cell composed of two slabs sustaining temperature wavelike oscillations on short timescales, is here introduced as an archetypal example [2]. The complex-valued dispersion relation for the temperature scalar field in TCs is investigated for the case of a localized temperature pulse [3]. The dispersion discloses frequency gaps, tunable upon varying the slabs thermal properties and dimensions, serving, for instance, as a frequency filter for a temperature pulse triggered by an ultrashort laser. Results are shown for the realistic case of a graphene- based TC, graphene having recently shown to sustain temperature wavelike oscillations at above liquid nitrogen temperatures [4]. The TC serves as a conceptual building block to manipulate nanoscale heat transfer by exploiting interference effects. The TC concept can be readily expanded to encompass other materials sustaining temperature waves in the hydrodynamic regime such as graphite and single-layer transition metal dichalcogenides, for the case of phononic temperature, and quantum materials [5], for the case of electronic and spin temperatures.

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Ultrafast quasiparticle dynamics in the layered semiconductor bismuth tri-iodide

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The discovery of graphene in 2004 has opened a new field of research about two-dimensional (2D) materials. Nowadays, by virtue of the tunability of their electronic and structural properties, 2D materials are applied in a great variety of areas like, for example, sensors, energy storage, and photonic devices. Among the emerging 2D materials, we have focused our attention on the van-der-Waals-layered semiconductor bismuth tri-iodide (BiI_3). Its photoconversion efficiency of 2% relies on a strong absorption resonance in the visible range and a nanosecond long electron-hole recombination time. This makes BiI_3 a promising material for photovoltaic application.
Here, we investigate the ultrafast optical response of BiI_3 single crystal by means of time-resolved broadband reflectivity. Our measurements reveal a multi-step electron relaxation dynamic with time constants that range from few hundreds of femtoseconds up to tens of nanoseconds, superimposed by a periodic intensity modulation ascribed to the generation of coherent optical phonons. As a first result, we unveil that the exciton is strongly coupled with the coherent phonon in BiI_3 and we identify the spectral fingerprints of this coupling on both the phonon and the excitonic resonance [1].
In the present poster, I will present the concurrent incoherent optical response of BiI_3. At all probed wavelengths, the early fs-long dynamics of the transient reflectivity are dominated by hot-carrier thermalization and cooling. These processes are followed by two ps-long dynamics, due to the electron- optical phonon scattering and a ns-long dynamic, ascribed to the electron-hole recombination via fluorescence [2,3].
Moreover, the energy position of the exciton resonance exhibits a photoinduced abrupt redshift followed bya blueshift that we assign to a change of the electronic band gap as well as of the exciton binding energy, induced by the dynamical screening.
All in all, our preliminary results indicate that the time and energy scale of the photoinduced relaxation dynamics of BiI_3 are suitable for photovoltaic applications.

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Photoexcitations in the Hubbard model –Loschmidt amplitude analysis of impact ionisation in small clusters

Clemens Watzenböck, Anna Kauch, Karsten Held

Light-induced phenomena in strongly correlated systems have gained attention for possible applications in the solar energy conversion [1]. The advantages of strong electron interaction in these systems include the usually large gap and the phenomenon called impact ionisation [2] that in principle allows for the generation of multiple electron-hole pairs per photon. In this talk I will focus on photoexcitations in small Hubbard clusters of up to 12 sites where the time-dependent electromagnetic field is introduced through Peierls substitution. Using exact diagonalization [3] with commutator-free Magnus integrators [4] for time evolution, we analyze the strong out of equilibrium dynamics of the double occupancy and the Heisenberg spin energy. We introduce a novel generalized Loschmidt amplitude to resolve which energy states are responsible for the impact ionization. We moreover demonstrate that the optical conductivity has a characteristic peak structure for one-dimensional chains. We show that these peaks originate solely from vertex corrections. We further apply our novel method which is capable of identifying the relevant energy states responsible for the long-time dynamics also to the Heisenberg spin energy. We find that the tendency toward spin ordering is of little importance in the systems we investigated [5, 6].

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Impurity induced flat band magnetism on the Fermi-Hubbard model

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Electronic flat bands represent a powerful platform to realize unconventional quantum many-body phenomena. Usually, flat bands are studied on their own, while flat-band mediated phenomena has remained largely unexplored. Here we put forward a method to create flat band electrons exchange coupled to local magnetic impurities. The hybridization of the correlated impurity with such flat band leads to flat- band mediated RKKY interaction, in strike comparison with conventional electron gases. We employ mean-field approach and state of art many-body methods dynamical mean-field theory (DMFT) and density matrix renormalization group (DMRG) to study novel emergent orders. Our results put forward flat-band mediated interactions as versatile new platform to control magnetism, providing a potential playground for heavy fermion flat band physics.

Observation of the gap inhomogeneity in $Bi_2Sr_2CaCu_2O_{8+\delta}$ by laser micro-ARPES

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The mechanism of the high-T_c superconductivity has not been clarified yet. The order parameter, the superconducting gap, of the high-T_c superconductivity has been extensively investigated. Angle-resolved photoemission spectroscopy (ARPES) is known as the powerful tool to prove the superconducting gap in a momentum-resolved manner, enabled fingerprinting the *d*-wave gap symmetry in cuprate superconductors. On the other hand, scanning tunneling spectroscopy/microscopy allows to observe the superconducting gap, and the nano-scale inhomogeneity in the real-space was reported in Bi2Sr2CaCu2O8+δ (Bi2212) [1]. However, such real-space inhomogeneity has not been fully considered in the conventional ARPES studies due to its low spatial resolution (~ mm-order scale). To overcome this problem and study the evolution of the superconducting gap in the real- and momentum-space, we have performed high-resolution micro-ARPES experiments on underdoped Bi2212 (T_c = 65 K) using a micro-focused laser ($h\nu$ = 6 eV) at the Hiroshima Synchrotron Radiation Center, Hiroshima University.

Figure 1 shows the ARPES image of the underdoped Bi2212 taken along the nodal direction (~~see~~ red line in the inset) in the superconducting state (T = 20 K). We have then measured such a clear band dispersion from the nodal to the off-nodal direction (~~see~~ blue line in the inset) and evaluated the momentum dependence of the gap. In addition, we have also examined the real-space dependence of the superconducting gap by performing the same measurement while slightly changing the measurement position on the sample surface. We found that the gap magnitude and its momentum dependence are clearly different in spite of the small difference (less than 0.1 mm) on the measurement position. In this talk, we will discuss the observed real-space and momentum-space dependence on the superconducting gap and the pseudogap in detail.

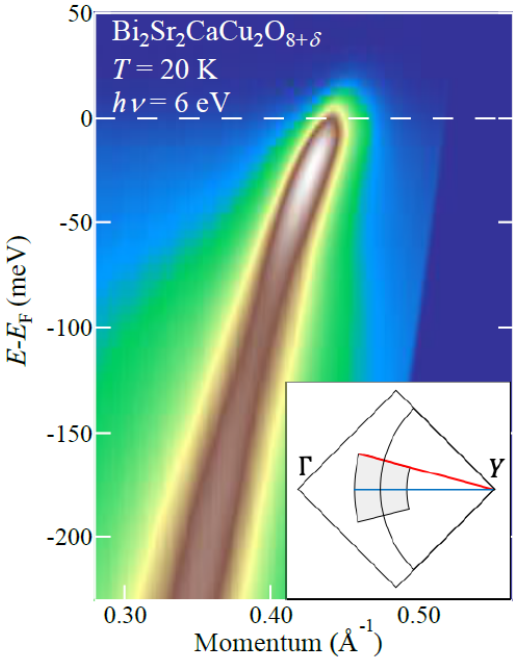

FIGURE 1.*ARPES image of underdoped Bi2212 (*Tc*= 65 K) taken along the nodal direction, where the insetshows the schematic diagram of the Fermi surfacedue to the antibonding bandof Bi2212.*

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Light-induced switching of magnetic order in the anisotropic triangular-lattice Hubbard model

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According to the Floquet theory, the Hamiltonian of the system is modified to a new effective one by introducing a time-periodic perturbation, e.g., continuous irradiation of a laser. This fact is utilized to obtain an artificial Hamiltonian whose quantum eigenstate has desired properties by adjusting the amplitude and the frequency of the external field [1]. The attempt to obtain the desired quantum state by changing the Hamiltonian in this manner is referred to as "Floquet engineering". Typical examples include the realization of the Floquet topological phase by controlling the band topology and the application to the ultrafast spintronics by varying the magnitude and sign of the Heisenberg exchange interaction. In our study, we aim to establish the way to control the magnetic order by a time-periodic external field [2]. Especially, we focus on a quantum system on a geometrically frustrated lattice since there are many competing magnetic orders in the ground state, and thus the switching among each magnetic order by external field is expected.

We use the Hubbard model at half-filling defined on an anisotropic triangular lattice, and the time-dependent Lanczos method [3] is used as a computational technique. When the on-site Coulomb interaction is sufficiently strong, the ground state of the model becomes Néel (120°) order in the small (large) next-nearest-neighbor hopping-integral region [4]. We consider the parameter where the ground state is in the 120° order. We find that, when the external periodic field has a frequency larger than the charge gap, the two kinds of regions emerge; one is the region where the spin correlation function of the 120° order is suppressed, and the other is the region where it is further enhanced. In each region, the spin correlation functions of the Néel order are complementarily enhanced and suppressed, respectively, implying that the switching of the magnetic order is realized in the former case. In addition, we also investigate the case where the ground state is in Néel order and find that the light-induced switching to 120° order is also possible.

These results can be interpreted using the effective Heisenberg exchange interactions obtained by the strong-coupling expansion of the Hubbard model and the high-frequency expansion by the Floquet theory [5,6]. The region where the magnetic order switching may occur is reproduced by using the ratio of the effective interactions. The quench dynamics of the Heisenberg model with these effective interactions is in good agreement with the Hubbard model in the time-periodic external field. We thus show that light irradiation can selectively control the magnetic order of a frustrated magnetic material.

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Roles of collective modes in third harmonic generation in excitonic insulators

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Recent progress in experimental techniques has made it possible to observe the dynamical properties of quantum many-body systems with laser light. Thus, the investigation of nonequilibrium states far away from equilibrium has become one of the central issues of condensed matter physics [1]. In addition, nonlinear optical responses in quantum materials, e.g., high-harmonic generation in strongly correlated electron systems [2,3], has actively been studied in recent years from both basic and applied aspects.

Motivated by such developments in the field, we study the nonlinear optical response of excitonic insulators theoretically. Specifically, using the extended Falicov-Kimball model (spinless two-band model), we investigate the nonlinear optical response of the excitonic insulator. We use the time-dependent mean-field theory to incorporate the dynamical behavior of the order parameter of the exciton insulator and evaluate the photocurrent by solving the equation of motion in the Anderson pseudospin representation. In addition, we carry out the analytical calculations using the perturbation expansion in terms of the nonequilibrium Green's function to investigate the behavior of the photocurrent.

In this talk, we will mainly present results for third-harmonics generation (THG) in the excitonic insulators. Fig. 1 shows the calculated third-order nonlinear optical response function. In the THG susceptibility, we find that the contribution of the excitonic collective mode is characteristically seen at half of the energy of the single-particle excitation gap. In order to identify the roles of the order parameter in THG, we will also compare these results with the response functions that ignore the collective-mode excitations. Then, together with the analytical calculations by the perturbation expansion, we will discuss the origin of the corrections of the THG profile induced by the collective-mode excitations in the excitonic insulator.

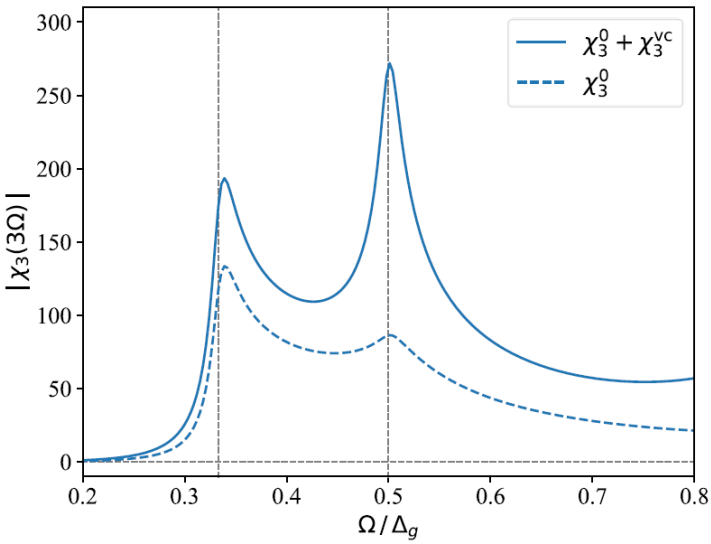

Figure 1: THG susceptibilities with (solid line) and without (dashed line) the collective-mode excitation

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Kondo physics in A-site ordered perovskite transition-metal oxides

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Kondo physics is observed widely in 4f rare-earth compounds, while it is elusive in transition-metal oxides with broader bands. However it was suggested experimentally that Kondo effect and heavy fermion like behavior take place in A-site ordered transition-metal perovskite oxides containing two different transition metals [1][2]; $CaCu_3Ir_4O_{12}$ and $CaCu_3Ru_4O_{12}$. The strong hybridization between localized spin (S=1/2) of Cu and Ir 5d (Ru 4d) bands may give rise to the Kondo states. However the question whether the materials can be viewed as the Kondo material is still under debate. We present a computational study of the electronic structures in $CaCu_3Ir_4O_{12}$ and $CaCu_3Ru_4O_{12}$ by means of local density approximation (LDA) + dynamical mean-field theory (DMFT).
Figure 1 shows LDA and LDA+DMFT density of states in $CaCu_3Ir_4O_{12}$. The localized Cu xy states are embedded in broad metallic bands composed of Ir t2g states. The LDA+DMFT result reveals a sharp Kondo peak near the Fermi energy. The calculated local spin correlation function result of Cu 3d electrons at different temperatures shows a screening of the Cu spin moment at low temperatures due to the Kondo coupling. In this talk, we discuss a crossover from a Fermi liquid state to a localized spin state by analyzing the temperature dependence of the self-energy and the density of states.

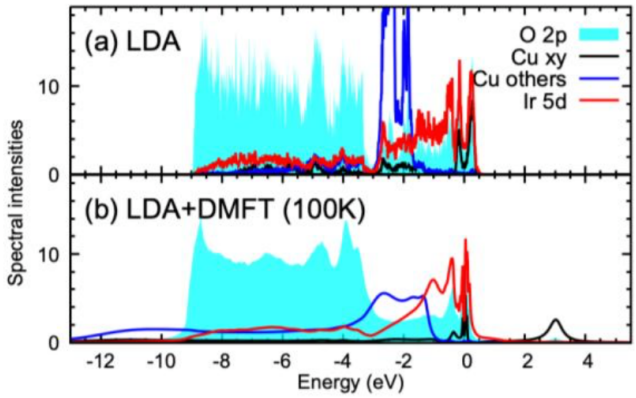

Figure 1: LDA and LDA+DMFT density of states in $CaCu_3Ir_4O_{12}$

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