December 11-15, 2022
Ambrož, Krvavec, SLOVENIA

BOOK OF ABSTRACTS

NQW

Nonequilibrium Quantum Workshop

December 11 - 15, 2022
Krvavec, Slovenia
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Ultrafast spin-lattice dynamics in FePt nanoparticles

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The dynamics of spins in magnetic materials initiated by a sub-picosecond laser pulse is an emerging and rapidly developing field in fundamental magnetism. The goal of this research is to understand and ultimately control the energy and angular momentum transfer processes in the laser-excited non-equilibrium state. The exploration of the excited-state electronic and magnetic structure has received much attention ever since femtosecond optical lasers have become available. The magneto-acoustic coupling of phonon and magnon modes offers novel functionality for spintronics applications in information technology. Magnon polarons can form via magnetoelastic coupling [1], circularly polarized phonons can form and transport angular momentum [2] or phonons can be used to generate spin currents in metallic contacts [3]. However, many of these phenomena are currently only demonstrated at GHz frequencies and micrometer dimensions. X-ray free electron lasers (XFELs) enable us to explore the potential of moving towards THz frequencies and nanometer dimensions that are far more attractive for applications. In this talk I will discuss how the non-equilibrium conditions reached during ultrafast demagnetization with a femtosecond laser pulse provide an efficient generation mechanism for the formation of spin-wave solitons [4]. We identify the coherent phonons generated by the spin-wave solitons' magnetization precession. The small magnetic exchange length of FePt determines the size of the spin-wave solitons of only several nanometers and up to THz frequency [5]. This is expected to open up new theoretical and experimental efforts towards the understanding of magnetism at its intrinsic length and time scales, with implications for further scaling strategies in magnetic information storage and processing.

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Electric Pulse Driven Spin and Charge Dynamics in Mott Insulators

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Electric pulse applied to materials changes states of matter and induces novel phenomena. Mott insulating states are a good playground for such phenomena. We firstly focus on a two-dimensional Mott insulator with square lattice, which is a parent compound of cuprate high temperature superconductors. Calculating momentum-dependent spin dynamics induced by pumping electric pulse numerically, we find an antiphase oscillation of spectral weight in the spin structure factor between momentum $q = (\pi,0)$ and $(0,\pi)$, which can be detectable by time-resolved resonant inelastic x-ray scattering. Such an oscillation is seen in the equal-time spin correlation function and the intensity of single-magnon excitations [1]. The oscillation partly originates from antiferromagnetic exchange interaction modified by the pumping pulse. In addition, we find that, after turning off a pump pulse tuned to an absorption edge, new magnetic signals clearly emerge well below magnon energy in both single- and two-magnon excitations (for two-magnon case, see Fig. 1) [2]. The low-energy excitations are predominantly created via excitonic states at the absorption edge. These exciton-assisted magnetic excitations may provide a possible explanation for low-energy spectral weight in a recent time-resolved two-magnon Raman scattering experiment for insulating $YBa_2Cu_3O_{6.1}$ [3].
We next examine photo-doping effect on a one-dimensional Mott insulator driven by pumping electric field, by calculating time-resolved optical conductivity numerically [4,5]. We find the appearance of photocarriers in the optical conductivity strongly depends on the frequency of the pumping pulse. In particular, strong mono- and half-cycle pulses inducing quantum tunneling strongly suppress spectral weights contributing to the Drude weight, even if we introduce a large number of carriers. This is in contrast to a metallic behavior in the Drude weight induced by photon absorption and chemical doping. The strong suppression of the Drude weight in the quantum tunneling regime is a result of the emergence of the Hilbert-space fragmentation, which makes pulse-excited states glassy [4]. The glassy state is accompanied by electric polarization breaking inversion symmetry [5]. We also demonstrate that, using an ultrashort subcycle pulse, one can generate a steady electric current because of an Aharonov-Bohm flux instantaneously introduced through the phase of an electric field. Consequently, time-reversal symmetry is broken [5]. Both symmetry breakings can be monitored by second harmonic generation. These findings propose a new methodology for designing the symmetries of electronic states and open up a new field of subcycle-pulse engineering.

[1] K. Tsutsui, K. Shinjo, and T. Tohyama, Phys. Rev. Lett. **126**, 127404 (2021).
[2] K. Tsutsui, K. Shinjo, S. Sota, and T. Tohyama, arXiv:2207.0341.
[3] J.-A. Yang et al., Nat. Commun. **11**, 2548 (2020).
[4] K. Shinjo, S. Sota, and T. Tohyama, Phys. Rev. Res. **4**, L032019 (2022).
[5] K. Shinjo, S. Sota, S. Yunoki, and T. Tohyama, arXiv:2211. 08694.

Quantum Domain Melting in a Quantum Annealer

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The ordering of systems emerging through non-equilibrium symmetry breaking transitions is inevitably accompanied by domain formation. The underlying microscopic physics that defines the system's energy landscape for tunneling between domain configurations is of interest in many different areas of physics, ranging from cosmology to solid state quantum matter [1-8]. Domains may reconfigure by thermally-driven microscopic processes [9,10], or - in quantum systems - by incoherent macroscopic quantum tunneling. Here, we report quantum domain melting dynamics in two embodiments: an electronic crystal 1T-TaS_2, and its matching simulation on a quantum computer [11]. We use scanning tunneling microscopy to measure the time-evolution of electronic domain reconfiguration dynamics in real time and compare this with the time evolution of domains in an ensemble of entangled correlated electrons in simulated quantum domain melting. The domain reconfiguration is found to proceed by tunneling between minima in a self-configuring energy landscape. A quantum charged lattice gas model is set up in a quantum annealer, that closely matches the experiment. Both are seen to exhibit characteristic ragged time evolution and temperature-dependence observed macroscopically averaged over the ensemble. Understanding the quantum processes involved in electronic domain melting opens the way to understanging non-equilibrium interacting many-body quantum systems at the microscopic level.

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[3] S. Coleman, Physical Review D 15, 2929 (1977)
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Visualisation of topology of a metastable domain state in 1T-TaS_2

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Systems with globally protected topological states that exhibit metastability are considered possible candidates for use in quantum computation and memory devices. Such systems can feature topological objects such as domain walls in ferroelectric[1] or magnetic[2] nanowires, which can be manipulated using electrical current and are already used in memory devices.
Here we present another system (material 1T-TaS_2), where the formation of a 'hidden' (*H*) metastable state with a topological domain wall network is observed after external current pulse excitation. Using multi-tip scanning tunnelling microscope (STM) we see how the emergent charge density wave (CDW) state evolves with electrical current pulsing and observe the annihilation dynamics of domain walls at higher currents. We interpret the domain state using Wigner-Seitz tessellation, which gives us insight into the topological protection of the metastable network of dislocations connected by domain walls. We also study how the emergent state is linked with the injected carriers using charge lattice gas model.

Intra- and Inter-Layer Charge Density Wave Dynamics of 1*T*-TaS_2

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1*T*-TaS_2 is a van der Waals transition metal dichalcogenide material with unique 'Star of David' charge density wave (CDW) states in thermal equilibrium [1]. Numerous studies have characterized these phases through observables such as resistivity, optical reflectivity, and scanning tunneling microscopy, but experiments to study the structural dynamics of the nonequilibrium 'hidden' CDW state and a seemingly probabilistic chiral switching have been less revealing [2-5].
We performed ultrafast pump-probe X-ray diffraction experiments to access dynamic observables, coherent oscillations of structural and electronic signals, to reveal directional and chiral dependencies that unveil the complexity of the domain structure that prior experiments failed to capture. In particular, distinct frequencies and modulations tied to specific positions in momentum space of both the equilibrium and nonequilibrium 'hidden' CDW orders shed light on the inter- and intra-layer dynamics.

[1] B. Sipos *et al.*, Nat. Mater. **7**, 960-965 (2008)
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Cavity control of metal insulator transition in TaS2

D. Fausti

Charge Dynamics in the Amorphous State of 1T-TaS_2

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The interest in 1T-TaS2 is not fading for the last 10 years thanks to its well-known metastable hidden (H) state, which can be reached only at non-equilibrium conditions at low temperatures [1]. The charge density wave (CDW) in the material forms domains and domain walls at such conditions. While being stable for extended periods of time at low temperatures, the H state relaxes back to the commensurate CDW (C state) upon heating [2].

While the H state is the most studied for 1T-TaS_2, the material can undergo other phase transitions to various states [3], including the amorphous (A) state [4], which is studied in this work.

We are presenting the results of the scanning tunnelling microscopy studies of the local charge dynamics in the laser-induced A state of 1T-TaS2 in the context of the time-domain phase diagram of the material.

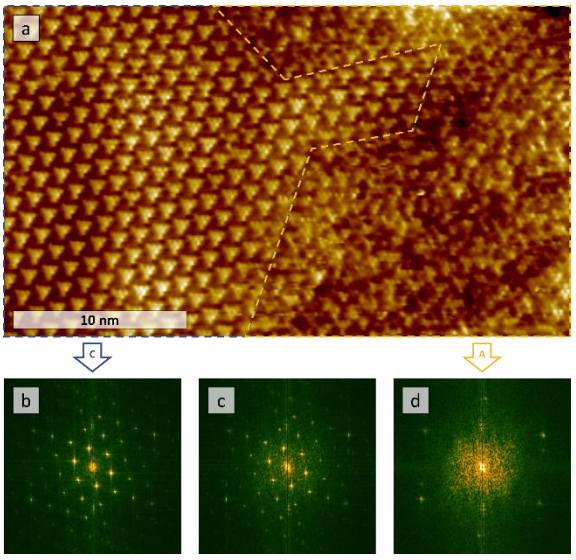

Fig. 1. a) STM image of the border between C (blue dashed line) and A (yellow dashed line) states of 1T-TaS2 after exposure to a laser pulse. b-d) Fourier transform of C state, the whole image and A state, as marked by lines in (a).

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[3] Ravnik J., et al. ACS Applied Nano Materials 2, 3743-3751 (2019)
[4] Gerasimenko, Y.A. et al. Nat. Mater. 18, 1078–1083 (2019)

Ground state symmetries and collective modes in Ta_2NiSe_5

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The origin of phase-transition from a high temperature orthorhombic phase to a low temperature monoclinic phase in Ta_2NiSe_5 is debatable. There are two competing scenarios, namely, a structural instability with a B_{2g} zone center optical phonon and electronic order parameter of excitonic nature breaking the discrete set of lattice symmetries due to a sponteneous interband hybridization between Ta and Ni mediated by Coulomb many-body interactions [1-4]. We further explore the ground state symmetries and nature of collective excitations in the excitonic ordered phase of this compound.
We perform a realistic modeling using Density Functional Theory as a starting point to construct a tight-binding Hamiltonian and describe the electronic correlations on a Hartree Fock level. The collective modes or excitonic susceptibilities in the ordered phase are computed within the linear response regime [5]. We see the breaking of discreet lattice symmetries due to the Ta-Ni hybridization makes the phase mode massive. We estimate the mass of this phase mode and show how the shape of the susceptibility depends on the strength of Ta-Ni hybridization, lattice geometry and temperature.

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Monday, December 12, 2022

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Ergodicity and dynamics of strongly disordered one- and two-dimensional interacting systems

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We consider a chain of interacting fermions with random disorder that was intensively studied in the context of many-body localization. We show that only a small fraction of the two-body interaction represents a true local perturbation to the Anderson insulator [1]. While this true perturbation is nonzero at any finite disorder strength *W*, it decreases with increasing *W*. This establishes a view that the strongly disordered system should be viewed as a weakly perturbed integrable model, i.e., a weakly perturbed Anderson insulator. As a consequence, the latter can hardly be distinguished from a strictly integrable system in finite-size calculations at large *W*. We then introduce a rescaled model in which the true perturbation is of the same order of magnitude as the other terms of the Hamiltonian and show that the system remains ergodic at arbitrary large disorder.

We study also a quench dynamics of interacting spinless fermions on a disordered, two-dimensional lattice [2]. First, we demonstrate that the semiclassical description provides the upper bound for the relaxation rates. We obtain this result by comparing the semiclassical dynamics with exact diagonalization and Lanczos propagation of one-dimensional chains. Next, we show that strongly disordered two-dimensional systems exhibit a transient, logarithmic-in-time relaxation which is well established for one-dimensional disordered chains.

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Probing real-time broadening of nonequilibrium density profiles via a local coupling to a Lindblad bath

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The Lindblad master equation is one of the main approaches to open quantum systems. While it has been widely applied in the context of condensed matter systems to study properties of steady states in the limit of long times, the actual route to such steady states has attracted less attention yet. Here [1], we investigate the nonequilibrium dynamics of spin chains with a local coupling to a single Lindblad bath and analyze the transport properties of the induced magnetization. Combining typicality and equilibration arguments with stochastic unraveling, we unveil for the case of weak driving that the dynamics in the open system can be constructed on the basis of correlation functions in the closed system, which establishes a connection between the Lindblad approach and linear response theory at finite times. This connection particularly implies that closed and open approaches to quantum transport have to agree strictly if applied appropriately. We demonstrate this fact numerically for the spin-1/2 XXZ chain at the isotropic point and in the easy-axis regime, where superdiffusive and diffusive scaling is observed, respectively.

[1] T. Heitmann et al., arXiv:2210.10528 (2022).

Suppression of dark-state polariton collapses in EIT-based cold-atom quantum memory

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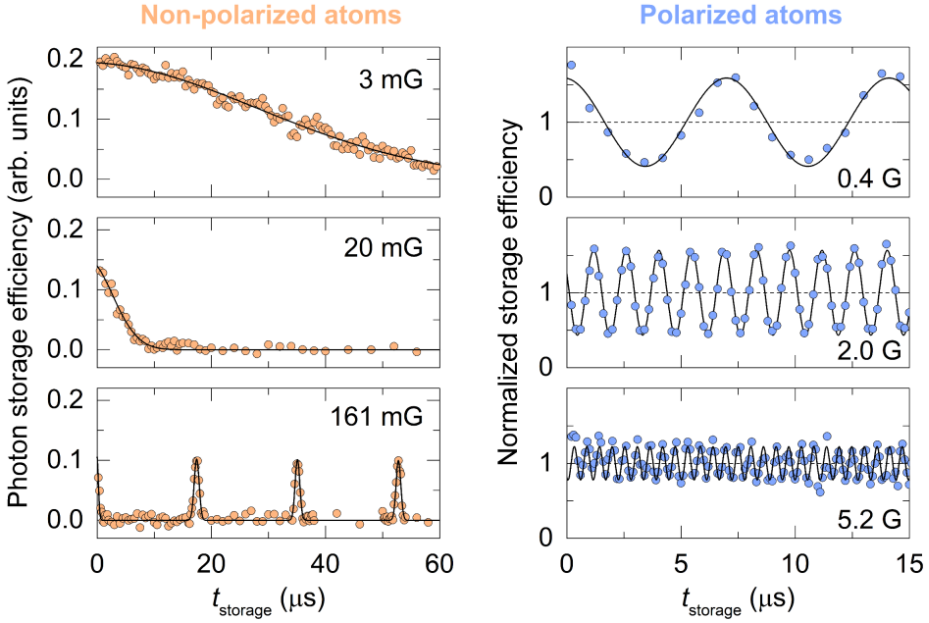
Cold atoms are an emerging quantum technology offering unparalleled accuracy, precision and control in a variety of applications, including gravimetry [1], magnetometry [2] and quantum computing [3]. They are also very promising as a light storage medium using the phenomenon of electromagnetically induced transparency (EIT). The group velocity of light passing through the atoms can be slowed down or even stopped, while the information of the light is written onto the atoms in the form of spin waves (dark state polaritons) [4]. We will discuss the optimisation of photon storage time in the presence of a magnetic field [5].



Left panel: The presence of a small magnetic field (B = 3 mG) causes the spin waves to interfere and collapse, effectively reducing the lifetime of the photon storage. At higher magnetic fields (B = 161 mG) the spin wave interference causes periodic collapses and revivals in the photon storage efficiency. Right panel: If the atoms are initially polarized, fewer different spin waves are created and consequently their interference is less destructive. The oscillations in photon storage efficiency become less pronounced at higher magnetic fields with storage times exceeding 500 μs [5].

[1] Iván Alonso *et al.*, *EPJ Quantum Technol*. **9**, 30 (2022).
[2] Katja Gosar, Tina Arh, Tadej Mežnaršič, Ivan Kvasič, Dušan Ponikvar, Tomaž Apih, Rainer Kaltenbaek, Rok Žitko, Erik Zupanič, Samo Beguš, and Peter Jeglič, *Phys. Rev. A* **103**, 022611 (2021).
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[5] Vesna Pirc Jevšenak, Katja Gosar, Tadej Mežnaršič, Samo Beguš, Erik Zupanič and Peter Jeglič, manuscript in preparation.

Photoinduced superconductivity by η pairs in a Mott insulator

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Recent experiments have clearly demonstrated that the non-equilibrium dynamics can induce many intriguing physics in strongly correlated materials. Among them, the most striking is the discovery of photo-induced transient superconducting behaviors in some of high-Tc cuprates and alkali-doped fullerenes. It has also been shown theoretically that superconductivity can be enhanced or induced by pulse irradiation in models for these materials. However, the main focus so far, both experimentally and theoretically, is a photo-induced state that may already exist in the equilibrium ground state phase diagram. Here, employing unbiased numerical methods, we show that pulse irradiation can induce superconductivity as photo-induced excited states in the Mott insulator of the Hubbard model. The superconductivity is due to the η-pairing mechanism and exhibits the pair-density-wave like staggered off-diagonal long-range correlation. Since the superconductivity is absent in the ground state phase diagram, i.e., not induced by photo-doping of carriers or due to a dynamical phase transition by effectively changing the physical parameters, our finding provides a conceptually different pathway to a nonequilibrium control of unraveling hidden excited states and may also give an alternative interpretation for the enhancement of superconductivity observed in the recent experiments.

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[2] T. Shirakawa, S. Miyakoshi, and S. Yunoki, Phys. Rev. B **101**, 174307 (2020).
[3] T, Kaneko, S. Yunoki, and A. J. Millis, Phys. Rev. Research **2**, 032027(R) (2020).

Behavior of spectral form factor and survival probability in systems with eigenstate transitions

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Recently it was shown, in the three-dimensional Anderson model [1] and the avalanche model of ergodicity breaking transitions [2], that the spectral form factor and the Thouless time extracted from the spectral form factor are useful measures for characterization of eigenstate transition. In the literature, an alternative definition of the Thouless time was given in terms of survival probability [3,4] which measure the stability of initial states. Motivated by this fact, we investigate the survival probability measure and possible connections to the spectral form factor measure.

We focus on differences in behavior of the survival probability across the eigenstate transitions. Remarkably, we observe scaling invariant power-law decay of the survival probability at the transition in three physically relevant models: the three-dimensional Anderson model, one-dimensional Aubry-Andre model, and the avalanche model of ergodicity breaking transitions. We discuss connections of this universality to the universality of the spectral form factor measure. Our study [5] demonstrate that both quantities, the survival probability and the spectral form factor, are useful tool for detection of the eigenstate transitions.

[1] J. Šuntajs, T. Prosen and L. Vidmar, Annals of Physics **435**, 168469 (2021)

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[5] M. Hopjan and L. Vidmar, in preparation

Ultrafast surface melting of electronic order in a manganite

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Key to understanding dynamics of phase transitions is to be able to track the dynamics of the order parameter. Time-resolved diffraction has been a key tool in this regard as it is senstive to both the amplitude and wave-vector of the order parameter. However, extacting the dynamics of the order parameter from a Bragg peak is still non-trivial and requires assumptions, such as which atoms are moving during the phase transition and the exact role of the heterogenity.

In first order phase transitions, surfaces play a key role, for example the surface electronic order in the manganite $La_{0.5}Sr_{1.5}MnO_4$ melts at a significantly lower temperature than the bulk order [1]. The role of surface effects in ultrafast phase transitions have been largely ignored to date, but experiments in the X-ray regime are often sensitive to the surface regime because they are performed in geometries that aim to limit the pump-probe penetration depth miss-match.

In this talk, I will present combined optical [2] and X-ray work that shows understanding this surface heterogenity is key to understanding the dynamics of the order parameter. By using time-resolved reflection anisotropy, we can extract the dynamics of the electronic order parameter and find that melting is an incoherent process that starts at the surface. By moving to X-ray surface scattering, we can extract the dynamics from the orbital truncation rod. We find that a huge degree of disorder is generated after exctitation, which first appears at long length-scales and takes longer to influence the short range order. Furthermore, while a coherent response is also seen in diffraction, showing many of the signs of a coherent structrual change, we show that the coherence is not associated with the order parameter, but arrises from a form of X-ray heterodyned detection of zone boundary modes.

Collapse of the band gap at the surface of *1T*-TaS_2 induced by strain

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Tantalum disulphide (1*T*-TaS_2) is a layered material that hosts a series of charge density wave (CDW) phases at temperatures below ~350K, and an insulating commensurate CDW (CCDW) phase below ~165 K. In 1976, already, it was recognized that the particular rearrangement of atoms in so-called Star-of-David within the CCDW phase might lead to a Mott phase due to the presence of strong electronic correlations and small electronic bandwidth of the Ta *5d* band [1]. Since then, more evidence in favour of a Mott phase has accumulated in the literature. However, recently, this picture has been challenged by the proposal that interlayer hybridization is in fact responsible for the insulating CCDW phase [2]. What is then the role of electronic correlations in this material?

In this talk, I will present angle resolved photoelectron spectroscopy (ARPES) measurements on 1*T*-TaS_2 combined with advanced electronic structure calculations (GW+EDMFT) showing actually that both pictures, the Mott correlations and the interlayer hybridization, are leading to band gap formation and thus the insulating character of the CCDW phase in 1*T*-TaS_2 [3].

In a second part, I will show how strain can be employed to modify the ground state of 1*T*-TaS_2 as probed by ARPES [5]. As a consequence of strain, a bandwidth-driven insulator-metal transition is observed upon reducing temperature. The collapse of the band gap and the presence of an emergent quasi-particle peak at the Fermi level further support that the system hosts Mott correlations.

All in all, the recent literature and our studies depict the layered material 1*T*-TaS_2 as a complex material for which a subtle combination of electronic correlations and interlayer stacking leads to a rich phase diagram.

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[3] Petocchi *et al.*, Phys. Rev. Lett. 129, 016402 (2022).
[4] Nicholson *et al.*, arXiv, 2204.05598 (2022).

Clocking superconducting fluctuations in cuprates: a covariance-based approach

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In both underdoped and optimally-doped cuprates, superconducting fluctuations survive well above the critical temperature, where either the presence of a competing charge order or the pair phase incoherence yet hinder the formation of a macroscopic superconducting state. Addressing the role of superconducting fluctuations is thus key to elucidate the pairing mechanism itself. However, standard spectroscopies are mostly based on a mean-value approach that, by integrating several stroboscopic repetitions to improve the signal-to-noise ratio, would flatten not only the environmental noise, but also the intrinsic photonic fluctuations (either classical or quantum) that can carry instead genuine information on the material properties. Here, we develop a covariance-based technique to study time-resolved electronic Raman scattering in cuprates. By probing the system with randomized pulses and implementing a single-shot frequency-resolved acquisition, we are able to unveil the spectral correlations imprinted in the pulses by the inelastic scattering from the pump-induced Cooper pair breaking. The momentum selectivity peculiar to Raman scattering, in combination with the sub-picosecond temporal resolution of the technique, allows to measure the correlation dynamics projected onto different regions of the Brillouin zone, thus enabling the isolation of the nodal and antinodal contributions. Our findings reveal gap-size correlations in the pseudogap phase, hinting at the presence of a local pairing that survives even when the superconducting state is macroscopically melted.

Slow diffusion in modulated spin chains: from periodic to random systems

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It is general observation that one-dimensional spin chains, and equivalently interacting fermionic chains, reveal a transition/crossover to many-body localization (MBL) when subjected **to** large random or quasiperiodic (QP) potentials, which is manifested in strong dependence of the d.c. transport quantities on potential strength W. The qualitative difference is that in random systems numerical results show large sample-sample fluctuations [1], while QP systems can/do not since the potential is deterministic. We present numerical results for the high-temperature dynamical and dc transport, i.e., the dc spin conductivity σ_0, in QP as well as in simpler periodic chains. In QP system σ_0 reveals an exponential-like dependence on W over several decades, without any clear indication of a well-defined transition to MBL. Moreover, replacing the QP potential with a simpler periodic one, the variation remains qualitatively similar up to intermediate values of W, whereas at large W the dc conductivity shows power-law decay consistent with the absence of MBL in such systems, which offers a new route to investigations of slow diffusion in such systems. The relation of dc transport to level statistics and matrix-element fluctuation is also investigated in QP system to establish the shifting of the effective MBL crossover with system size.

[1] J. Herbrych, M. Mierzejewski, and P. Prelovšek, Phys. Rev. B **105**, L081105 (2022)

Localization challenges quantum chaos in finite two-dimensional Anderson model

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It is believed that the two-dimensional (2D) Anderson model exhibits localization for any nonzero disorder in the thermodynamic limit and it is also well known that the finite-size effects are considerable in the weak disorder limit. Here, we numerically study the quantum-chaos to localization transition in finite 2D Anderson models, using standard indicators used in the modern literature, such as the level spacing ratio, spectral form factor, variances of observable matrix elements, participation entropy and the eigenstate entanglement entropy. We show that many features of these indicators may indicate emergence of single-particle quantum chaos at weak disorder. However, we argue that a careful numerical analysis is consistent with the one-parametric scaling theory and predicts the breakdown of quantum chaos at any nonzero disorder value in the thermodynamic limit. Among the hallmarks of this breakdown are the universal behavior of the spectral form factor at weak disorder and the universal scaling of various indicators as a function of the parameter $u=(W\ln V)-1$, where W is the disorder strength and V is the number of lattice sites.

[1] J. Šuntajs, T. Prosen and L. Vidmar, *Localization challenges quantum chaos in finite two-dimensional Anderson model* (Manuscript in preparation).

Quantum chaos to integrability crossover in weakly disordered spin chains

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The one-dimensional anisotropic Heisenberg chain (XXZ) subjected to weak disorder is one of the paradigmatic models that exhibit quantum chaos and eigenstate thermalization hypothesis. However, when one of the model parameters becomes much smaller or much larger than the others, the quantum dynamics may exhibit intriguing features and a complete relaxation may require extremely long times. Having that in mind, we explore the scaling behavior of time scales close and far away from integrability.

Tuesday, December 13, 2022

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Overcoming the Critical Slowing Down of Magnetization Dynamics

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In order to develop ultrafast and energy efficient storage devices based on magnetic media, it is usually believed that magnetization must undergo a longitudinal dynamic [1,2] as opposed to a precessional one [3,4]. It must then be completely quenched at the sub-picosecond timescale [5] before recovering in the opposite direction. However, when magnetization approaches zero, its dynamics slows down, a phenomenon called Critical Slowing Down (CSD) [6,7] which generally exists when a system is close to a phase transition [8].
In order to explain CSD and explain how it can be avoided in magnetic systems, we introduce a two-level mean field model for localized spins [9]. Magnetization dynamics is then understood as transfers of energy and angular momentum, and to each magnetic configuration, one can define a temperature for the spin system even under out of equilibrium conditions. We then show that only angular momentum transfers can lead to magnetization reversal and suppress CSD via two mechanisms referred to as spin heating and spin cooling: the heating and respectively cooling of the magnetic system via exchange of spin with an external bath. These effects are simulated using a s-d model of magnetization dynamics [10], consistent with this framework. Experimentally, we demonstrate the existence of these two mechanisms by monitoring the ultrafast magnetization dynamics of a ferromagnetic [Co/Pt] multilayer when it is subjected to an external spin current emitted by a GdFeCo alloy [11]. We show that magnetization crosses zero in 400 fs and reaches equilibrium in 2 ps. Moreover, using the bipolarity of the source spin current [12], we show that magnetization can be reversed twice consecutively in 650 fs. This shows that one can achieve a complete control of magnetization dynamics at the sub-picosecond timescale, close to the ferromagnetic/paramagnetic phase transition, using ultrashort pulses of spin with tunable polarization.

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Nonequilibrium DMFT simulation of time-resolved X-ray absorption

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We present a formalism based on nonequilibrium dynamical mean field theory which allows to compute the time-resolved X-ray absorption spectrum (XAS) of photo-excited solids. By applying this formalism to the photo-doped half-filled and quarter-filled two-orbital Hubbard models in the Mott insulating regime we clarify how the time-resolved XAS signal reflects the nonequilibrium population of different local states. Apart from the missing broadening associated with continuum excitations, the atomic XAS spectrum computed with the nonthermal state populations provides a good approximation to the full nonequilibrium DMFT result [1].

[1] P. Werner et al. Phys. Rev. B 106, 165106 (2022)

Time resolved X-ray absorption in charge-transfer insulators

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Charge excitations across electronic band gaps are a key ingredient for transport in optoelectronics and light-harvesting applications. We will present how X-ray absorption spectroscopy can act as a sensitive probe of excited electron dynamics in charge transfer insulators. I will start with the spectral properties of the photo-doped state in charge-transfer insulators. The latter is described within the three-band Emery model as relevant for copper oxides. The main effect of photodoping is a strong renormalization of the charge-transfer gap and a substantial broadening of bands. We will present how these photoinduced changes in the spectrum are encoded in the dynamics of the X-ray absorption spectrum. The dominant effect is a renormalization of the exciton between the core hole and valence electrons and we will elucidate the role of electronic screening in the binding energy of the exciton. Finally, we will show what information on photo-induced changes in screening can be extracted from the satellite features of the main exciton resonance.

Perturbed integrable systems

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Integrable systems typically exhibit non-generic transport properties. The spin 1/2 Heisenberg model is particularly rich, with ballistic transport of energy and different regimes of spin transport, including ballistic, diffusive, and super-diffusive ones. I will discuss the fate of the diffusive and super-diffusive regimes under different types of Hamiltonian perturbations and show that symmetry of perturbations can play an important role. For example, perturbations that respect the SU (2) symmetry of the isotropic Heisenberg model can cause anomalous transport behavior even away from exact integrability, for all magnetization sectors.
In the second part, I will focus on Markovian perturbations and propose a new Krylov space-type approach for an efficient steady-state description of weakly driven and open, nearly integrable systems. Lindblad dissipator will be used to add the most necessary conservation laws iteratively and thus increase the interpretability of stabilized non-thermal steady states.

[1] P. Prelovšek, S. Nandy, Z. Lenarčič, M. Mierzejewski, J. Herbryh, arXiv:2205.11891 (2022)

Approaching the classical limit of Lindblad dynamics - emergence of limit cycles, fixed points and algebraic decay

M. Haque

Iconic features of classical dissipative dynamics include persistent limit-cycle oscillations and critical slowing down at the onset of such oscillations, whereby the system relaxes purely algebraically in time. On the other hand, quantum systems subject to generic Markovian dissipation decohere exponentially in time, approaching a unique steady state. Here we show how coherent limit-cycle oscillations and algebraic decay can emerge in a quantum system governed by a Markovian master equation. We illustrate these mechanisms using a single-spin model motivated by Landau-Lifshitz-Gilbert dynamics, and using a bosonic model with dissipation.

Autoencoder – assisted learning of Hamiltonians

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Reconstructing (effective) Hamiltonians from local measurements has several appealing applications. In the realm of quantum simulators, it can serve verification purposes. In condensed matter field, it can reveal the effective minimal models for quantum materials. Away from equilibrium, such as in Floquet driven setups, it can reconstruct the generator of effective stroboscopic evolution. Here we propose an algorithm for Hamiltonian reconstruction, assisted by machine learning pre-processing of data, with dataset that is diagnosed to contain thermal measurements of local operators. Efficient and precise reconstruction of local Hamiltonians is achieved, while long-range interacting Hamiltonians are reconstructed approximately. As a nontrivial application, we use this algorithm to diagnose the effective description of the prethermal and heating regime of Floquet and random multipolar driven setups.

Ultrafast dynamics of symmetry-broken states: From mean-field theory to a microscopic description of inhomogeneous disorder

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Using ultrashort laser pulses, it has become possible to probe the dynamics of long-range order in solids on microscopic timescales. In the conventional description of symmetry-broken phases within time-dependent Ginzburg-Landau theory, the order parameter evolves coherently along an average trajectory. Recent experiments, however, indicate the profound effect of order parameter fluctuations on the dynamics. An extreme scenario is ultrafast inhomogeneous disordering, where the average order parameter is no longer representative of the state on the atomic scale. While this has a profound effect on the dynamics, a theoretical approach which takes into account atomic scale inhomogeneities of both the electronic structure and the order parameter is challenging. In my talk, I will report on results for the Holstein model, which are based on a nonequilibrium generalization of statistical dynamical mean-field theory, coupled to stochastic differential equations for the order parameter [1]. The results show that ultrafast disordering can occur already in this minimal model for the Peierls charge-density wave transition. Similar techniques may help in future to solve the coupled electron lattice dynamics for strongly interacting electrons [2].

[1] A. Picano, F. Grandi, M. Eckstein, arXiv:2112.15323
[2] A. Picano, F. Grandi, Ph. Werner, M. Eckstein, arXiv:2209.00428

The space-time fabric of a doped Wigner crystal

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New experimental evidence of characteristic polaronic local structural distortions well above CDW ordering temperatures from X-ray local structure analysis of 1T-TaS_2, implies that the complex charge ordering in this material is better described in terms of a polaronic Wigner crystal than a conventional CDW. The application of the Wigner crystal paradigm leads to significant progress in understanding its complex metastable behaviour. In particular, charge injection is shown to lead to the charge fractionalization and entanglement with strong non-local effects that explains the remarkable robustness of the metastable state to local perturbations. The entangled fractionally charged network that results upon charge injection presents a topologically robust gapless space-time fabric for the propagation of single particle excitations that are measured by conventional transport measurements.

Pulsed excitations of 2H-$NbSe_2$

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We investigated 2H-$NbSe_2$ which is a two-dimensional material that has recently drawn a lot of interest due to the coexistence of charge density wave and superconductive states at low temperatures. While the equilibrium phase diagram of the material has already been well experimentally studied, the material's response to pulsed excitations and the possible existence of non-equilibrium metastable states is yet to be fully explored [1, 2].
We used an optical pump-probe setup to look at the ultrafast response of the 2H-$NbSe_2$ by transient reflectivity measurements at 1.55 eV photon probe energy. We observe a long-lived ultrafast response as the charge density wave state is formed that is similar to the previously reported response at 1.03 eV [1]. In addition, we observe a tiny change in the amplitude of the ultrafast response below the critical temperature for the superconducting state. Similar to Anakin et al. [2], we do not observe any coherent oscillations due to the amplitude modes within the explored ranges of temperatures and pump fluences. Additionally, we do not see the appearance of any distinct long-lived metastable state despite a high-fluence laser excitation.
By means of a scanning tunneling microscope, we performed also tip excitation of the 2H-$NbSe_2$ surface. With a high-voltage electrical pulse excitation, we were able to transform the surface from 2H to 1T polytype which has a $\sqrt{13} \times \sqrt{13}$ charge density wave phase.

[1] D. T. Payne et al. arXiv:2010.09826 (2020).
[2] A. Ankin et al. Phys. Rev. B 102, 205139 (2020)

DFT+DMFT calculations of electronic Raman scattering of Sr2RuO4

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We compute the electronic Raman scattering of Sr_2RuO_4 for different channels using DFT+DMFT calculations. We find that the B2g channel can be represented mostly by contributions of the xz/yz orbitals of the material, while the B1g channel shares contributions of xy and xz/yz orbitals. This is a different interpretation than the one proposed in a recent experiment of polarization-resolved Raman spectroscopy. By studying the role of the self-energy and the vertex separately, we are able to identify interband contributions due to the nesting of beta and gamma sheets of Sr2RuO4 that are important to the B2g channel, and identify it as the reason for a higher mass enhancement than the B1g channel.

Non-equilibrium superconductivity in THz driven two-band superconductor MgB_2

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Excitation of a superconductor (SC) with a low energy electromagnetic pulse may lead to a non-equilibrium state, which may profoundly differ from a quasi-thermal one, driven by optical excitation. Such a non-equilibrium may be especially pronounced in multi-band superconductors. Here, we report on studies of the dynamics of the SC order in ultra-clean thin films of MgB_2 [1], the prototype two-band SC with two distinct superconducting gaps opening in the two bands with weak interband coupling [2,3]. We performed systematic time-resolved studies of gap dynamics following excitation with intense narrow-band THz pulses with photon energies tuned between the two superconducting gaps. We demonstrate that the temperature and excitation density dependent dynamics qualitatively follows the behavior predicted by the phenomenological Rothwarf-Taylor model for dynamics in a single gap BCS superconductor [4]. This implies strong coupling between the two condensates on the ps timescale. Tracking the dependence of the amplitude of the THz driven gap suppression, however, displays a pronounced minimum near ~ 0.6 Tc, that cannot be accounted by the phenomenological model. Comparison of the results to those obtained by excitation with near-infrared pulses suggests that excitation with narrowband THz pulses results in long-lived (100 ps timescale) non-thermal quasiparticle distribution, which gives rise to Eliashberg-type enhancement of superconductivity [5,6], competing with pair-breaking.

[1] S. Kovalev, et al., Phys.Rev. B 104, L140505 (2021).
[2] A.Y. Liu, I.I. Mazin, J. Kortus, Phys. Rev. Lett. 87, 087005 (2001).
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[4] V.V. Kabanov, J Demsar, and D Mihailovic. Phys. Rev. Lett. 95, 147002 (2005).
[5] G.M. Eliashberg, JETP Lett 11, 114 (1970).
[6] M. Beck, et al., Phys. Rev. Lett. 110, 267003 (2013).

Superconductivity in Giant Poisson-Effect Strained 1T-TaS_2 Thin Films Grown by Molecular Beam Epitaxy

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Due to its rich phase diagram which includes multiple charge density wave (CDW) transitions, 1T-TaS_2 is regularly used as a prototype layered material. It is also known for metastable states, as well as the superconducting phase induced by hydrostatic pressure, cation substitution, doping or intercalation. When moving from the bulk crystals to the thin films, 1T-TaS_2 exhibits transition temperature strongly dependent on the substrate-induced strain.

In this work, we show that thin polycrystalline films of 1T-TaS_2 grown by molecular beam epitaxy (MBE) on $(LaAlO_3)_{0.3}(Sr_2TaAlO_6)_{0.7}$ (LSAT) substrates have a suppressed CDW transition to a commensurate phase. Instead, a metallic behavior is observed via resistivity, critical current and magnetoresistance measurements with the onset to a superconducting state below T_c = 3.8 K.

We are showing, that appearance of superconductivity is driven by in-plane tensile differential strain, which is caused by LSAT substrate when cooled after the growth. As a result, a strongly amplified out-of-plane compressive strain is triggered by the Poisson effect, which is confirmed by X-Ray data.

The experiments show that tensile substrate strain can be applied to achieve the desired functional properties, which are otherwise only accessible through hydrostatic pressure. Moreover, such strain can be used for investigation of the effects of anisotropic strain in 2D materials.

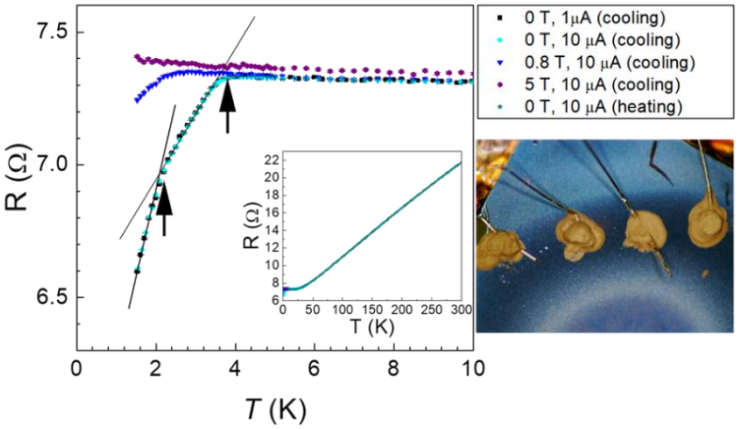

Fig. 1. 4-probe resistance measurements with and without the external magnetic field. The resistance curve at low temperatures, indicating the presence of two transitions (arrows) as a function of T at B = 0 T, 0.8 T and 5 T is measured on cooling and heating. The resistance slope and T_c are comparable to the one obtained under a hydrostatic pressure >8 Gpa. The insert shows the full measurement up to room temperature. The contact area on the sample is shown on the right.

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Scrambling in quantum glasses

A. Silva

Single-particle eigenstate thermalization and its effect on nonequlibrium dynamics in many-body systems

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First, we demonstrate the concept of single-particle eigenstate thermalization [1] on the example of three-dimensional Anderson model with an additional spin-polarized triplet p-wave pairing interaction, which breaks the particle number conservation [2]. We consider the subspace of the Hilbert space with a single Bogoliubov quasiparticle. Specifically, we show the finite size scaling of eigenstate-to-eigenstate fluctuations and variances of the diagonal matrix elements of a local observable. Moreover, we compare the ratio between the variance of the diagonal and offdiagonal matrix elements with the prediction of the random matrix theory. We perform an analogous comparison for the distributions of the diagonal and offdiagonal matrix elements. Finally, we discuss the existence of highly localized modes in the middle of the energy spectrum, i.e., Majorana-like modes.
Next, we prove that the observables which exhibit eigenstate thermalization in a single-particle sector equilibrate in many-body sectors of quadratic models [3]. Remarkably, the same observables do not exhibit eigenstate thermalization in many-body sectors (there are exponentially many outliers). Therefore, the generalized Gibbs ensemble is generally needed to describe their expectation values after equilibration, and it is characterized by Lagrange multipliers that are smooth functions of single-particle energies.

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[2] P. Tokarczyk, L. Vidmar and P. Łydżba, in preparation (2022).
[3] P. Łydżba, M. Mierzejewski, M. Rigol and L. Vidmar, arXiv:2210.00016 (2022)

Tight-binding billiards

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Recent works have established universal entanglement properties and demonstrated validity of single-particle eigenstate thermalization in quantum-chaotic quadratic Hamiltonians. However, a common property of all quantum-chaotic quadratic Hamiltonians studied in this context so far is the presence of random terms that act as a source of disorder. Here we introduce tight-binding billiards in two dimensions, which are described by non-interacting spinless fermions on a disorder-free square lattice subject to curved open (hard-wall) boundaries. We show that many properties of tight-binding billiards match those of quantum-chaotic quadratic Hamiltonians: the average entanglement entropy of many-body eigenstates approaches the random matrix theory predictions and one-body observables in single-particle eigenstates obey the single-particle eigenstate thermalization hypothesis. On the other hand, a degenerate subset of single-particle eigenstates at zero energy (i.e., the zero modes) can be described as chiral particles whose wavefunctions are confined to one of the sublattices.

[1] Iris Ulčakar and Lev Vidmar, Phys. Rev. E 106, 034118 (2022)

A Novel Spin Liquid on the Triangular Lattice

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Quantum spin liquid nowadays represents one of the key paradigms in the field of quantum materials [1-3]. This fascinating magnetic state of matter that is highly quantum entangled but lacks long-range magnetic order, has been in recent years experimentally observed in various geometrically frustrated materials, including realizations of the two-dimensional triangular spin lattice. However, most of these materials are plagued by structural disorder, which can dramatically affect the magnetic ground state and lead to states that resemble a quantum spin liquid. This makes the detection and characterization of possibly intrinsic spin-liquid states in these systems highly challenging.
Recently, we discovered a quantum-spin-liquid state in a new triangular lattice antiferromagnet neodymium heptatantalate, $NdTa_7O_{19}$, with no detectable structural disorder [4]. Our in-depth study utilizing several complementary experimental techniques, including neutron scattering, muon spin relaxation and electron spin resonance, showed that this material does not undergo magnetic ordering even at temperatures of only a few tens of millikelvins, which is far below the magnitude of the dominant exchange interaction. Nevertheless, significant diffuse magnetic scattering was observed at low temperatures, characteristic of Ising-like spin correlations between the nearest neighbors on the triangular lattice. Furthermore, persistent spin dynamics was detected in the ground state, suggesting that in the investigating compound quantum fluctuations may be induced by components of the exchange interaction perpendicular to the dominant Ising exchange. The properties of the discovered spin-liquid state have thus been attributed to large magnetic anisotropy, which is rather typical for rare-earth ions. In this respect, it is quite intriguing to imagine various exotic magnetic states and excitations that could be observed withing the vast family of isostructural rare-earth- based heptatantalates in the future.

[1] L. Balents, Nature 464, 199 (2010)
[2] L. Savary et al., Rep. Prog. Phys. 80, 016502 (2017)
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Beyond perturbation theory: multi-photon and non-radiative recombination effects in spectroscopies

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The conventional calculation of scattering cross sections relies on a treatment based on time-dependent perturbation theory that provides formulation in terms of Green's functions in the frequency domain. In equilibrium, it boils down to evaluating a simple spectral function equivalent to Fermi's golden rule, which can be solved efficiently by a number of numerical methods. However, away from equilibrium, the resulting expressions require a full knowledge of the excitation spectrum and eigenvectors to account for all the possible allowed transitions and intermediate states, a seemingly unsurmountable complication. We have recently presented a new paradigm to overcome these hurdles [1-3]: we explicitly introduce the scattering particles (neutron, electron, photon, positron) and simulate the full scattering event by solving the time-dependent Schrödinger equation. The spectrum is recovered by measuring the momentum and energy lost by the scattered particles, akin an actual energy-loss experiment. I here show how these ideas can be generalized to study multi-photon processes such as coincidence ARPES, and the interplay between radiative and non-radiative recombination channels in X-ray spectroscopies.

[1] Krissia Zawadzki, Luhang Yang, Adrian E. Feiguin; Phys. Rev. B **102**, 235141 (2020).
[2] Krissia Zawadzki, Adrian Feiguin; Phys. Rev. B **100**, 195124 (2019).
[3] Krissia Zawadski, Alberto Nocera, and Adrian E. Feiguin arXiv: 1905.08166

Ultrafast and ultraefficient light modulator for EUV and X-rays based on photoinduced phase transition

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With the rapid development of bright coherent light sources, which can deliver short EUV and X-ray pulses, it is now possible to extend the traditionally optical spectroscopic techniques to the high photon energy regime overcoming the main limitations of optics: relatively poor spatial resolution (restricted by the optical wavelength) and limited energy range, inadequate for probing core level-to-conduction band electronic transitions. The extended energy range has opened numerous possibilities for studying complex materials and electronic phase transitions allowing also resonant probing of different sub-components in the system etc. While being extremely useful, the high photon energy creates a lot of experimental difficulties due to the absence of efficient optical elements, which can deflect or manipulate such ionizing beams.
Here we report on a novel device, which can be used as an ultrafast beam deflector or spatial light modulator for EUV or X-ray photons. The deflection efficiency of the device can be tuned in a broad range from as low as 1e-10 and up to a few precents. By using two crossed FEL beams, we show that the metastable periodic structure can be imprinted in the sample, which acts as a tunable diffraction grating for the EUV light. Unlike usual transient gratings, which are frequently caused by thermal effects, the reported effect is electronically driven and is long-lived. Alternatively, similar structure can be potentially recorded electrically via an array of metallic contacts deposited on the sample surface.
The underlying effect is based on the metastable insulator-to-metal phase transition, which is accompanied by extremely large change of the lattice constant in quasi 2D transition metal dichalcogenide. The periodic variation of the lattice constants translates into the change of the surface morphology creating phase grating with the nm-scale period and ~0.1 nm groove height. The switching speed between the different states is expected to be limited by the frequency of the amplitude mode of the charge density wave as was shown before for the optically excited 1T-TaS_2.

Light-induced symmetry breaking via nonlinear phononics

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Intense midinfrared light can be used to selectively pump the phonon modes of materials that couple to light. However, it is not obvious how the oscillations of the pumped mode about its equilibrium position can coherently break the point-group or translation symmetries of the material. I will discuss how a $Q_h^2 Q_l^2$ nonlinear coupling between the pumped mode Q_h and a symmetry-breaking mode Q_l can be used to stabilize a broken-symmetry phase of the material through the duration of the pump pulse. First principles calculations show that a $Q_h^2 Q_l^2$ nonlinearity is large in KTaO3 between the highest- and lowest-frequency optical phonon modes at the Brillouin zone center, and this nonlineary is such that the Q_l mode softens while the Q_h mode has a finite value. Furthermore, the Q_l mode breaks the inversion symmetry of the material, and the solutions of the coupled equations of motion of the two modes in the presence of external pump pulse show that a transient ferroelectric state can be stabilized for pump pulse intensities that are achievable using currently available laser sources [1]. Additionally, similar $Q_h^2 Q_l^2$ coupling is present at the Brillouin zone boundary, which can in principle be used to break the translation symmetry of this material [2].

[1] A. Subedi, Phys. Rev. B 95, 134113 (2017).
[2] A. Gómez Pueyo and A. Subedi, arxiv:2208.05293 (2022).

On the classical limit of the polaron mass in the Holstein model

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We consider the polaron mass in the limit of large Holstein polaron in 1D where phonons have dispersion. The mass does not have exponential suppression typical for small polarons. The spatial dispersion of polaron is described by the Klein-Gordon equation. When polaron velocity becomes larger than typical velocity (analog of the speed of light) the motion becomes damped because of the Cherenkov radiation.

Magnetic spectroscopy studies of quasi-one-dimensional superconductors

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$A_2Mo_3As_3$, where A stands for K, Rb or Cs, is a family of quasi one-dimensional conductors, where MoAs form quasi one-dimensional double-walled subnanotubes, with A ions in between tubes. It is isostructural to the $A_2Cr_3As_3$, family, which was shown to be superconducting at low temperatures, with T_c = 6.1 K [1], T_c = 4.8 K [2] and T_c = 2.2 K [3], for A = K, Rb and Cs respectively. The Molybdenum family achieves higher critical temperatures of 10.4 K [4], 10.5 K [5] and 11.5 K [6] for A = K, Rb and Cs respectively.
A comprehensive ^{87}Rb nuclear magnetic resonance (NMR) and ^{75}As nuclear quadrupole resonance (NQR) study of $Rb_2Mo_3As_3$ is presented. Intriguingly they show different behavior. ^{87}Rb NMR shows a power-law temperature dependence of spin-lattice relaxation rate in the normal phase, which is a fingerprint of the Tommonaga-Luttinger liquid. ^{75}As NQR, on the other hand, shows a linear relationship, suggesting Korringa relation. Even is the superconducting phase, they show a different value of a superconducting gap, with ^{75}As showing a BCS value of a gap and ^{87}Rb showing a reduced gap value [5].
In $K_2Mo_3As_3$ even different spectral lines of ^{75}As NQR show different temperature dependence of the spin lattice relaxation rate. Different spectral lines correspond to different crystallographic sites, which suggests that the multi-orbital physics is of utmost importance.
Additionally, muon spin rotation/relaxation (μSR) study of $Rb_2Mo_3As_3$ is presented. The transverse field μSR signal shows enhanced damping below T_c, which is due to the formation of a vortex lattice. Comparison of vortex lattice broadening against single gap s−, p− and d−wave models shows the best agreement for the s−wave scenario but with the anomalously small superconducting gap (Δ_0) to T_c ratio of $2\Delta_0/T_c$ = 2.74. The alternative nodal p−wave or d−wave scenarios with marginally worse goodness of fits yield more realistic $2\Delta_0/T_c$ = 3.50 and $2\Delta_0/T_c$ = 4.08, respectively, and thus they cannot be ruled out to account for the superconducting state in $Rb_2Mo_3As_3$ [7].

[1] J.-K. Bao, et al, Phys. Rev. X. 5, 011013 (2015)
[2] J. Yang, et al, PRL. 115, 147002 (2015)
[3] Z.-T. Tang, et al, Sci China Mater. 58: 16–20 (2015)
[4] Q.-G. Mu, et al, Science Bulletin. 63, 952-956 (2018)
[5] Ž. Gosar, et al, PRB. 101, 220508(R) (2020)
[6] K. Zhao, et al, APL Mater. 8, 031103 (2020)
[7] Ž. Gosar, er al, *in preparation*

Optically driven electron-electron attraction in a model with nonlinear electron-phonon interaction

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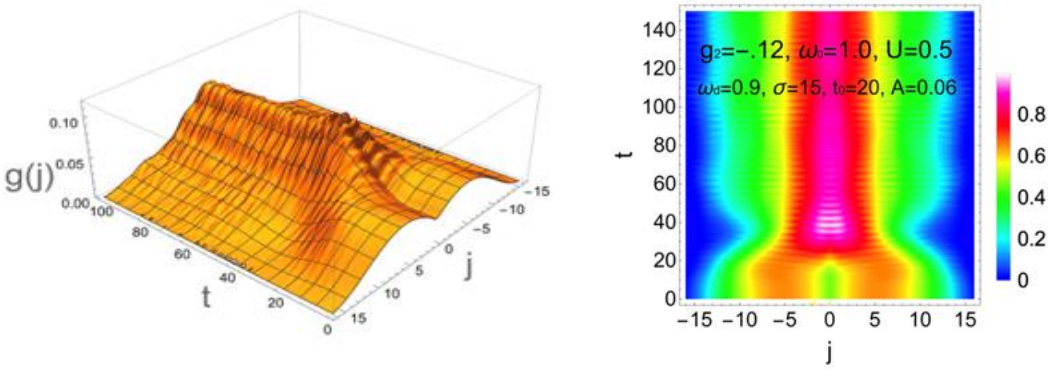
We analyze a model with two electrons nonlinearly coupled to quantum phonons subject to a short optical pulse tuned to the phonon frequency. Nonlinear electron-phonon coupling can either soften or strengthen the phonon frequency in the presence of electron density. In the atomic limit, both cases lower the energy of the doubly occupied site compared to the single-occupied one. When two electrons are free to propagate on a lattice subject to nonlinear coupling to phonons that soften phonon frequency, an external optical pulse can induce a strong attraction between electrons. Electrons remain bound long after the optical pulse is switched off [1].



Figures show the time evolution of a density – density correlation function starting from an unbound state at t=0 subcject to an optical pulse.

[1] *Work in progress* ☺

Ultrafast dichroism in bulk transition metal dichalcogenides

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The present semiconductor technology largely exploits the manipulation of the electronic charge, although additional electronic degrees of freedom could be used to encode further information. In particular, recently it has been shown how to potentially take advantage from the so-called valley degree of freedom, by selectively populating inequivalent valleys with electrons, holes or excitons.
This possibility has become realistic after realizing that group-VI layered (2D) transition metal dichalcogenides (TMDs) like MoS_2, $MoSe_2$, WS_2 and WSe_2 display an hexagonal semiconducting electronic structure dominated by two inequivalent valleys occurring at the ±K points of the Brillouin zone. This fact, together with the broken inversion symmetry of the monolayer compounds and the strong spin-orbit coupling, constitutes the playground for making possible the control of spin and valley in these materials. Here, we perform broadband time-resolved optical spectroscopy on bulk WSe_2 and, by using a circularly polarized pump pulse, we show that a large transient anisotropic reflectivity signal, associated to the rotation of the reflected polarization, is obtained. This signal is bound in in the spectral region of the A exciton at ≈1.6 eV. At room temperature, its dynamics, which is connected to the valley depolarization time, equals ≈400 fs and it is considerably faster than that of the valley exciton lifetime (showing a 10s of ps decay). We experimentally prove that, provided that the excitation is nearly resonant to the A exciton, the valley degree of freedom can be exploited also in bulk materials when referring to the (transient) macroscopic optical properties. This fact is confirmed by a microscopic modelling of the dielectric properties of multi-layer non-centrosimmetric TMDCs, and paves the way to the exploitation of transition-metal dichalcogenides bulk materials for valleytronics-related applications beyond the stringent monolayer limit.

Ultrafast dynamics in $(TaSe_4)_2I$ triggered by valence and core-level excitation

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Dimensionality plays a key role for the emergence of ordered phases like charge-density-waves, that in turn can couple to and modulate the topological properties of matter. In this work, we study the out-of-equilibrium dynamics of the paradigmatic quasi-one-dimensional material $(TaSe_4)_2I$, that exhibits a transition into an incommensurate charge-density-wave (CDW) phase when cooled down just below room temperature, at T_{CDW} = 263 K [1,2]. We make use of both optical laser and free-electron laser (FEL) based time-resolved spectroscopies in order to study the effect of a selective excitation of the material on the charge-density-wave phase, by probing the near-infrared/visible optical properties both along and perpendicularly to the direction of the charge-density-wave. Excitation of the core-levels by ultrashort X-ray FEL pulses at 47 eV and 119 eV induces reflectivity transients resembling those recorded when exciting the valence band of the compound - by near-infrared pulses at 1.55 eV – in the case of the insulating sub-system [3]. Conversely, the metallic sub-system displays a relaxation dynamic, which depends on the energy of the photoexcitation. Moreover, excitation of the CDW amplitude mode is recorded for excitation at low photon-energy [3,4]. This fact suggests that the coupling of light to ordered states of matter can predominantly be achieved when directly injecting delocalized carriers in the valence band, rather than localized excitations in the core levels. On a complementary side, table-top experiments allow us to prove the unidirectional nature of the CDW phase in $(TaSe_4)_2I$, which fingerprints are detected along the c-axis only. Our results provide new insights on the symmetry of ordered phase of $(TaSe_4)_2I$ perturbed by a selective excitation, and suggest a novel approach based on complementary tabletop and FEL spectroscopies for the study of complex materials.

[1] Z. Wang et al., Solid State Communications 46, 325-328 (1983)
[2] J. Gooth et al., Nature 575, 315-319 (2019)
[3] W. Bronsch et al., Faraday Discussions 237, 40 – 57 (2022)
[4] H. Schaefer et al., The European Physical Journal Special Topics 222, 1005 – 1016 (2013)

Thursday, December 15, 2022

	Chair: Federico Cilento	
09:00 - 09:30	**Jacek Herbrych:** Hund bands in spectra of multiorbital systems	52
09:30 – 10:00	**Tomaž Mertelj:** Ultrafast optical polarimetry in magnetic phases of Kondo semimetal CeSb	53
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Hund bands in spectra of multiorbital systems

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Spectroscopy experiments are routinely used to characterize the behavior of strongly correlated systems. An in-depth understanding of the different spectral features is thus essential. Here, we show that the spectrum of the multiorbital Hubbard model exhibits unique Hund excitations that occur at energies given only by the Hund coupling J_H, as distinct from the Hubbard satellites following the interaction U. We focus on the experimentally relevant single-particle and optical spectra that we calculate for a model related to iron chalcogenide ladders. The calculations are performed via the density-matrix renormalization group and Lanczos methods and the generality of the implications is verified by considering a generic multiorbital model within the dynamical mean-field theory.

[1] arXiv:cond-mat/2210.11209

Ultrafast optical polarimetry in magnetic phases of Kondo semimetal CeSb

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The CeSb magnetic phase diagram is one of the most complex among lanthanide monopnictides. It contains at least 16 different magnetic phases in the H-T plane [1] comprising different sequences of ferromagnetic, with either up or down spin orientation, and paramagnetic (001) planes stacked along the c-axis. The complexity is thought to arise from the interplay of Kondo, spin orbit and crystal field effects. [1, 2] Lattice modulation in the magnetic phases was also observed [3].
The phase diagram [4, 5] and the magnetic excitations [1] were thoroughly studied by neutron scattering. Recently the sensitivity of the electronic structure to the magnetic phase has been demonstrated [6] and additional magnetic excitations were found in the ordered phases [7].
While the main features of the magnetic behavior are understood and successfully modeled using effective interaction approach [8] the microscopic origin of the interactions is still puzzling [2, 7]. An insight into non equilibrium dynamics of different phases might therefore shed some light to interplay of the different degrees of freedom. Here we present and discuss our investigation of the ultrafast non-equilibrium dynamics upon photo excitation in different magnetic phases in CeSb with focus on the magnetic excitations in the weakly nonequilibrium photoexcited state.

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Interface spin-Hall effect at metal-insulator border

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Most often the spin torque induced by heavy metal layer to the layer of ferromagnetic metal in spintronic devices is described by either spin-Hall effect related to the bulk of heavy metal or by Rashba-Edelstein effect that exist only near the interface between heavy metal and some other material. However, recent experiments [1] show that modification of the second surface of heavy metal can significantly change the spin torque.
We show that when the surface of heavy metal and insulator contains impurities, the skew scattering form this impurities produces several novel effects. The skew scattering itself leads to spin polarization that span over mean free path into the bulk of heavy metal. When the spin relaxation at the surface is taken into account, the interface spin Hall effect appears that leads to the current conversion to spin-current at the heavy metal – insulator interface.
Both the phenomena depend on properties of insulator and impurities allowing the control of spin torque with surface engineering.

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Light-driven antiferromagnetic magnonics

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Magnonics is a research field complementary to spintronics, in which quanta of spin waves (magnons) replace electrons as information carriers, promising lower dissipation and a wider range of functionality [1,2]. The development of future nanoscale magnonic logic circuits calls for new tools and materials to generate coherent spin waves with frequencies as high, and wavelengths as short, as possible [3]. Antiferromagnets can host spin waves at terahertz (THz) frequencies and are therefore seen as a future platform for the fastest and the least dissipative transfer of information [4]. Yet, the antiferromagnetic magnonics has so far remained elusive, being limited by the lack of the efficient THz sources for the generation of antiferromagnetic magnons.
Here I will show you how ultrashort pulses of light can be used for the efficient emission and detection of a nanometer-scale wavepacket of coherent propagating magnons in various antiferromagnets [5]. The subwavelength confinement of the laser field due to large absorption creates a strongly non-uniform spin excitation profile, enabling the propagation of a broadband continuum of coherent THz spin waves (see Fig. 1). The wavepacket features magnons with detected wavelengths down to 100 nm that propagate with supersonic velocities V_0 of more than 10 km/s. This long-sought source of coherent short-wavelength spin carriers opens up new prospects for THz antiferromagnetic magnonics and nanoscale coherence-mediated logic devices at THz frequencies. I will also demonstrate you that the light-induced antiferromagnetic magnons are highly nonlinear waves and their interaction goes well beyond of a linear superposition.

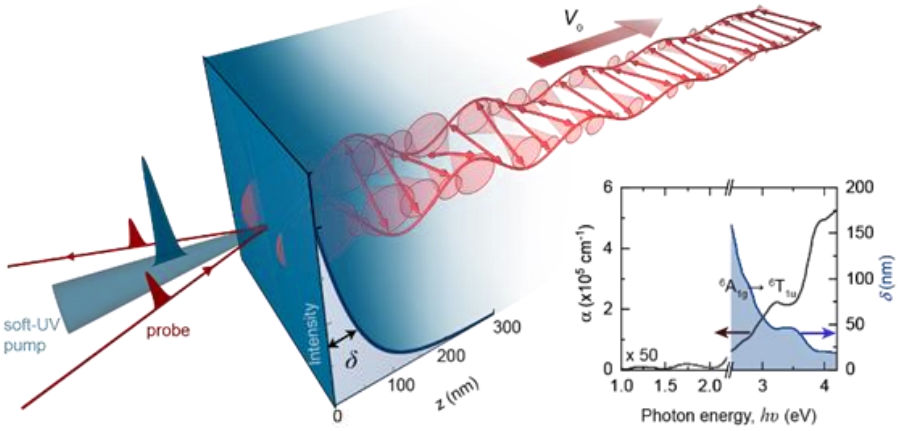

Figure 1. Schematic of the generation of propagating AFM spin waves after above bandgap soft-UV photoexcitation. The optical penetration depth δ defines the excited region Inset: absorption coefficient α (left axis) and corresponding penetration depth δ (right axis) for the AFM $DyFeO_3$ as a function of photon energy.

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Thermoelectric diffusive modes

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Quantum simulations of strongly correlated quantum matter have recently reignited the attempts to understand transport dynamics of correlated electrons at high temperatures, e.g., the measured charge resistivity in the 2-dimensional Hubbard model. A common assumption in the analyses of these systems is that thermoelectric effects are either absent or too small to influence the measurements. The thermoelectric spin Seebeck coefficient in the Hubbard model was, on the contrary, found to vastly exceed both the atomic limit and the Kelvin approximate value [1]. To describe these effects faithfully in the hydrodynamic regime, we make use of a wider set of transport equations that describe diffusion in terms of transport and susceptibility matrices. I will introduce the mathematical formalism and discuss the impact of thermoelectric effects on heat and charge diffusion in the 2-dimensional Hubbard model [2].

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Extending third quantization with commuting observables: a dissipative spin-boson model

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We consider the spectral and initial value problem for the Lindblad- Gorini-Kossakowski-Sudarshan master equation describing an open quantum system of bosons and spins, where the bosonic parts of the Hamiltonian and Lindblad jump operators are quadratic and linear respectively, while the spins couple to bosons via mutually commuting spin operators. Needless to say, the spin degrees of freedom can be replaced by any set of finite level quantum systems. A simple, yet non-trivial example of a single open spin-boson model is worked out in some detail.

Equilibrium States in 1*T*-TaS_2: Are There More?

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1*T*-TaS_2 is a very versatile and well-studied system, which supports a plethora of different charge density wave (CDW) states, and also shows superconductivity [1] and an unusual quantum spin liquid [2]. In the recent years, a lot of attention is given to its non-equilibrium states, which can be reached via electrical or laser excitations. These include a textured metallic state [3,4] and an amorphous state [5] among others. On the other hand, the equilibrium phase diagram has long been established and is not very commonly investigated nowadays, especially at higher temperatures, even though some uncertainties still exist. Nevertheless, another state that appears only in a very narrow temperature window on heating was recently found in 1*T*-TaS_2 [6]. Wang et. al. have used ARPES to show that on heating from the low temperature C state, a new state appears at 220 K and persists for around 20 K until transitioning to the triclinic state at 240 K. They claim that this is the true Mott insulating state of 1*T*-TaS_2, while the low temperature C state is a band insulator and not a Mott insulator, as it is widely believed. The authors observe the state only with ARPES, while no trace of the state is seen using X-ray diffraction.
Since the authors observe the new state only using surface measurements, we have designed an X-ray scattering experiment to probe separately the surface and the bulk of the material and try to identify in what regime the newly discovered state appears. We used X-ray beam with the photon energy of 9.8 keV at two different grazing incidence angles (5 degrees and 0.4 degrees) to probe the bulk and a few of the top layers of the material respectively. Here we show the results, comparing the scattering peaks in the temperature range between 100 K and 300 K on both cooling and heating.
This project has received funding from the European Union's Horizon 2020 research and innovation program under the Marie Skłodowska-Curie grant agreement No 701647.

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POSTERS

The Charge Density Wave State in a System of Coupled Chains

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The 1T-TaS_2 polytype of TaS_2 is a layered compound exhibiting a series of charge density wave (CDW) transitions, including a low temperature insulating state, considered a consequence of electron correlation effects. We aim to devise a minimal model of such materials to better understand the factors contributing to the stability of the observed phases.

We consider a one-dimensional coupled electron-lattice system, described by the Fröhlich Hamiltonian [1]. The system adopts the CDW ground state, characteristic of highly anisotropic systems. To include interlayer hopping in the description, two copies of the single-chain system are coupled through inter-chain hopping and an on-site Coulomb repulsion is introduced. The mean-field solution is used to characterise the various phases adopted based on the relative strength of phonon coupling and inter-chain hopping. A Peierls insulator to band insulator transition is observed.

We also look at the dynamics of the system. The influence of an electric field pulse, applied in various orientations, is measured. The response of the system provides information on various observables, e.g., optical conductivity [2], which can be related back to experimental observations.

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Ultrafast demagnetization and transient magnetization reversal in ferromagnetic Co_xPt_{1-x} thin films

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Recent studies of the ultrafast demagnetization process in multi-component magnetic alloys have ignited the question of the importance of the dynamics of the different sublattices for driving emergent effects, such as all-optical magnetization switching [1, 2, 3, 4]. The development of table-top sources such as high harmonic generation setups and the capabilities offered at large-scale free electron laser facilities allow experimentalists to resonantly probe the element-specific response to photoexcitation and separate the contributions of different sub-lattices.
We have investigated the demagnetization process in ferromagnetic Co-Pt thin films of different stoichiometry (50:50 and 70:30) and thickness (10 nm, 20 nm, and 30 nm) using femtosecond magneto-optical Kerr spectroscopy in the extreme ultraviolet region. The experiments were performed at the MagneDyn beamline at the FERMI free electron laser at the cobalt M and the platinum N edges.
For both stoichiometries we observe thickness dependent demagnetization. While we have not observed full demagnetization in the 10 nm 70:30 sample, the thicker 30 nm sample exhibits complete demagnetization and complex magnetization dynamics. In the case of partial demagnetization, the dynamics can be described by two exponential functions corresponding to fast de- and slow re-magnetization, but this description is no longer sufficient at higher photoexcitation fluences, where the demagnetization proceeds in multiple stages. Immediately after excitation the magnetization is quenched by about 90 % and persists for about 2 ps, after which the sample proceeds to demagnetize further, crossing zero and, about 4 ps after excitation, finally transiently reversing its direction, reaching about 2-3 % of its static magnitude before slowly remagnetizing. Behavior of the 50:50 samples is again distinct. We have observed complete demagnetization at subpicosecond timescales in all samples, but interestingly, only the 20 nm thick sample exhibits transient magnetization reversal. The reversal proceeds quicker with the magnetization reaching its minimum already around 1.5 ps after excitation. Moreover, there is no clear multicomponent response, highlighting that the dynamics are distinctly different compared to the 70:30 composition sample exhibiting reversal. In addition to demonstrating small transient magnetization reversal in a ferromagnetic thin film, our experiments highlight the importance of external parameters, in this case film thickness, on the demagnetization/remagnetization process, suggesting that non-local effect might be responsible for the reversal.

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Small polaron problem – electrons coupled to hard-core bosons

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Holstein-Hubbard model is a tight-binding lattice model which was introduced to describe a small polaron. The basis of states of the Holstein-Hubbard model applied to a one-dimensional chain consisting of N sites is infinite. By replacing phonons with hard-core bosons (HCB) we limit the infinite-dimensional basis to a finite-dimensional subspace of states with the most one boson per site [1]. This enables us to numerically analyze bigger systems getting closer to the thermodynamic limit.

We analyzed, analytically and numerically, the properties of the HCB model applied to one-dimensional one-electron and two-electron systems such as energy dispersion of the ground state and lowest excited states, the expected number of bosons, the kinetic energy of charge carriers in these states, the quasiparticle weight, the polaron's effective mass, and the spectral function. In a two-electron system, in which electron-phonon interaction is strong enough to suppress the Coulomb repulsion, polarons can bind and form a bipolaron. We found out that not only do the electron-electron and electron-phonon interaction play an important role to determine whether the bound state will be favorable, but phononic dispersion also has a great impact on bipolaron formation.

Comparing the HCB model with the phononic Holstein-Hubbard model [2, 3] shows many parallels between the two, but also many deviations. As expected, the behavior of models is quite similar in the weak-coupling regime, where the number of excited phonons is low. In the strong coupling limit, a phononic cloud forms around the electron in the Holstein model resulting in a diverging number of phonons and polaron's effective mass. On the other hand, in the HCB model, the hard-core restriction prevents the excitation of a large number of bosons resulting in converging effective mass. Difference between the two also reflects in the spectral function of electron addition.

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Optically triggered Néel vector manipulation of a metallic antiferromagnet Mn_2Au under strain

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The absence of stray fields, their insensitivity to external magnetic fields, and ultrafast dynamics make antiferromagnets promising candidates for active elements in spintronic devices. Here, we demonstrate manipulation of the Néel vector in the metallic collinear antiferromagnet Mn_2Au by combining strain and femtosecond laser excitation. Applying tensile strain along either of the two in-plane easy axes and locally exciting the sample by a train of femtosecond pulses, we align the Néel vector along the direction controlled by the applied strain [1]. The dependence on the laser fluence and strain suggests the alignment is a result of optically triggered depinning of 90° domain walls and their motion in the direction of the free energy gradient, governed by the magneto-elastic coupling. The resulting, switchable, state is stable at room temperature and insensitive to magnetic fields. Such an approach may provide ways to realize robust high-density memory device with switching timescales in the picosecond range.

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Extending third quantization with commuting observables: a dissipative spin-boson model

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We consider the spectral and initial value problem for the Lindblad- Gorini-Kossakowski-Sudarshan master equation describing an open quantum system of bosons and spins, where the bosonic parts of the Hamiltonian and Lindblad jump operators are quadratic and linear respectively, while the spins couple to bosons via mutually commuting spin operators. Needless to say, the spin degrees of freedom can be replaced by any set of finite level quantum systems. A simple, yet non-trivial example of a single open spin-boson model is worked out in some detail.

Influence of oxygen on transport properties of Iron in liquid outer Earths' core

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First principle evaluations of thermal conductivities of iron under inner- and outer Earth's core conditions found higher values than previously assumed from the extrapolation of the data from the experimentally available temperature window, affecting the geophysical modelization of Earth's intereior. [1,2] disregarded electronic correlations, but their effect is believed to be insignificant [3,4]. It is known that iron is alloyed with lighter elements, such as silicon and oxygen. The influence of oxgyen is especially interesting as it could reduce the iron occupancy towards the half-filling where the electron corellations are strongest. We performed the density functional theory calculations combined with molecular dynamics on up to ~100 atom supercells including oxgyen impurities and evaluated the electronic correlations using the dynamical mean-field theory [5]. We found the oxygen significantly enhances the electron-electron scattering but the final effect on the conductivities is still limited due do the domination of the thermal disorder, confirming the picture proposed in [4].

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Photoinduced dynamics of flat bands in the Kagome metal CoSn by TR-ARPES

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In Kagome systems, the geometry of the lattice localizes the electrons in real space, enhancing the correlations and giving rise to flat bands [1]. In CoSn two flat bands with nontrivial topological character lie below the Fermi level [2]. In order to study the response of the localization mechanism to impulsive excitation, we performed the first time- and angle-resolved photoelectron spectroscopy study on CoSn. At temporal overlap we observe an increase in the electronic temperature, along with a shift and broadening of the flat bands by few meV. A smaller broadening of the flat band persists for the whole duration of the investigated time delay range (about 6 ps). A possible explanation for this broadening is the partial disruption of the real-space electron localization, because of the increased mobility of the carriers due to the energy injected by the infrared pump pulse.

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Ultrafast all-optical manipulation of the charge-density-wave in VTe_2

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By means of broadband time-resolved optical spectroscopy (TR-OS) we investigated the ultrafast reflectivity changes caused by collective and single particle excitations in the charge-density wave (CDW) system VTe_2. This material has been recently subject of investigation since the modifications in its electronic structure triggered by the CDW formation are strongly orbital-dependent and may give rise to a topological change in specific bands [1].
In our contribution, we show by means of TR-OS measurements the possibility to optically excite the amplitude mode (AM) of the CDW phase and therefore couple to the CDW condensate [2]. Moreover, through double pump experiments, we show the possibility to control the intensity and the phase of the amplitude mode of the system.

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Influence of metal-organic interface on magnetic anisotropy in Co thin films

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Metal-organic interfaces are principally interesting from the technological point of view because of potential applications in electronics as well as in the emerging field of spintronics.

We investigated the influence of various surface capping materials on the magnetic anisotropy in 5 nm thick ferromagnetic Co thin films grown by electron-beam evaporation. To assess the magnetic anisotropy, we measured femtosecond laser-pulse induced transient magnetization precession by means of the time-resolved magneto-optical Kerr effect (MOKE) spectroscopy.

We compare the effects of capping the Co films by a nonmagnetic metal (Al), a metalorganic complex tris(8-hydroxyquinoline) gallium (Gaq_3) as well as a naturally grown Co(II) oxide (CoO) antiferromagnetic passivation layer.

In general, the transient MOKE signals were found to exhibit damped coherent oscillations with frequencies up to several tens of GHz, corresponding to the precession of the magnetization in the effective magnetic field.

Detailed analysis of the magnetization precession frequency and the dephasing, extrapolated to zero field, allowed us to qualitatively compare the influence of different surface cappings and determine that the films capped with the metal-organic complex gallium quinoline (Gaq_3) exhibit markedly larger magnetic anisotropy than either of the other samples. Strong damping of the precession observed in the organic sample also points to large disorder in the probed volume.

The frequency response of the Co/Al film can be described with a simple two axis anisotropy model. The same model can be also used for Co/CoO film for temperatures above 100K. In this temperature range, the CoO capping induces an increase in the in-plane anisotropy. On the other hand, we observed signatures of a metamagnetic magnetic phase transition in the Co/CoO film below 100 K, which we tentatively attribute to the spin-flop transition in the antiferromagnetic CoO.

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