December 12-16, 2021 Ambrož, Krvavec, SLOVENIA

BOOK OF ABSTRACTS

Nonequilibrium Quantum Workshop

December 12 - 16, 2021 Krvavec, Slovenia Webpage: <u>https://nqw.ijs.si/</u> E-mail: <u>nqw@ijs.si</u>

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Phenomenology of spectral functions in disordered spin chains

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Studies of disordered spin chains have recently experienced a renewed interest, inspired by the question to which extent the exact numerical calculations comply with the existence of a many-body localization phase transition. For the paradigmatic random field Heisenberg spin chains, many intriguing features were observed when the disorder is considerable compared to the spin interaction strength. Here, we introduce a phenomenological theory that may explain some of those features. The theory is based on the proximity to the noninteracting limit, in which the system is an Anderson insulator. Taking the spin imbalance as an exemplary observable, we demonstrate that the proximity to the local integrals of motion of the Anderson insulator determines the dynamics of the observable at infinite temperature. In finite interacting systems our theory quantitatively describes its integrated spectral function for a wide range of disorders [1].

[1] Lev Vidmar, Bartosz Krajewski, Janez Bonca, Marcin Mierzejewski, arXiv:2105.09336

Relaxation at different length-scales in models of many-body localization

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We study dynamical correlation functions in the random-field Heisenberg chain, which probe the relaxation times at different length scales. Firstly, we show that the relaxation time associated with the dynamical imbalance (examining the relaxation at the smallest length scale) decreases with disorder much faster than the one determined by the dc conductivity (probing the global response of the system). We argue that the observed dependence of relaxation on the length scale originates from local nonresonant regions. The latter has particularly long relaxation times or remains frozen, allowing for nonzero dc transport via higher-order processes. Based on the numerical evidence, we introduce a toy model that suggests that the nonresonant regions' asymptotic dynamics are essential for the proper understanding of disordered chains. In addition, the toy model explains the exponential dependence of the transport properties on the disorder and the broad distribution of dc conductivity.

Time-Resolved Spectroscopy of Anisotropic Compounds – an Overview

F. Cilento

Coherent Modulation of Quasiparticle Scattering Rates in a Photoexcited Charge-Density-Wave System

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Fundamental quasiparticle interactions in solids such as electron-electron and electron-phonon scattering are of fundamental importance e.g. for electronic and optical material properties. While for simple systems such as quasi-free electron gases, fairly good descriptions have been reached, for more complex solids, it remains highly challenging to unravel their intricate interplay, and to identify the dominant channels. Additional challenges arise from broken-symmetry ground states emerging due to strong correlations in complex quantum materials. A way to tackle this problem is by tracking a material's dynamical response after ultrafast optical excitation, as this approach yields direct insight into energy dissipation and scattering processes on their intrinsic timescales. In addition, tailored photoexcitation also provides a way to dynamically control specific material properties, and thereby modify the material's intrinsic interaction channels.

Here, we combine these two approaches, by tracking the fundamental quasiparticle interactions during a photoinduced insulator-to-metal phase transition in a charge-density-wave (CDW) material. Using timeand angle-resolved photoemission spectroscopy (trARPES), we study the transient electronic structure of the prototypical CDW compound TbTe₃. By employing strong optical excitation, we suppress the CDW energy gap at the Fermi level, thereby driving the system into a transient metallic state, followed by a coherent evolution of the system within the transient CDW potential [1]. Simultaneously, we track the relaxation of highly excited, hot quasiparticles, and find a highly unusual modulation of their relaxation rate. State-of-the-art calculations based on non-equilibrium Green's functions provide a microscopic view onto the interplay of quasiparticle scattering and the (transiently modified) electronic band structure, which allow us to quantify the modification of particle-hole scattering processes due to the influence of the CDW energy gap [2].

- [1] J. Maklar, et al., Nat. Commun. 12, 2499 (2021)
- [2] J. Maklar, et al., arXiv:2108.12323 (2021)

Nanocryotron-driven Charge Configuration Memory devices

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For some time, cryo-computing has been severely limited by the absence of a suitable fast and energy efficient low-temperature memory^{1,2}making it an ideal platform for energy efficient memories. Conventional superconducting memories use an architecture based on Josephson junctions (JJs. Ideally, such memory should be compatible with single-flux quantum (SFQ) logic in terms of speed, switching energy and matching impedance. Here we present an implementation of non-volatile charge configuration memory (CCM)^{3,4} in a cryo-computing environment with a hybrid device incorporating a superconducting nanowire cryotron (nTron)⁵. The dynamical response of the device is modelled in terms of the superconducting order parameter in a confined channel of a current-controlled nanowire with a CCM shunt⁶ geared towards understanding and controlling coherence and dissipation in nanowires. The dynamics is probed by measuring the evolution of the V-I characteristics and the distributions of switching and retrapping currents upon varying the shunt resistor and temperature. Theoretical analysis of the experiments indicates that as the value of the shunt resistance is decreased, the dynamics turns more coherent presumably due to stabilization of phase-slip centers in the wire and furthermore the switching current approaches the Bardeen's prediction for equilibrium depairing current. By a detailed comparison between theory and experimental, we make headway into identifying regimes in which the quasi-one-dimensional wire can effectively be described by a zero-dimensional circuit model analogous to the RCSJ (resistively and capacitively shunted Josephson junction. Analysis of time-dynamics and current-voltage characteristics based on measured device parameters show that single flux quantum (SFQ)-level pulses can drive non-volatile CCM on the picosecond timescale. We also present first measured current-voltage characteristics and read operation of actual hybrid memory devices showing expected behaviour.

The inherent high energy efficiency and ultrahigh speed makes this hybrid device an ideal memory for use in cryo-computing and quantum computing peripheral devices.

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- [3] I. Vaskivskyi et al. Nat. Comm. 7, 11442 (2016).
- [4] D. Mihailovic *et al.*, APL **119**, 013106 (2021).
- [5] A.N. McCaughan, & K.K. Berggren, A Nano Letters 14, 5748–5753 (2014).
- [6] M.W.Brenner, et al., Phys. Rev. B 85, 224507 (2012).

Nontrivial Damping of Quantum Many-Body Dynamics

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Understanding how the dynamics of a given quantum system with many degrees of freedom is altered by the presence of a generic perturbation is a notoriously difficult question. Recent works predict that, in the overwhelming majority of cases, the unperturbed dynamics is just damped by a simple function, e.g., exponentially as expected from Fermi's Golden Rule. While these predictions rely on random-matrix arguments and typicality, they can only be verified for a specific physical situation by comparing to the actual solution or measurement. Crucially, it also remains unclear how frequent and under which conditions counterexamples to the typical behavior occur. In this work, we discuss this question from the perspective of projection-operator techniques, where exponential damping of a density matrix occurs in the interaction picture but not necessarily in the Schrödinger picture. We show that a nontrivial damping in the Schrödinger picture can emerge if the dynamics in the unperturbed system possesses rich features, for instance due to the presence of strong interactions. This suggestion has consequences for the time dependence of correlation functions. We substantiate our theoretical arguments by large-scale numerical simulations of charge transport in the extended Fermi-Hubbard chain, where the nearest-neighbor interactions are treated as a perturbation to the integrable reference system.

[1] T. Heitmann, J. Richter, J. Gemmer, R. Steinigeweg, arXiv:2103.06646.

Detecting delocalization-localization transitions from full density distributions

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Characterizing the delocalization transition in closed quantum systems with a many-body localized phase is a key open question in the field of nonequilibrium physics. We exploit the fact that localization of particles as realized in Anderson localization and standard many-body localization (MBL) implies Fock-space localization in single-particle basis sets characterized by a real-space index. Using a recently introduced quantitative measure for Fock-space localizationcomputed from the density distributions, the occupation distance [1], we systematically study its scaling behavior across delocalization transitions [2].

We first identify critical points from scaling collapses of numerical data with an excellent agreement with literature results for the critical disorder strengths of noninteracting fermions, such as the one-dimensional Aubry-André model and the three-dimensional Anderson model. We then observe a distinctively different scaling behavior in the case of interacting fermions with random disorder consistent with a Kosterlitz-Thouless transition. Finally, we use our measure to extract the transition point as a function of filling for interactsing fermions [2].

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- [2] M. Hopjan, G. Orso and F. Heidrich-Meisner, arXiv:2105.10584, to appear in Phys. Rev. B

Monday, December 13, 2021

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Microscopic dynamics of propagating and localized excitations across interfaces analyzed by femtosecond solid state spectroscopy

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An excited electron propagates in condensed matter with its momentum \mathbf{k} at an energy $E(\mathbf{k})$ and experiences elastic and inelastic scattering processes, which lead to electronic relaxation and energy transfer to microscopic excitations of the lattice and spin systems. Experiments employing femtosecond time-resolved photoelectron spectroscopy exploited so far very successfully the surface sensitivity of the method and probed such scattering processes locally at or near the surface in the time domain [1]. Here, we report on experimental results which analyze the non-local dynamics of excited electrons in two-photon photoemission (2PPE) and demonstrate sensitivity to buried media [2]. In these experiments one photon excites in Au/Fe/MgO(001) heterostructures electrons in Fe. Electron propagation through the layer stack to the Au surface is detected in 2PPE in back side pump – front side probe experiments in a time-of-flight like scheme. We observe pronounced differences between front and back side pumping of the heterostructure which are attributed to electron transport contributions through the layer stack. Furthermore, competition of e-e with e-ph scattering will be discussed in [Fe/MgO], heterostructures. Pump-probe experiments of element specific spectroscopy in combination with electron diffraction provide here unprecedented insights regarding the mechanism of energy transfer across interfaces and emphasize the importance of coupling hot electrons to non-thermalized interface phonons [3]. Extension of these experimental tools to address effects of strong electron correlation [4] and spin-dependent dynamics across interfaces [5] will be discussed.

This work was funded by the Deutsche Forschungsgemeinschaft through the Collaborative Research Center CRC 1242.

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- [3] N. Rothenbach, M. E. Gruner, K. Ollefs, C. Schmitz-Antoniak, S. Salamon, P. Zhou, R. Li, M. Mo, S. Park, X. Shen, S. Weathersby, J. Yang, X. J. Wang, R. Pentcheva, H. Wende, U. Bovensiepen, K. Sokolowski-Tinten, A. Eschenlohr, Phys. Rev. B 100, 174301 (2019).
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Coherent Control of a Metastable Hidden Phase

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Controlling material properties by illumination with ultrashort optical pulses is a promising new pathway to extend the functionality of complex solids. Prominent examples of this rapidly growing research field include photostabilization of superconductivity [1] and switching to metastable states not accessible in thermal equilibrium [2]. A metastable state of particular interest is the optically or electrically induced hidden phase of 1T-TaS₂, as it features an order-of-magnitude change in resistivity [3], which allows for novel energy-efficient high-speed memory devices [4]. However, so far a clear understanding of the microscopic processes that govern the dynamic pathways to metastable states is still missing, limiting controllability due to empirical and unspecific switching protocols.

Here, using time- and angle-resolved photoemission spectroscopy (trARPES), we investigate the electronic band structure and ultrafast photoinduced phase transition from commensurate charge-density-wave (CDW) ground state to the hidden state in 1T-TaS₂. Mapping the band structure of the hidden state reveals suppression of correlation effects and confirms metallization, suggesting a critical role of interlayer stacking order of the TaS₂ sheets in the hidden state. Next, we track the fluence-dependent electron dynamics upon photoexcitation and find strong evidence that the CDW amplitude mode governs a collective, ultrafast switching pathway to the hidden state. This is further corroborated by demonstrating coherent control of the switching efficiency into the hidden phase by controlling the CDW amplitude mode using a multi-pump-pulse excitation scheme. We envision that the amplitude-mode governed transition applies to a range of CDW compounds [5].

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Ultraweak electron-phonon coupling strength in cubic boron arsenide unveiled by ultrafast dynamics

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We report a time-resolved ultrafast quasiparticle dynamics investigation of cubic boron arsenide (c-BAs), which is a recently discovered highly thermal conducting material. The excited state ultrafast relaxation channels dictated by the electron-phonon coupling (EPC), phonon-phonon scattering, and radiative electron-hole recombination have been unambiguously identified, along with their typical in-

teraction times [1]. Significantly, the EPC strength is obtained from the dynamics, with a value of $\lambda_{T_2} = 0.008$, demonstrating an unusually weak coupling between the electrons and phonons. As a comparison, an ultraweak EPC strength for graphene is also expected. Notably, during our analysis we have generalized the fluence-dependence method for obtaining the EPC strength to room temperature, which can be applied to many other types of quantum materials in the future.

Time permits, I will also talk about two other recent progresses: (1) We have conceived and constructed an *on-site in situ* high-pressure ultrafast pump-probe spectroscopy instrument that facilitates ultrafast pump-probe dynamics measurements under high pressure condition [2]. (2) We demonstrate that second harmonic generation (SHG) is a local microscopic process—it does not rely on macroscopic broken inversion symmetry [3]. An AB-type superstructure can generate SHG easily and an ABC-type super-structure is not necessary. Our results introduce a scheme for SHG, extending the generation and control of SHG in nano-photonics to nearly all the accessible centrosymmetric materials.

- Z. Y. Tian, Y. W. Xiao, Q. Y. Zhang, G. A. Gamage, F. Tian, S. Yue, V. G. Hadjiev, Jiming Bao, Zhifeng Ren, Erjun Liang,[†] and Jimin Zhao^{*}, Ultraweak electron-phonon coupling strength in cubic boron arsenide unveiled by ultrafast dynamics, *Submitted* (2021).
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Phonons in metals and Eliashberg function

V. Kabanov

Taking the temperature of a pure quantum state

J. Goold

Universal Magnetic Oscillations of dc Conductivity in the Incoherent Regime of Correlated Systems

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Using the dynamical mean field theory we investigate the magnetic field dependence of dc conductivity in the Hubbard model on the square lattice, fully taking into account the orbital effects of the field introduced via the Peierls substitution. In addition to the conventional Shubnikov–de Haas quantum oscillations, associated with the coherent cyclotron motion of quasiparticles and the presence of a well-defined Fermi surface, we find an additional oscillatory component with a higher frequency that corresponds to the total area of the Brillouin zone. These paradigm-breaking oscillations appear at elevated temperature. This finding is in excellent qualitative agreement with the recent experiments on graphene superlattices. We elucidate the key roles of the off-diagonal elements of the current vertex and the incoherence of electronic states, and explain the trends with respect to temperature and doping.

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Time resolved ARPES: a glance to the past-present-future

F. Parmigiani

Quantum billiards in metastable heterostructures

D. Mihailović

Relaxation mechanisms in a disordered system with the Poisson level statistics

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I will discuss the interplay between many-body localization and spin-symmetry. I will present the time evolution of several observables in the anisotropic t – J model. Like the Hubbard chain, the studied model contains charge and spin degrees of freedom. Yet, it has a smaller Hilbert space and thus allows for numerical studies of larger systems. I will compare the field disorder that breaks the Z_2 spin symmetry and a potential disorder that preserves the latter symmetry. In the former case, sufficiently strong disorder leads to localization of all studied observables, at least for the studied system sizes. However, in the case of symmetry-preserving disorder, we observe that odd operators under the Z_2 spin transformation relax towards the equilibrium value at relatively short time scales that grow only polynomially with the disorder strength. On the other hand, the dynamics of even operators and the level statistics within each symmetry sector are consistent with localization. Our results indicate that localization exists within each symmetry sector for symmetry preserving disorder. Odd operators' apparent relaxation is due to their time evolution between various symmetry sectors.

Single-particle eigenstate thermalization in quantum-chaotic quadratic Hamiltonians

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In this presentation, we study single-particle properties of quantum-chaotic quadratic models, which are identified with quadratic models having random matrix theory correlations in single-particle spectra, i.e., exhibiting single-particle quantum chaos. We analyze matrix elements of local and nonlocal operators in two paradigmatic Hamiltonians, i.e., the quadratic Sachdev-Ye-Kitaev model and the three-dimensional Anderson model below the localization transition. We demonstrate that their matrix elements display single-particle eigenstate thermalization. Specifically, we show that the diagonal matrix elements exhibit vanishing eigenstate-to-eigenstate fluctuations, and the variance proportional to the inverse Hilbert space dimension. We also demonstrate that the ratio between the variance of diagonal and off-diagonal matrix elements agrees with the prediction of random matrix theory. We also study distributions of matrix elements, and establish the conditions under which they are (not) Gaussian.

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Topological defects on demand in the charge density wave of SmTe3

M. Trigo

Non-equilibrium electron dynamics of the bulk VSe2 charge-density-wave system

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By means of time- and angle-resolved photoemission spectroscopy (tr-ARPES), we investigate the effect of the charge density wave (CDW) phase transition on the equilibrium and out-ofequilibrium electronic properties 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]. However, at present, only a few studies on the effect of an ultrafast optical excitation are available [1,3]. In our contribution we present a study on the bulk material. By selecting the polarization of the probe pulses, tr-ARPES allows us to disentangle states with different orbital character, originating from the V and Se valence bands. 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 filling of novel photoinduced states near the Fermi level, lasting for several picoseconds after photoexcitation.

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- [3] Majchrzak et al., arXiv:2011.06358v1 (2020).

Optical signatures of photoinduced phase transitions in IrTe₂

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 $IrTe_2$, a Van-der-Waals transition metal dichalcogenide, is known to host a complicated phase diagram: two first order phase transitions into charge ordered stripe phases of different periodicity are observed in bulk undoped samples [1]; superconductivity emerges in bulk doped samples resulting in the familiar superconducting dome behavior [1]; superconductor – normal metal switching was demonstrated in undoped quenched nanoflakes [2]; and superconductivity has been shown to emerge in thin flakes resulting in a superconducting dome as a function of flake thickness [3]. Most interestingly however, fast cooling of undoped bulk samples has resulted in the formation of superconducting hexagonal-like surface patches appearing at three-fold stripe phase intersections [4].

We have studied the possibility to control the low temperature charge order in $IrTe_2$ with ultrafast pulses using optical time domain spectroscopy. High fluence photoexcitation gives rise to non-thermal behavior of transient reflectivity on sub-picosecond timescales, indicative of a transient photoinduced phase transition thought to be associated with Ir dimer breaking and recovery [5]. Following the trajectory of the system in double-pump measurements we observe definite evidence of a transition to a mixture of higher temperature equilibrium phases several picoseconds after the arrival of the strongly perturbing pulse, as well as the material's subsequent relaxation into the low temperature equilibrium state some 100 to 150 picoseconds after excitation. We conclude that the phase transitions at these timescales are driven by the increase in the transient lattice temperature imposed by laser excitation.

On the other hand, by tracking the response to increasing intensity of the pump beam at a fixed delay in the double-pump experiment we observe threshold-like behavior in the temporal as well as in the spectral domain, thus shedding light on the connection between the dimer breaking transition at sub-picosecond timescales and the transient lattice temperature driven transitions at longer timescales.

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Nonthermal electronic orders

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Recent experiments and theoretical studies suggest that electronic orders such as superconductivity or excitonic insulator phases can be realized in highly nonthermal systems. In this talk, I will discuss some examples which have been demonstrated in nonequilibrium dynamical mean field theory simulations of Hubbard-type models. After briefly reviewing results for nonthermal magnetic order and the eta-pairing state in photo-doped Mott insulators, I will discuss in more detail two recent studies on nonthermal excitonic order in a two-orbital Hubbard model with Hund coupling and crystal field splitting [1] and on a nonthermal form of composite order (or odd-frequency orbital order) in a three-orbital Hubbard model which is relevant for the description of A3C60 [2]. The excitonic insulator study reveals a new entropy-trapping mechanism for nonthermal orders, while the fulleride example demonstrates a nonthermal electronic order which is stabilized by the kinetic energy of the photo-excited charge carriers.

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[2] P. Werner and Y. Murakami, Phys. Rev. B 104, L201101 (2021).

Photoinduced spinful excitons in Hubbard systems with magnetic superstructures

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The possibility to form excitons in photo-illuminated correlated materials is central from fundamental and application oriented perspectives. We show how the interplay of electron-electron interactions and a magnetic superstructure leads to the formation of a peculiar spinful exciton, which can be detected in ARPES-type experiments and optical measurements. We study this by using matrix product states (MPS) to compute the time evolution of single-particle spectral functions and of the optical conductivity following an electron-hole excitation in a class of one-dimensional correlated band-insulators, simulated by Hubbard models with on-site interactions and alternating local magnetic fields. An excitation in only one specific spin direction leads to an additional band in the gap region of the spectral function only in the spin direction unaffected by the excitation and to an additional peak in the optical conductivity. Recombination of the excitation happens on much longer time scales than the ones amenable to MPS. We discuss implications for experimental studies in correlated insulator systems.

[1] C. Meyer and S.R. Manmana, arXiv:2109.07037 (2021)

Assigning temperatures to many-body eigenstates

M. Haque

Ultrafast manipulation of the NiO antiferromagnetic order via sub-gap optical excitation

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M. Beye,³ W. Bronsch,⁴ F. Parmigiani,⁴ C. Schüssler-Langheine,⁵ A. Steyervoyedov,⁶
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Wide-band-gap insulators such as NiO offer the exciting prospect of coherently manipulating electronic correlations with strong optical fields [1]. Contrary to metals where rapid dephasing of optical excitations via electronic processes occurs, the sub-gap excitation in charge-transfer insulators has been shown to couple to low-energy bosonic, probably phonon, excitations [2]. Here we use the prototypical charge-transfer insulator NiO to demonstrate that sub-gap excitation leads to a renormalized NiO bandgap in combination with a significant reduction of the antiferromagnetic order. We employ element-specific x-ray absorption spectroscopy at the FLASH free electron laser [3] to demonstrate the reduction of the upper band-edge at the O 1s-2p core-valence resonance whereas the antiferromagnetic order is probed via x-ray magnetic linear dichroism (XMLD) at the Ni 2p-3d resonance. Comparing the transient XMLD spectral lineshape to ground-state measurements [4] allows us to extract a spin temperature rise of more than 60 K for time delays longer than 400 fs. This is accompanied by a band-gap reduction. Before 400 fs a non-equilibrium state is formed characterized by O 2p mid-gap states. We will discuss these results in terms of a transient Ni-O charge transfer during the optical driving field. The energetic proximity of our 800 nm excitation wavelength to phonon-assisted NiO d-d transitions facilitates the bosonic dressing of the laser field. Finally, laser-excited phonons [5] couple to magnons on a ~400 fs timescale enabling the quenching of the NiO magnetic order [6].

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Resonant excitations of spins, orbitals and the lattice probed by x-rays

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Results will be presented of how the spins, the orbitals and the lattice react to phase stable excitations of low energy phonons, electromagnons or orbitals. Examples will cover soft mode driving of the ferro-electric mode in $SrTiO_3$, [1] electromagnon excitation in hexaferrites and orbital excitation in magnetically frustrated $Tb_2Ti_2O_7$. These ultrafast changes caused by the excitations are probed by resonant and non-resonant X-ray diffraction to obtain the lattice the spin and/or the orbital dynamics. Recent results from SwissFEL will be presented.

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Transient Enhancement of the Ferroelectricity in the Rashba Semiconductor α-GeTe

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 α -GeTe(111) is a bulk ferroelectric Rashba semiconductor which exhibits the largest known Rashba-type

spin splitting of so-far known materials, one of the most promising mechanism to reversibly manipulate spin polarization. Its electronic structure in the occupied states has been intensively studied by Angle Resolved Photoemission Spectroscopy (ARPES) and Spin ARPES (SARPES) [1], the key technique to understand the spin texture of materials. Using operando SARPES, it has been demonstrated that it is possible to reversibly manipulate spin polarization by an external electric field in α -GeTe(111) [2]; a promising behavior for spintronics applications. A stimulating direction of research is to investigate whether it is possible to coherently modify the ferroelectric properties of GeTe upon photoexcitation.

Using a 800 nm photoexcitation, we drive α -GeTe(111) out-of-equilibrium and probe its transient low-energy electronic structure with time-resolved ARPES. We reveal that the Rashba splitting of its bulk states is *enhanced* after 200 fs. By comparison with density functional theory calculations, we show that this change of the electronic structure is driven by a shift of the Ge atomic layer towards the Te atomic layer, meaning an *increase* of the ferroelectric distortion. A coherent phonon oscillation linked to this ferroelectric distortion is also observed, with a frequency consistent with the amplitude mode of the related polar mode.

We identify a surface photovoltage effect as the mechanism responsible for this transient enhancement of the ferroelectricity at the surface of GeTe and link it to a delayed displacive excitation of the coherent phonon of the ferroelectric distortion.

- J. Krempaský, S. Muff, F. Bisti, M. Fanciulli, H. Volfová, A.P. Weber, N. Pilet, P. Warnicke, H. Ebert, J. Braun, F. Bertran, V.V. Volobuev, J. Minár, G. Springholz, J.H. Dil, and V.N. Strocov, Nat. Commun. 7, 13071 (2016).
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Characterizing microscopic interactions via photo-induced lifetime changes

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Charge excitations across electronic band gaps are a key ingredient for transport in optoelectronics and light-harvesting applications. In contrast to conventional semiconductors, studies of above-band-gap photo-excitations in correlated materials are still in their infancy. The new idea presented in this talk is that lifetime changes after a photo-excitation in correlated systems carry essential information about the competition between active degrees of freedom. We will exemplify the concept by a comparative analysis between theoretical many-body simulations and time-resolved ARPES on the excitonic insulator candidate Ta2NiSe5, where the interplay between electronic and lattice degrees of freedom is a matter of hot debate. We will employ photo-induced changes in the lifetime to quantify the competition between electron-driven versus lattice-driven situation is apparent as in the former, the photoinduced lifetime changes are substantial, while in the latter, they are strongly suppressed. The quantitative comparison between experiment and theory demonstrates the pivotal (but not necessarily sole) contribution of electron-electron interactions to stabilizing the electronic gap in the material.

[1] DG, Sydney Dufresne, et al., to be published.

Dynamics of quantum geometry in the fractional quantum Hall effect

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Intermediate-scale quantum technologies provide unprecedented opportunities for scientific discoveries while posing the challenge of identifying important problems that can take advantage of them through algorithmic innovations. A major open problem in quantum many-body physics is the table-top generation and detection of emergent excitations analogous to gravitons -- the elusive mediators of gravitational force in a quantum theory of gravity. In solid state materials, fractional quantum Hall phases are one of the leading platforms for realizing graviton-like excitations, however their direct observation remains an experimental challenge. Here, we generate these excitations on the IBM quantum processor. We first identify an effective one-dimensional model that captures the geometric properties and graviton dynamics of fractional quantum Hall states. We then develop an efficient, optimal-control-based variational quantum algorithm to simulate geometric quench and the subsequent graviton dynamics, which we successfully implement on the IBM quantum computer. Our results [1] open a new avenue for studying the emergence of gravitons in a new class of tractable models that lend themselves to direct implementations on the existing quantum hardware.

[1] A. Kirmani et al., arXiv:2107.10267

Quantum Domain Melting of a Wigner Crystal 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 macroscopic quantum tunneling. Here, we report quantum domain melting dynamics in two embodiments: an electronic crystal 1T-TaS₂, 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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Ultrafast dynamics of Mott-state quench and formation in strongly correlated BEDT-TTF molecular conductors observed by three-pulse pump probe spectroscopy

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We investigate the quench and real-time formation of the Mott state and photoexcited carrier relaxation dynamics in the Mott insulator κ -(BEDT-TTF)₂Cu[N(CN)₂]Cl (κ -Cl) and the superconductor κ -(BEDT-TTF)₂Cu[N(CN)₂]Br (κ -Br) using three-pulse femtosecond optical spectroscopy. In both salts, we find that transient reflectivity amplitude recovers on 2 ps timescale after a strong near-infrared pulse quench. The transient reflectivity relaxation time is nearly constant throughout indicating that the energy gap for charge excitations is filled rather than closed, by photoinduced carriers of only 0.5% per dimer site. The Mott state is re-formed on a few-picosecond timescale with the disappearance of the in-gap photo-to-doping induced states near the Fermi energy. In κ -Br, a similar behavior to that in κ -Cl is observed and attributed to the disorder induced phase-separated Mott insulating regions [2].

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Nonthermal control of excited quantum materials via laser interaction quench

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Quantum material systems upon applying ultrashort laser pulses provide a rich platform to access excited material phases and their transformations that are not entirely like their equilibrium counterparts. The addressability and potential controls of metastable or long- trapped out-of-equilibrium phases have motivated interests both for the purposes of understanding the nonequilibrium physics and advancing the quantum technologies.

Thus far, the dynamical spectroscopic probes eminently focus on microscopic electronic and phonon responses. For characterizing the long-range dynamics, such as order parameter fields and fluctuation effects, the ultrafast scattering probes offer direct sensitivity. Bridging the connections between the microscopic dynamics and macroscopic responses is central toward establishing the nonequilibrium physics behind the light-induced phases.

Learning from the quantum gases microscope experiments and the nonequilibrium sciences on atomic and molecular systems, we present a path to understand the nonequilibrium many-body dynamics using excited quantum material phases as a platform. We first highlight the synergies based on phenomenology to identify common open questions and potentially different manifestations in hard condensed matter systems. To this end, we give the basic theoretical framework on describing the non-equilibrium scattering problems and describe how such framework relates to the out-of-equilibrium phenomena.

On the experimental realizations, the focus will be placed on the short-time behaviors mediated by interaction quench. We give effective models outlining the emergences of nonthermal critical points, and hidden phases setting the initial condition for the long-time relaxation dynamics as the system re-establish the thermal states[1]. In particular, the inhomogeneity embedded in the system formation and their impacts on the dynamical evolutions into especially the long-time trapped states stemming from interaction quench are of particular interests.

Following the phenomenology, rich scenarios as those involve competitive broken-symmetry orders, vestigial orders, and the intertwined ground states could be identified, leading to intriguing nonequilibrium phenomena from vacuum- suspended rare-earth tritellurides[2], tantalum disulfides[3] thin films, and vanadium dioxide nanocrystalline materials[4] upon light excitations re-examined in recent experiments.

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Ultra-efficient resistance switching between charge ordered phases in 1T-TaS, with a single picosecond electrical pulse

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Resistance switching between charge ordered phases of the 1T-TaS₂ has shown to be potentially useful for the development of high-speed, energy efficient non-volatile memory devices^{1,2}. While ultrafast switching was previously reported with optical pulses³, determination of the intrinsic speed limits of actual devices that are triggered by electrical pulses is technically challenging and hitherto still largely unexplored.

Using an optoelectronic "laboratory-on-a-chip" especially designed for measurements of ultrafast memory switching, we are able to accurately measure the *electrical* switching parameters with sub-100 fs temporal resolution. A photo-switch is used for ultrashort electrical pulse generation, while its propagation along a coplanar transmission line, and across the memory device, is detected using electro-optical sampling using a purpose-grown highly-resistive electro-optic (Cd,Mn)Te crystal substrate.

We observe *non-volatile* resistance switching with single 1.9 ps electrical pulses, with a switching energy of 0.47 atto-Joules. This represents a significant advance over existing non-volatile memory device concepts in terms of both parameters. The ground-breaking result suggest that electrical charge manipulation in $1T-TaS_2$ could become a new technological platform for cryogenic, ultrahigh-speed, energy efficient memory devices.

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Many-body tunnelling in a symmetric double-well potential

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Tunnelling is one of the most fascinating phenomena in quantum physics, whose implications on the dynamics of many-body systems are still unclear. Recently, it has been argued that the presence of inter-particle interactions may lead to cooperative effects, such as the modification of the single-particle tunnelling between wells or the simultaneous tunnelling of a few particles as a single object through a potential barrier. Under certain conditions, these non-standard Hubbard terms are considerably more important than previously assumed, due to correct account of the Wannier functions, which tails were disregarded in many estimations. In this talk, we will examine some preliminary results about possible cooperative effects shown by two particles in a double-well potential, under the effect of different types of interaction. Our results show that, under certain conditions, the non-standard density-induced tunnelling amplitude may suppress the single-particle tunnelling even for repulsive two-particle interactions. This would correspond to a bound state localized in one well, which cannot decay but only propagate between the wells due to the non-standard pair-tunnelling mechanism.

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Ultrafast magnetic switching by resonant excitation of optical phonons

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Identifying an efficient pathway to change the order parameter via a subtle excitation of the coupled high-frequency mode is the ultimate goal of the field of ultrafast phase transitions [1,2]. This is an especially interesting research direction in magnetism, where the coupling between spin and lattice excitations is required for magnetization reversal [3]. Despite several attempts [4,5] however, the switching between magnetic states via resonant pumping of phonon modes has not yet been demonstrated.

To provide resonant excitation of the phonon modes, we use pulses from FELIX (Free Electron Lasers for Infrared eXperiments, Nijmegen, The Netherlands). The IR/THz light with photon energy ranging between 25 meV and 124 meV (wavelength 10-50 μ m) is typically focused onto the sample. The pulses of FELIX have been shown to be Fourier-transform limited [6], with their bandwidth experimentally tunable in the range of 0.5-2.0%, corresponding to the typical pulse width of 1-10 ps, depending on the wavelength range.

And thus we show how an ultrafast resonant excitation of the longitudinal optical phonon modes in magnetic garnet films switches magnetization into a peculiar quadrupolar magnetic domain pattern, unambiguously revealing the magneto-elastic mechanism of the switching [7]. In contrast, the excitation of strongly absorbing transverse phonon modes results in thermal demagnetization effect only. The mechanism appears to be very universal, and is shown to work in samples with very different crystallographic symmetry and magnetic properties.

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Ultrafast Amplification and Nonlinear Coupling of Coherent Magnon Modes in an Antiferromagnet

D. Bossini

Manipulation of a collinear metallic antiferromagnet with femtosecond optical pulses and external strain

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Optical control of magnetization in numerous ferro and ferrimagnets¹⁻³ has been demonstrated in recent years. While the absence of stray fields, the insensitivity to external magnetic fields and ultra-fast dynamics make antiferromagnets promising candidates for active elements in spintronic devices, optical control has been limited to a few insulating antiferromagnets with specific spin configurations at cryogenic temperatures.^{4,5} Here, we demonstrate optical manipulation of the staggered magnetization in the metallic collinear antiferromagnet Mn₂Au by combining tensile strain and excitation with femtosecond optical pulses at room temperature. By applying tensile strain along one of the two orthogonal in-plane easy axes and exciting the sample at room temperature by a train of intense femtosecond pulses, we are able to manipulate the direction of the Néel vector, resulting in a stable magnetically aligned state. The dependence of optically induced Néel vector alignment on excitation density and strain suggests the alignment is a result of induced depinning of 90° domain walls and their montion in the direction of the free-energy gradient, governed by the magneto-elastic energy. Such an approach may be applicable to a wider range of collinear antiferromagnets.

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On many body localization in random and quasiperiodic potentials

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Our recent numerical results on many-body localization in disordered and quasiperiodic spin chains will be presented. The time dynamics in 1D disordered Heisenberg spin-1/2 chain is studied focusing on a regime of large system sizes and a long time evolution. Performing extensive numerical simulations of the imbalance, a quantity often employed in the experimental studies of MBL, we show that the regime of a slow power-law decay of imbalance persists to disorder strengths exceeding by at least a factor of 2 the current estimates of the critical disorder strength for MBL. Even though we investigate time evolution up to few thousands tunneling times, we observe no signs of the saturation of imbalance that would suggest freezing of system dynamics and provide a smoking gun evidence of MBL. We demonstrate that the situation is qualitatively different when the disorder is replaced by a quasiperiodic potential. In this case, we observe an emergence of a pattern of oscillations of the imbalance that is stable with respect to changes in the system size. This suggests that the dynamics of quasiperiodic systems remain fully local at the longest time scales we reach provided that the quasiperiodic potential is sufficiently strong. The results for time dynamics are further confirmed by a finite-size scaling analysis of eigenstates and spectral statistics across the many-body localization in quasiperiodic systems. The analysis shows the many-body localization transition in quasiperiodic systems belongs to the Berezinskii-Kosterlitz-Thouless class, the same as in the case of uniformly disordered systems. However, the finite size effects are less severe in quasiperiodic systems than in chains with random disorder. Also interestingly, deep in the ergodic regime, we find an unexpected double-peak structure of distribution of onsite magnetizations. Our studies identifies challenges in an unequivocal experimental observation of the phenomenon of MBL [1,2].

The numerical calculations have been possible thanks to PL-Grid Infrastructure. The research has been supported by National Science Centre (Poland) under project 2019/35/B/ST2/00034 (A.S.A., J.Z.). The work of T.C. was realised within the QuantERA grant QTFLAG, financed by National Science Centre (Poland) via grant 2017/25/Z/ST2/03029. We acknowledge the support of Foundation for Polish Science (FNP) through scholarship START (P.S.) as well as via first Polish-French Maria Skłodowska – Pierre Curie award received by D. Delande and J. Zakrzewski.

- [1] P.Sierant, J. Zakrzewski, arXiv:2109.13608
- [2] A.S. Aramsthottil, T. Chanda, P.: Sierant, J. Zakrzewski, arxiv:2109.08408, Phys. Rev. B in press.

Universal behavior beyond multifractality of wave-functions at measurement-induced and localization phase transitions

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The competition between unitary evolution that spreads information throughout the manybody system, and the monitoring action of an environment gives rise to dynamical phases separated by measurement-induced phase transitions. The first part of the talk will be devoted to numerical investigations of the structure of many-body wave functions of 1D random quantum circuits with local measurements across a measurement-induced transition between phases with volume-law and area-law scaling of entanglement entropy. The many-body wave functions are investigated by means of the participation entropies. The leading term in system size dependence of participation entropies indicates a multifractal scaling of the wavefunctions at any non-zero measurement rate. The sub-leading term contains universal information about measurement-induced phase transitions and plays the role of an order parameter, being non-zero in the volume-law phase and vanishing in the area-law phase. We provide an analytical interpretation of this behavior expressing the participation entropy in terms of partition functions of classical statistical models in 2D. The second part of the talk will concern the structure of many-body wave functions. The ensuing measures of localization transitions – both in presence and in absence of interactions. The ensuing measures of localization in the system alongside with the more conventional quantities will be used to discuss the stability of many-body localization in the Kicked Ising model.

[1] P. Sierant, X. Turkeshi, arXiv:2109.06882

Study of critical dynamics close to the many-body localisation transition

S. Nandy

Resolving chicken-or-egg causality dilemma in physics of magnetostructural phase transition in FeRh

A. V. Kimel

Nonequilibrium Quantum Workshop, Krvavec, Slovenia December 12 – 16, 2021

TBA

D. Fausti

Correlation functions in perturbed dual unitary circuits

T. Prosen

Signatures of transient Hubbard exciton formation and recombination in Sr2IrO4

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To date, excitons have mainly been studied in rigid band semiconductors. Due to the irrelevance of electron-electron correlations in these systems, the same hydrogenic excitonic models apply to many material classes. In Mott insulators, however, strong interactions between electronic, spin, and orbital degrees of freedom create pathways for other excitonic binding mechanisms. These so-called Hubbard excitons are predicted to exhibit novel non-hydrogenic properties that rely critically on the microscopic description of the host material. I will report the spectroscopic signatures of transient exciton formation in the antiferromagnetic spin-orbital Mott insulator Sr2IrO4 obtained by employing an ultrafast terahertz probe that is sensitive to transitions between different excitonic states. A near-infrared photoexcitation is used to generate a conductive particle-hole gas, which decays into insulating excitonic states. Strong spin-exciton coupling is deduced from an analysis of the excitonic recombination dynamics as a function of temperature. To develop a microscopic picture of the excitonic states, I will compare the experimental results against numerical exact diagonalization calculations. These results stimulate the search for novel excitonic states in other Mott insulating systems.

Seebeck coefficient in skewed non-Fermi liquids: application to Nd-LSCO

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We consider thermoelectric transport in correlated metals with disorder within a simple phenomenological approach. We allow for a particle-hole asymmetry in the inelastic scattering rate. We find that the effects of this asymmetry disappear at low temperatures in Fermi liquids (where electronic contribution to resistivity $\rho \sim T^2$) but not in non-Fermi liquids ($\rho \sim T^v$; $v \le 1$), which can lead to changes of sign of the Seebeck coefficient at low temperatures with respect to that found in a band theory. We apply the theory [1] to recent measurements of thermoelectric transport in Nd-LSCO cuprate close to the pseudo-gap ending point [2] and show that both the inplane and outofplane measured resistivity and the Seebeck coefficient are consistently described.

[1] A. Georges and J. Mravlje, Phys. Rev. Research 3, 043132 (2021).

[2] A. Gourgot et al., arXiv:2106.05959

Dissipative Floquet dynamics and measurement induced criticality in trapped-ion chains

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Quantum systems evolving unitarily and subject to quantum measurements exhibit various types of non-equilibrium phase transitions, arising from the competition between unitary evolution and measurements. Dissipative phase transitions in steady states of time-independent Liouvillians and measurement induced phase transitions at the level of quantum trajectories are two primary examples of such transitions. Investigating a many-body spin system subject to periodic resetting measurements, we argue that many-body dissipative Floquet dynamics provides a natural framework to analyze both types of transitions. We show that a dissipative phase transition between a ferromagnetic ordered phase and a paramagnetic disordered phase emerges for long-range systems as a function of measurement probabilities. A measurement induced transition of the entanglement entropy between volume law scaling and area law scaling is also present, and is distinct from the ordering transition. The ferromagnetic phase is lost for short range interactions, while the volume law phase of the entanglement is enhanced. An analysis of multifractal properties of wave function in Hilbert space provides a common perspective on both types of transitions in the system. Our findings are immediately relevant to trapped ion experiments, for which we detail a blueprint proposal based on currently available platforms.

[1] P. Sierant, G. Chiriaco et al. arXiv:2107.05669 (2021)

Heat transport in the 2d Hubbard model

M. Ulaga

Thursday, December 16, 2021

	Chair: Tomaž Prosen	
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Nonequilibrium Quantum Workshop, Krvavec, Slovenia December 12 – 16, 2021

TBA

G. Aeppli

Spectral properties of the three-dimensional Anderson model

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The three-dimensional Anderson model represents a paradigmatic model to understand the Anderson localization transition. Using modern numerical approaches, we investigate the model's spectral properties, focusing particularly on the quantitative comparison between the level sensitivity statistics and the level statistics. While the former probes the susceptibility of the Hamiltonian eigenlevels towards the introduction of the magnetic flux to the system, the latter deals with the unperturbed energy levels. We define two versions of the dimensionless conductance, the first corresponding to the width of the level curvature distribution relative to the mean level spacing, and the other corresponding to the ratio of Heisenberg and Thouless times obtained from the spectral form factor. We show that both conductances display remarkably similar behaviour around the localization transition, in particular, they predict a nearly identical critical point consistent with other well-established measures of the transition.

Motivated by the pioneering work of Edwards and Thouless [J. Phys. C. 5, 807 (1972)], we then calculate the characteristic energy, defined as the mean change of the eigenlevels upon switching the hopping along one of the lattice edges from periodic to antiperiodic boundary conditions. Making use of the modern hardware to perform a systematic analysis, we obtain results for system sizes much greater than the ones available to the authors of the original study. By accurately pinpointing the location of the critical point, we establish the latter method as a reliable tool for detecting the localization transition in noninteracting systems. In the context of the spectral form factor, we show that at the critical point it enters a broad time-independent regime, in which its value is consistent with the level compressibility obtained from the level variance. Finally, we test the scaling solution of the average level spacing ratio in the crossover regime using the cost function minimization approach introduced recently in [Phys. Rev. B., 102, 064207 (2020)]. The latter approach seeks for the optimal scaling solution in the vicinity of the crossing point, while at the same time allowing for the drift of the crossing point due to finite-size corrections. We find that the extracted transition point and the scalling coefficient accurately agree with those obtained from the literature.

- [1] J. Šuntajs et. al. Annals of Physics, 168469 (2021)
- [2] J. Šuntajs et. al. Phys. Rev. B 102, 064207 (2020)
- [3] J. Edwards, E. Thouless, J. Phys. C. 5, 807 (1972)

Boundary Chaos

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Spatiotemporal correlation functions provide the key diagnostic tool for studying spatially extended complex quantum many-body systems. In ergodic systems scrambling causes initially local observables to spread uniformly over the whole available Hilbert space and causes exponential suppression of correlation functions with the spatial size of the system. In this talk, we present a perturbed free quantum circuit model, in which ergodicity is induced by a unitary impurity placed on the system's boundary and that allows for demonstrating the underlying mechanism governing the asymptotic scaling of correlations with system size.

This is achieved by mapping dynamical correlation functions of local operators in a system of linear size L at time t to a partition function with complex weights defined on a two-dimensional lattice of smaller size $t/L \times L$ with a helix topology. We evaluate this partition function in terms of suitable transfer matrices. As this drastically reduces the complexity of the computation of correlation functions, we are able to treat system sizes far beyond what is accessible by exact diagonalization. By studying the spectra of transfer matrices numerically and combining our findings with analytical arguments we determine the asymptotic scaling of correlation functions with system size.

For impurities that remain unitary under partial transpose, we demonstrate that correlation functions at times proportional to system size L are generically exponentially suppressed with L. In contrast, for generic unitary impurities correlations show persistent revivals with a period given by the system size.

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

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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 (BiI₃).

First of all, BiI_3 exhibits a clear and isolated absorption resonance in the visible range, detectable also at room temperature. Besides this, the lattice vibration is dominated by an out-of-plane A_g mode. The co-presence of these two degrees of freedom makes BiI_3 an ideal candidate to be used in the investigation of exciton-phonon coupling.

However, how exciton-phonon coupling manifests in the time and energy domains is still an open debate between experiment and theory. Through time-resolved broadband reflectivity, we investigate the ultrafast optical response of Bil₃ single crystal. Our measurements reveal a multi-step electron relaxation dynamic with time constants that range from a few hundreds of femtoseconds up to tens of nanoseconds, superimposed by a periodic intensity modulation ascribed to the generation of coherent optical phonons. Here, we will focus only on the coherent optical response of Bil₃.

Our joint theoretical and experimental effort allows uncovering the relationship between the photoinduced periodic excitonic energy modulation and the generation of coherent optical phonons. Moreover, employing ab-initio DFT calculation coupled with a transient analysis of the experimental results, we were able to extrapolate the photoinduced atomic displacement in the real space from the excitonic energy modulation.

In conclusion, with our work([1]), we set the spectral fingerprints for the optical detection of exciton-phonon coupling in layered semiconductors. Moreover, our findings represent a step forward on the road to coherent manipulation of the excitonic properties on ultrafast timescales.

[1] S. Mor et al. Phys. Rev. Research, accepted

Electronic and lattice properties of Ta2NiSe5- an excitonic insulator candidate

B. Chatterjee

Subgap states in superconducting islands

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The local magnetic moment of an interacting quantum dot can be screened by a Bogoliubov quasiparticle from a nearby superconductor. This gives rise to a long lived discrete spin singlet state inside the superconducting gap, known as the Yu-Shiba-Rusinov (YSR) state.

We study the nature of the subgap states in a quantum dot coupled to one or two superconducting islands. These are described by a number conserving Richardson model of superconductivity, which allows us to account for the charging energy of the superconducting islands. For charging energy comparable to the superconducting gap, the subgap states are stabilized by a combination of Kondo exchange screening and charge redistribution driven by the Coulomb interaction. The model predictions match experimental results very well.

There are two singlet subgap states in the case of a quantum dot embedded between two superconducting channels, corresponding to the formation of a YSR singlet in each channel. The system can be tuned to a regime where the subgap states can be put into a superposition and coherently manipulated by electronic pulses. Such a qubit could be implemented using known technology.

In the doublet spin sector we investigate the overscreened state. Overscreening in normal state systems leads to a fixed point in the renormalization flow with non Fermi liquid properties, while for superconducting islands it emerges as a doublet subgap state with curious spin properties.

- [1] L. Pavešič et al., arXiv:2101.10168
- [2] J. C. Estrada Saldaña et al., arXiv:2101.10794
- [3] L. Pavešič, R. Žitko, arXiv:2110.13881

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Nonequilibrium Quantum Workshop, Krvavec, Slovenia December 12 – 16, 2021

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Nonequilibrium Quantum Workshop, Krvavec, Slovenia December 12 – 16, 2021

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