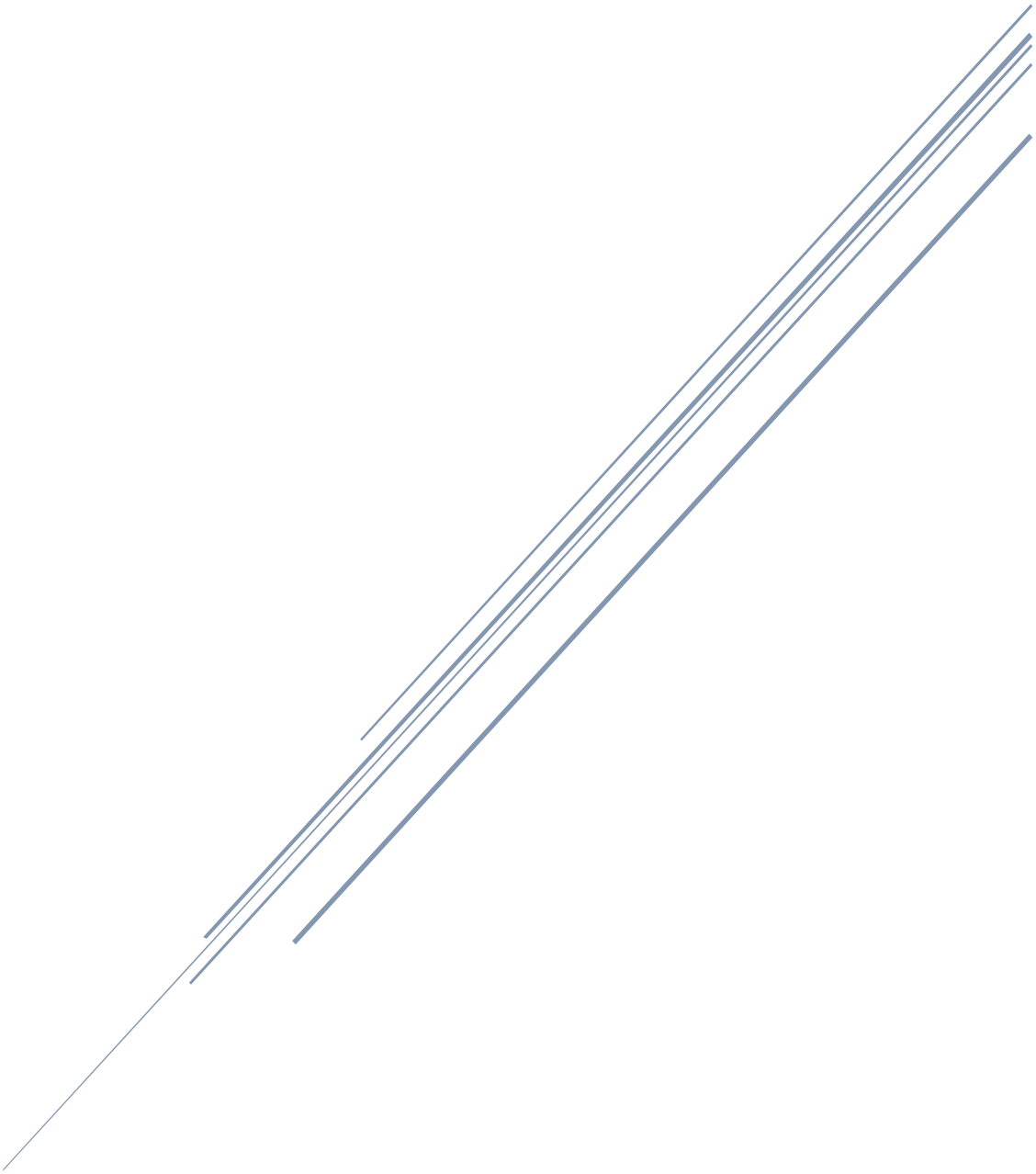
# QUANTUM MANY-BODY SYSTEMS IN AND OUT OF EQUILIBRIUM

## Book of Abstracts



Jožef Stefan Institute, Ljubljana, Slovenia
February 13 – 16, 2023

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Contact e-mail: joze.gasperlin@ijs.si

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*Department of Theoretical Physics, Jožef Stefan Institute, Ljubljana, Slovenia*

Denis Golež
*Department of Theoretical Physics, Jožef Stefan Institute, Ljubljana, Slovenia*
*Faculty of Mathematics and Physics, University of Ljubljana, Ljubljana, Slovenia*

Janez Bonča
*Department of Theoretical Physics, Jožef Stefan Institute, Ljubljana, Slovenia*
*Faculty of Mathematics and Physics, University of Ljubljana, Ljubljana, Slovenia*

| **Tuesday, 14. 2. 2023** | | |
|---|---|---|
| 9:00 - 11:00 | *Open discussions* | |
| 11:00 - 11:30 | Peter Prelovšek | Spin-liquid state in planar Heisenberg models |
| 11:30 - 11:50 | Kazuhiro Seki | Quantum-classical hybrid algorithm for microcanonical ensembles |
| 11:50 - 12:10 | Jure Kokalj | Transport and diffusion in a square lattice Hubbard model |
| 12:10 - 12:30 | Janez Bonča | Optically driven electron-electron attraction in a model with nonlinear electron-phonon interaction |
| 12:30 - 14:00 | *Lunch break* | |
| 14:00 - 14:20 | Seiji Yunoki | Quantum simulation for quantum many-body systems: variational quantum algorithms and beyond |
| 14:20 - 14:40 | Tomonori Shirakawa | Photo-induced eta-pairing states in Kondo lattice |
| 14:40 - 15:00 | Madhumita Sarkar | η-pairing in photodoped mix-D Hubbard model |
| 15:00 - 15:20 | Yuta Murakami | Spin, charge and η-spin separation in one-dimensional photo-doped Mott insulators |
| 15:20 - 18:00 | *Open discussions* | |
| 18:00 - 19:30 | *Dinner* | |

| **Wednesday 15. 2. 2023** | | |
|---|---|---|
| 9:00 - 12:00 | *Open discussions* | |
| 12:00 - 12:30 | Sadamichi Maekawa | Nonreciprocity in spin transport |
| 12:30 - 12:50 | Zala Lenarčič | Spin transport in perturbed integrable systems |
| 12:50 - 13:10 | Kazuya Shinjo | Subcycle pulse-induced nonequilibrium dynamics |
| 13:10 - 13:40 | *Coffee break* | |
| 13:40 - 14:00 | Jernej Mravlje | Spectroscopy of Hund's metals |
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| 14:20 - 17:00 | *Open discussions* | |

# Spin-liquid state in planar Heisenberg models

P. Prelovšek[1]

[1]*Jozef Stefan Institute, Jamova 39, 1000 Ljubljana, Slovenia*

An overview of recent and ongoing studies of frustrated spin systems and related models will be presented. They are motivated partly by experiments, revealing spin liquid state in layered 1T-$TaS_2$ [1], but as well on other materials, well described by the Heisenberg model on frustrated triangular and kagome lattices [2]. Using mostly the numerical FTLM approach based on the exact diagonalization of small clusters, we show that the frustration enables reliable results for thermodynamical and dynamical properties to considerably lower $T$ [3], relative to unfrustrated lattices. The hallmark of the similarity of spin-liquid properties is the generalised Wilson ratio which vanishes at low temperatures, indicating the predominant role of low-lying singlet excitations over the triplet ones [4]. While most studies so far were focused on extended isotropic Heisenberg models, recent experiments indicate that also easy-axis models might be relevant for an alternative but as well challenging spin-liquid physics.

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# Quantum-classical hybrid algorithm for microcanonical ensembles

Kazuhiro Seki[1]

[1]*Quantum Computational Science Research Team, RIKEN Center for Quantum Computing (RQC), Saitama 351-0198, Japan*

We propose a method to calculate finite-temperature properties of many-body systems for a microcanonical ensemble, which may find a potential application of near-term quantum computers [1]. In our formalism, a microcanonical ensemble is specified with a target energy and a width of the energy window, by expressing the density of states as a sum of Gaussians centered at the target energy with its spread associated with the width of the energy window. Using the Fourier representation of the Gaussian, we then show that thermodynamic quantities such as entropy and temperature can be calculated by evaluating the trace of the time-evolution operator, which is thus unitary, and the trace of the time-evolution operator multiplied by the Hamiltonian of the system. We also describe how these traces can be evaluated using random diagonal-unitary circuits suitable for quantum computation. We demonstrate the proposed method by numerically calculating thermodynamic quantities of the one-dimensional spin-1/2 Heisenberg model on small clusters and show that the proposed method is most effective for the target energy around which a larger number of energy eigenstates exist.

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# Transport and diffusion in a square lattice Hubbard model

J. Kokalj, [1,2] M. Ulaga, [1] J. Mravlje, [1] P. Prelovšek[1]

*[1]Jozef Stefan Institute, Jamova 39, 1000 Ljubljana, Slovenia*
*[2]Faculty of Civil and Geodetic Engineering , University of Ljubljana, Jadranska 19, 1000 Ljubljana, Slovenia*

Recent studies of transport in strongly correlated electron systems are using the Nernst-Einstein relation, which relates the conductivity to the static quantity like susceptibility and dynamic quantity, i.e., the diffusion constant. I will present numerical finite-temperature Lanczos model results obtained on the square lattice Hubbard model. Results on charge diffusion [1] will be discussed also in relation to the cold atom experiment [2]. Related experiment on spin diffusion will be discussed and also its discrepancy with numerical model results [3,4]. Further, results on thermal transport and thermal diffusion will be shown [5]. Connection to the Mott-Ioffe-Regel limit and some relations to the experiments on cuprates will be mentioned.

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

J. Bonča,[1,2] D. Golež,[1,2] K. Kovač,[2] and M. Mierzejwski[3]

[1]*Jozef Stefan Institute, Jamova 39, 1000 Ljubljana, Slovenia*
[2]*Faculty of Mathematics and Physics, University of Ljubljana, Jadranska 19, 1000 Ljubljana, Slovenia*
[3]*Department of Theoretical Physics, Faculty of Fundamental Problems of Technology, Wrocław University of Science and Technology, 50-370 Wrocław, Poland*

We investigate a model with two electrons nonlinearly coupled to quantum phonons. We simulate the dynamical response of a system subject to a short spatially uniform optical pulse that couples to dipole-active vibrational modes. 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 two singly-occupied ones [1]. When two electrons are free to propagate on a lattice subject to non-linear coupling to phonons that soften phonon frequency, an external optical pulse with well tuned frequency can induce attraction between electrons. Electrons remain bound long after the optical pulse is switched off. Changing the frequency of the pulse the attractive electron–electron interaction can be switched to repulsive. Two sequential optical pulses with different frequencies can switch between attractive and repulsive interaction [2].

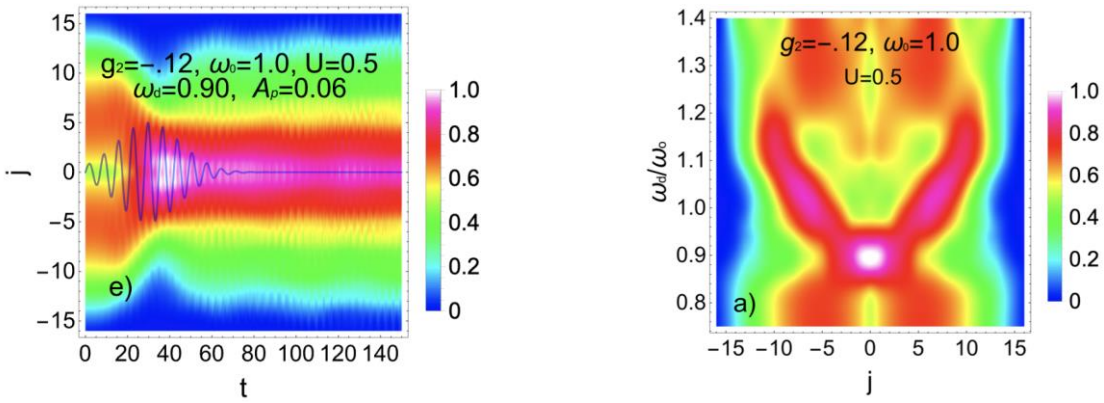


***Figure:*** *Left: the time evolution of a density–density correlation function g(j,t) starting from an unbound state at t=0 subject to an optical pulse. Right: time-averaged g(j) vs. driving frequency* $\omega_d$.

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# Quantum simulation for quantum many-body systems: variational quantum algorithms and beyond

Seiji Yunoki[1]

[1]*RIKEN*

As R. Feynman originally suggested in 1982, quantum many-body systems are the most promising application for quantum computing. Considering noisy near-term quantum devices with a relatively small number of qubits, one of the main focuses in the current quantum simulation research is to identify what one can do with such noisy quantum devices that is not too trivial but still interesting. In this talk, I would like to present some of our recent attempts to simulate quantum many-body systems based on a quantum variational approach and beyond [1-5].

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# Photo-induced eta-pairing states in Kondo lattice

Tomonori Shirakawa[1,2]

[1]*RIKEN Center for Computational Science, Kobe, Hyogo 650-0047, Japan*
[2]*RIKEN Center for Quantum Computing, Wako, Saitama 351-0198, Japan*

We have found that pulse irradiation to the Mott insulating state in the Hubbard model can induce the eta-pairs in the photo-excited states [1], which is a pair density wave with phase pi and is associated with the transverse components of pseudospin 1/2 operators, first introduced by C. N. Yang. We have also shown that the eta pairs are preferentially excited by the optical pulse field because of the selection rule forced by the symmetry of eta-pairing operators.
In this talk, we report that the same mechanism can be applied to another class of models, the Kondo lattice model, known as an effective model to describe electronic states in heavy electron systems [2]. We demonstrate numerically that the pulse irradiation onto the Kondo insulating ground state induces the enhancement of the eta-pairing correlation. The enhancement of the eta-pairing correlation is due to the increase of the number of eta pairs that are selectively generated by the pulse optical field as shown in Figure. We also show that this selection rule of the excitation can be well understood by using the symmetry analysis of the time-dependent perturbation expansion.

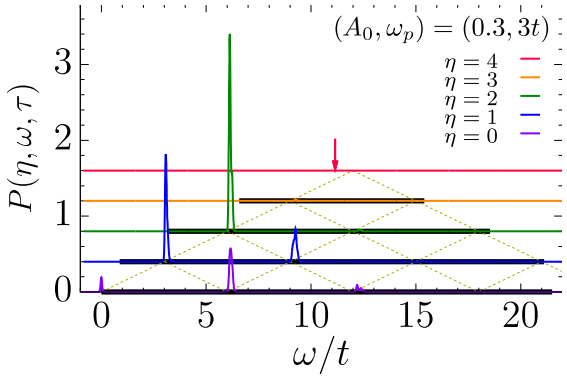


***Figure:*** *Spectral function resolved by the value of eta-pairing, η, in the photoexcited state for half-filled. For visibility, the spectral functions with different values of eta are shifted vertically. Black solid lines indicate the energy region where the eigenstates of Hamiltonian exist for each value of eta-pairing. Red arrows indicate the excitation energy of the vacuum state. Crossing points between dashed lines and black solid lines indicate $\omega=2n\omega_p$ for $\eta$ even and $\omega=(2n+1)\omega_p$ for $\eta$ odd, where n=0,1,2... and $\omega_p$ indicates the frequency of incident light.*

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# η-pairing in photodoped mix-D Hubbard Model

Madhumita Sarkar,[1] Zala Lenarčič,[1] Denis Golez[1,2]

[1]*Jozef Stefan Institute, Jamova 39, 1000 Ljubljana, Slovenia*
[2]*Faculty of Mathematics and Physics, University of Ljubljana, Jadranska 19, 1000 Ljubljana, Slovenia*

Strong excitations of correlated quantum materials give rise to various non-thermal phases which are not present in their equilibrium counterpart. Recently, it was shown that the one-dimensional Fermi Hubbard Model features charge density wave and η-pairing phases upon photo-doping.
Here, we present a study of such non-thermal phases in the mix-D Fermi Hubbard model. Using the Schrieffer-Wolff transformation, we map the mix-D Fermi Hubbard model to a t-J-like model, which gives a simplified and effective equilibrium description of the photo-doped states. An applied electric field allows us to tune the asymmetry in between the intra-chain J, and inter-chain exchange energy $J_1$. Our main finding is that the binding energy of photo-doped charge carriers changes compared to a chemically doped one due to the η-pairing in such a system. We characterize the ground state of this system using appropriate correlators at both the isotropic ( $J = J_1$) and strong anisotropic coupling ( $J >> J_1$) limits. At strong anisotropy, the ground state includes a strongly bound doublon-hole pair along the rung, and inter-chain singlets. Next, we plan to study the effect of a periodic drive on η-pairing.

# Spin, charge and η-spin separation in one-dimensional photo-doped Mott insulators

Y. Murakami[1], S. Takayoshi[2], D. Golež[3], T. Kaneko[4], Z. Sun[5], A. J. Millis[5], A. Läuchli [6], P. Werner [7]

[1]*Center for Emergent Matter Science, RIKEN, Wako, Saitama 351-0198, Japan*
[2]*Department of Physics, Konan University, Kobe 658-8501, Japan*
[3]*Jozef Stefan Institute, Jamova 39, 1000 Ljubljana, Slovenia*
[4]*Department of Physics, Osaka University, Toyonaka, Osaka 560-0043, Japan*
[5]*Department of Physics, Columbia University, New York, New York 10027, USA*
[6]*Laboratory for Theoretical and Computational Physics, Paul Scherrer Institute, 5232 Villigen, Switzerland*
[7]*Department of Physics, University of Fribourg, 1700 Fribourg, Switzerland*

Doping charge carriers into Mott insulators provides a pathway to produce intriguing emergent phenomena. In equilibrium systems, the doping can be chemically controlled. On the other hand, photo-doping, where particles are excited across the Mott gap, provides an alternative way. Compared to chemical-doping, photo-doping creates a wider variety of carriers, which may lead to the emergence of fascinating nonequilibrium states. In particular, when the gap is large, the life-time of photo-carriers becomes exponentially enhanced, which can lead to a metastable states after the intraband cooling of photo-carriers occurs.

In this talk, we reveal the peculiar features of such metastable states realized in the one dimensional extended Hubbard model [1,2]. Namely, we show that the corresponding wave function in the larger on-site interaction limit can be expressed as $|\Psi\rangle = |\Psi_{\mathrm{charge}}\rangle|\Psi_{\mathrm{spin}}\rangle|\Psi_{\eta-\mathrm{spin}}\rangle$, which indicates the separation of spin, charge and η−spin degrees of freedoms. Here η−spin represents the type of the photo-carriers. This state is analogous to the Ogata-Shiba state of the doped Hubbard model in equilibrium. $|\Psi_{\mathrm{charge}}\rangle$ is determined by spinless free fermions, $|\Psi_{\mathrm{spin}}\rangle$ by the isotropic Heisenberg model in the squeezed spin space, and $|\Psi_{\eta-\mathrm{spin}}\rangle$ by the XXZ model in the squeezed η-spin space. In particular, the metastable η-pairing and charge-density-wave (CDW) states correspond to the gapless and gapful states of the XXZ model. The specific form of the wave function allows us to accurately determine correlation functions, and suggests that the central charge of the η-pairing state is 3 and that of the CDW phase is 2. Our results demonstrate that the emergent degrees of freedom activated by photo-doping can lead to peculiar types of quantum liquids absent in equilibrium.

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# Nonreciprocity in spin transport

Sadamichi Maekawa[1]

[1]*RIKEN Center for Emergent Matter Science (CEMS), Wako, 351-0198, Japan*

"Nonreciprocity" means "not going the same way backward as forward". The well-known is the rectification by using PN junctions in electronics where electrons flow in one direction but not the other. The spin Hall effect and its inverse are the interconversion mechanism between electron current and spin current. It has been shown that the interconversion is reciprocal and described by the Onsager reciprocal relation [1]. On the contrary, many of the spin transport phenomena are nonreciprocal. Here, the nonreciprocity in spin transport is discussed together with various examples. The key is that the spin current is a flow of spin angular momentum, in contrast to the electric current. A flow of electrons can have the orbital angular momentum, which is called "vorticity", and may be interconverted with spin current [2]. However, since the vorticity of electron flow is highly nonlinear, the conservation mechanism, i.e., the spin-vorticity coupling, is also nonlinear [1]. As a result, we find a variety of nonreciprocal phenomena in spin transport. The nonreciprocity of surface acoustic waves in magnetic films [3,4], the magnetic skyrmion generation and annihilation by electric current in magnetic films with notch structure [5], and the spin current generation in the graded materials [6] will be discussed.

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# Spin transport in perturbed integrable systems

Z. Lenarčič,[1] S. Nandy,[1] E. Ilievski,[2] M. Mierzejewski[3], J. Herbrych[3], P. Prelovšek[1]

[1]*Jožef Stefan Institute, Jamova 39, 1000 Ljubljana, Slovenia Herbrych*
[2]*University of Ljubljana, Faculty for Mathematics and Physics, Jadranska 19, 1000 Ljubljana, Slovenia*
[3]*Department of Theoretical Physics, Faculty of Fundamental Problems of Technology, Wrocław University of Science and Technology, 50-370 Wrocław, Poland*

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 behaviour even away from exact integrability, for all magnetization sectors.

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# Subcycle pulse-induced nonequilibrium dynamics

Kazuya Shinjo[1]

[1]*Computational Quantum Matter Research Team,*
*RIKEN Center for Emergent Matter Science (CEMS), Wako, Saitama 351-0198, Japan*

The elucidation of nonequilibrium states in strongly correlated systems holds the key to emergence of novel quantum phases. The nonequilibrium-induced insulator-to-metal transition is particularly interesting since it reflects the fundamental nature of competition between itinerancy and localization of the charge degrees of freedom. We investigate pulse-excited insulator-to-metal transition of the half-filled one-dimensional extended Hubbard model [1,2]. Calculating the time-dependent optical conductivity with the time-dependent density-matrix renormalization group, we find that broad mono- and half-cycle pulses inducing quantum tunnelling strongly suppress spectral weights contributing to the Drude weight $\sigma_{\mathrm{D}}$, even if we introduce a large number of carriers $\Delta n_{\mathrm{d}}$ [1]. This is in contrast to a metallic behavior of $\sigma_{\mathrm{D}} \propto \Delta n_{\mathrm{d}}$ induced by photon absorption and chemical doping. The strong suppression of $\sigma_{\mathrm{D}}$ in quantum tunnelling is accompanied by electric polarization breaking inversion symmetry [2], which can lead to glassy dynamics. Also, an ultrashort subcycle pulse can generate exotic nonequilibrium states. We demonstrate that one can generate a steady electric current in a photoexcited state due to an Aharonov-Bohm flux instantaneously introduced through the phase of an electric field [2]. Consequently, time-reversal symmetry is broken. The breaking of inversion and time-reversal symmetries in a photoexcited state can be monitored by second harmonic generation. These findings provide a new methodology for designing the localization and symmetry of electronic states and open up a new field of subcycle-pulse engineering.

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# Spectroscopy of Hund's metals

M. Środa[1], J. Mravlje[2], J. Herbrych[1]

[1]*Wroclaw University of Science and Technology, Poland*
[2]*Jozef Stefan Institute, Jamova 39, 1000 Ljubljana, Slovenia*

Multiplet splittings due to the Hund's rule coupling can cause strong correlations for interaction strengths far below the one for the Mott critical value[1]. The two key aspects of resulting »Hund's metal« behavior are different scales for the screening of spin and orbital moments[2] and large charge fluctuations. I will review the dynamical mean-field theory predictions of spectroscopic signatures in Hund's metals, discuss the inner structure of the quasiparticle peak[3], with side-peaks caused by the spin-orbital separation, the multiplet splittings of the Hubbard bands[4], but especially focus on additional features, that are none of the two and that we dubbed Hund's bands[5], because they vary only with Hund's coupling. I will discuss what these are and highlight their relation to holon-doublon side peaks noted in models for orbital-selective Mott transition[6].

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# Metastable metallic state in Ca2RuO4

D. Golež[1,2], Andy Millis, Anita Verma, Andrej Singer

[1]*Jozef Stefan Institute, Jamova 39, 1000 Ljubljana, Slovenia*
[2]*Faculty of Mathematics and Physics, University of Ljubljana, Jadranska 19 1000 Ljubljana, Slovenia*

Technology moves towards ever faster switching between different electronic and magnetic states of matter. Yet, in many Mott insulators, the electronic transition is accompanied by the nucleation and growth of percolating domains of the changed lattice structure, leading to slow coarsening dynamics. I'll present a comparison between time-resolved X-ray diffraction and reflectivity measurements and numerical analysis based on time-dependent dynamical mean-field theory for photoinduced insulator-to-metal transition in an epitaxially strained Mott insulator $Ca_2RuO_4$. The main result is that above a fluence threshold, the initial electronic excitation drives a fast lattice rearrangement, followed by a slower electronic phase transition into a metastable non-equilibrium state. This work highlights the importance of combined electronic and structural studies to unravel the physics of dynamic transitions and highlights the importance of strain for tuning the timescales of photoinduced processes.