

## 45. EAS - Meeting “Extreme Atomic Systems”

23 – 28 February 2025, Riezlern/Kleinwalsertal

– list of abstracts –

**Mohanad Awad**, Friedrich Schiller University, Jena

### **Few-cycle laser pulse characterization on-target using high-harmonic generation from nano-scale solids**

Pulse characterization techniques based on strong-field physics, such as attosecond streaking and TIPTOE, have proven effective in accurately characterizing the waveform of laser fields. While these techniques are powerful, they often require highly complex setups or high intensities, which can be challenging to achieve with mid-IR laser drivers.

We utilize high harmonic generation for time domain observation of the electric field (HHG-TOE) in thin films of ZnO and monolayers of  $WS_2$ . This method involves perturbing the harmonic yield of the driver with a weak replica. By varying the delay between the two beams, we measure the duration of few-cycle pulses at 3200 nm. Our results show good agreement with established pulse characterization techniques, validating the reliability of this method.

**Baghdasar Baghdasaryan**, Friedrich Schiller University, Jena

### **Feasibility of long-distance multi-photon interference in satellite-based quantum networks**

Quantum interference of multi-photon states is foundational for the realization of a global quantum network. A typical multi-photon interference consists of the interaction of two indistinguishable photons on a beam splitter, where their simultaneous arrival is essential for interference to occur. Temporal indistinguishability can be achieved with time-synchronized pulsed photon sources by controlling photon generation times and propagation distances. However, time synchronization can be challenging in satellite-based communication systems due to continuous satellite motion. A more promising alternative is the use of photon sources with continuous emission, where photons are generated randomly over time. Time-synchronized photon pairs can be post-selected by carefully measuring the respective arrival times. While post-selection eliminates the need for active time synchronization, the finite resolution of detectors limits the precision of time-resolved detection. This study explores whether the realization of a global quantum network is feasible based on sources with continuous emission. We especially examine the impact of limited detector resolution on the efficiency of multi-photon interference with a focus on entanglement swapping. We estimate the maximum achievable entangled photon pair rate by optimizing the performance of the source and analyzing potential losses in a realistic Earth-satellite communication link.

**Loïc Bassement**, Albert Ludwigs University, Freiburg

### **Optimization of a nanoparticle injector for ultrafast imaging experiments**

The intense X-ray pulses from free-electron laser (XFEL) sources open new opportunities for the investigation of single nanoparticles in the gas phase. So far, efficient sample delivery is a bottleneck for conducting experiments with individual nanoscale samples at XFEL facilities. One of the most promising approaches is the generation of an aerosol [1] that is then delivered and focused through an aerodynamic lens stack to the interaction point [2].

We define general requirements, report and compare the performance of an aerosol jet for a commercial instrument and a custom-made design from EuXFEL [1]. The new injector presents better results, a larger flexibility and more sample tunability. A workflow for the aerosol source characterization is established. The transmission of the sample delivery system is assessed through water-based condensation particle counting, the dispersity is estimated via scanning mobility particle sizing, and real-time tuning of the sample delivery system is made possible with a Rayleigh scattering set-up [3].

[1] Rafie-Zinedine, S., Varma Yenupuri, T., Worbs, L., Maia, F. R. N. C., Heymann, M., Schulz, J., & Bielecki, J. (2024). Enhancing electrospray ionization efficiency for particle transmission through an aerodynamic lens stack. *Journal of Synchrotron Radiation*, 31(2).  
<https://doi.org/10.1107/s1600577524000158>

[2] Roth, N., Awel, S., Horke, D. A., & Küpper, J. (2018). Optimizing aerodynamic lenses for single-particle imaging. *Journal of Aerosol Science*, 124, 17–29.

<https://doi.org/10.1016/j.jaerosci.2018.06.010>

[3] Hantke, M. F., Bielecki, J., Kulyk, O., Westphal, D., Larsson, D. S. D., Svenda, M., Reddy, H. K. N., Kirian, R. A., Andreasson, J., Hajdu, J., & Maia, F. R. N. C. (2018). Rayleigh-scattering microscopy for tracking and sizing nanoparticles in focused aerosol beams. *IUCrJ*, 5, 673–680.

<https://doi.org/10.1107/S2052252518010837>

**Buca Berislav**, Niels Bohr International Academy, Copenhagen

### **Eternal equilibrium**

This talk is based on a previous proof that quantum many-body systems, rather than merely reaching a Gibbs ensemble in the long-time limit, are, following a quench, always in a time-dependent Gibbs ensemble with chemical potentials that can decay in time. The corresponding conservation laws are called "transient dynamical symmetries"

In this talk I will show how to use Krylov subspace methods to identify these "transient dynamical symmetries". Moreover, I will provide analytical results for these based on the universal operator growth hypothesis and a careful truncation of the Krylov space - chaotic systems have only a finite number of different complex frequencies giving the corresponding decay rates of the chemical potential of the transient dynamical symmetries. The transient dynamical symmetries can likewise be identified in the generic chaotic, integrable and free cases.

This approach of eternal equilibrium can give universal analytical result for dynamics of local observables far from equilibrium and efficient numerical calculations in concrete example systems.

References: N. Loizeau, B. Buca, D. Sels. In preparation.

B. Buca. *Phys. Rev. X* 13, 031013 (2023)

D. E. Parker, X. Cao, A. Avdoshkin, T. Scaffidi, E. Altman. *Phys. Rev. X* 9, 041017 (2019)

**Andreas Buchleitner**, Albert Ludwigs University, Freiburg

**tbd**

tbd

**Ronald Cárdenas**, MPI for the Physics of Complex Systems, Dresden

**Machine learning for transient spectroscopy**

Transient spectroscopy captures ultrafast changes in molecular systems, generating complex datasets that can be challenging to analyze using traditional methods. The use of machine learning techniques can ease the treatment of this data and allowing to get insights on the nature of the studied system. It can help to identify key spectral patterns and correlate them with physical processes, such as electronic transitions or molecular dynamics. It can also allow to infer reaction mechanisms, dynamics, or photophysical properties from experimental data while at the same time reduce the computational cost associated to the simulation of these features. The use of ML in transient spectroscopy allows to obtain faster, more accurate insights into molecular dynamics and energy transfer processes.

**José R. Crespo López-Urritia** , MPI for Nuclear Physics, Heidelberg

**Highly charged ions in the lab**

The talk will present an overview of the activities on spectroscopy and frequency metrology in the Heidelberg EBIT laboratory at MPIK.

**Tim Ehret**, Albert Ludwigs University, Freiburg

**Dipole-dipole interactions of strongly driven two-level atoms**

We formulate a Floquet-Markov master equation for two spatially separated atoms driven by an intense electromagnetic field and coupled to a common bath. This equation features a modified form of dipolar interactions as compared to the case of weakly driven atoms, giving rise to new shifts in the Floquet quasienergy spectrum of the system. We provide a detailed physical interpretation of the modified dipole-dipole interactions, discuss their manifestations in two-atom resonance fluorescence, and extract the distance-dependence of the dipole force between the atoms.

**Jiahao Fan**, City University, Hongkong

**Quantum light enabled ultrafast spectroscopy**

Classical light such as laser and thermal radiation has long been utilized for spectroscopy to explore material structures and dynamics. However, quantum states of light open new avenues for ultrafast optics and spectroscopy, by the variation of their unique properties, e.g., entanglement and photons statistics, after interacting with materials. Quantum light possesses unique characteristics that distinguish it from classical light, particularly the phase-space distribution which reflects its fundamental quantum statistics that may take advantage of noise-reduction. We focus on spectroscopic applications using entangled photons and squeezed light. A microscopic theory for the spectroscopy and corresponding signals induced by certain transition processes is developed. The stimulated Raman spectra (SRS) are investigated. We further extend our efforts to the transient absorption process that enables real-time monitoring of the exciton transport in the transition metal dichalcogenides (TMDs), namely, using the WS<sub>2</sub> monolayer. This series of works on nonlinear optical spectroscopy using quantum light explicitly demonstrates the quantum supremacy in ultrafast spectroscopy by jointly enhancing the time and energy scales beyond the classical bound.

**Peter Förderer**, Albert Ludwigs University, Freiburg  
**Testing Born's rule via photoionization of helium**

The ever-increasing stability and controllability of available light sources promise the synergy of attosecond physics and quantum information science. Here, we propose how state-of-the-art photoionization experiments can be used to test Born's rule - a postulate of quantum mechanics - via the so-called Sorkin test. In particular, we show how to realize a three-path interferometer, required to perform the Sorkin test, in the photoionization of helium via a combination of an ultrashort extreme ultraviolet pulse and a trichromatic infrared pulse. A simulation of the Sorkin test under consideration of typical experimental noise and data acquisition efficiencies infers an achievable measurement precision in the range of the best Sorkin tests to date.

**Stefan Fritzsche**, Helmholtz Institute Jena  
**Uncommon atomic excitation and decay pathways**

Aside of the well-known photo- and auto-ionization of atoms and ions, there are several less common "atomic processes" which determine the measurements and observations in

**Miriam Gerharz**, MPI for Nuclear Physics, Heidelberg  
**Quantum dynamics of nuclear many-body systems driven by an XFEL**

Mössbauer nuclei are an extreme platform for quantum optics because of their narrow transitions in the x-ray regime. These narrow transitions feature long lifetimes, but on the other hand also allowed to only study single excitations for decades. This has recently changed with first experiments at X-ray free electron lasers, where now multiple photon excitations and the subsequent dynamics can be studied.

This technological progress immediately raises the question whether there are new effects expected depending on the number of resonant photons. In this project we theoretically explore quantum dynamics of nuclear many-body systems after multiple photon excitations.

**Lukas Germeroth**, University of Kassel  
**Photon-recoil imaging: X-ray Raman spectroscopy of molecules**

L. Germeroth (1), M. Agåker (2), T. Baumann (3), R. Boll (3), A. De Fanis (3), S. Eisebitt (4), M. Génévriez (5), V. Kimberg (6), H. Lee (1), E. Marin-Bujedo (5), T. Mazza (3), M. Meyer (3), Y. Ovcharenko (3), S. Patchkovskii (4), D. Reiser (3), J.-E. Rubensson (2), J. Söderström (2), P. Schmidt (3), B. Senfftleben (3), A. Senfftleben (1), S. Usenko (3), J. Mikosch (1) and U. Eichmann (4) — (1) Universität Kassel — (2) Uppsala University — (3) XFEL Hamburg — (4) MBI Berlin — (5) UCLouvain — (6) KTH Stockholm

Non-linear Raman spectroscopy was originally developed for narrowband lasers. It has since become important in the spectroscopy and microscopy of technological and biological processes. Stimulated Raman scattering with optical femtosecond lasers is routinely used to excite coherent vibrational and rotational wavepackets. The advance of ultrabright FELs enabled the extension of non-linear physics to the X-ray domain. Some of us have recently established photon-recoil imaging as a background-free technique to detect stimulated X-ray Raman scattering (SXRS) [1]. This process is similar to STIRAP, a form of state-to-state coherent control well known in the optical domain. Here we extend the pioneering experiments on Neon atoms to molecules. Near and far-off resonance SXRS in CO molecules populates efficiently an electronically excited long-lived metastable final state. Demonstration of far-off resonance SXRS in molecules opens new possibilities to study site-selective non-linear processes avoiding spontaneous decays.

[1] Eichmann et al., Science 369, 1630 (2020)

**Andre Giraldi**, MPI for Nuclear Physics, Heidelberg

**Towards experimental studies of interatomic Coulombic electron capture (ICEC)**

This work targets the experimental detection of an environment assisted atomic decay mechanism, referred to in literature as “excitation transfer ionization”. The process constitutes the resonant excitation of a neon atom in a cluster by electron impact to a  $2p^5 3s$  or  $2p^5 3p$  state (excitation energy on the range of 16 – 19 eV), and subsequent deexcitation by ionizing a neighboring Ar atom (ionization potential of 15.8 eV). This reaction has been evidenced by laser-induced excitation of neon, but remains to be detected by means of an electron beam as the excitation mechanism. The confirmation of such process could provide insight into the role of the atomic environment on energy transfer and help gather information about ICD- and ICEC-like reactions. Presently we are adapting an electron and ion momentum spectrometer (reaction microscope) and are optimizing the formation of neon-argon dimers or bigger mixed clusters which requires the determination of the optimal conditions (nozzle temperature, gas pressure and mixing ratio). First results will be presented.

**Frank Großmann**, TU Dresden

**Quantum enhancement of thermalization**

Relaxation to equilibrium in Bose-Hubbard rings is numerically investigated in the time domain. We show that for small mean site-populations in the Mott insulator regime, characterized by strong onsite interaction as compared to hopping, equipartition starting from nonequilibrium initial states is significantly faster in these bosonic quantum many-body systems than in their classical counterparts, described by discrete Gross-Pitaevskii lattices. We attribute this phenomenon of thermalization enhancement to a genuine quantum transport mechanism akin to tunneling, allowing for pathways that are more efficient than chaotic diffusion across the ergodic domain of the classical systems.

**Sebastian Hell**, Institute for Optics and Quantum Electronics, Jena

**Two-photon double ionization of argon - powered by our new table-top high-flux XUV source**

Electron correlations in atoms, molecules and solids are a fundamental aspect of quantum physics and have been a subject of interest for decades. The advent of intense and ultrafast XUV sources, such as free-electron lasers (FELs) and high-field harmonic generation (HHG) in gases, has now made it possible to study electron correlations on the attosecond timescale. Utilizing our advanced high-flux HHG source, driven by 515 nm laser pulses at a repetition rate of 100 kHz, we have measured ions and electrons from the two-photon double ionization (TPDI) of Argon in coincidence. The electron energy and ion momentum spectra, supported by calculated ionization and excitation cross-sections, reveal comparable contributions of sequential, non-sequential, and auto-ionization pathways to TPDI in our experiment.

**Markus Ilchen**, University of Hamburg

### **Exploring chiral dynamics with x-ray lasers**

Polarization-controlled FELs provide unique access to nonlinear and time-resolving investigations of transient and otherwise inaccessible states of matter. They have demonstrated rich potential for magnetization studies at a variety of facilities, but also open new avenues for gas-phase science. The emerging field of site-specific investigations of dynamics in (transient) chiral matter, i.e., matter that possesses a handedness, is an important example in this regard. Chirality has a profound relevance for a multitude of reasons. In fact, it influences our all-day-life and is discussed to shape the fabric of our existence to a great extent. Gas-phase studies of chiral molecules at FELs can unprecedentedly add new perspectives on their (re-)formation dynamics, their ultrafast response to light of different energies in general, their ionization dynamics and ionic functionality, and the relevance of a stereocenter-site for an effective choice of methodology.

The rapid evolution of technological advances at (X)FELs has leveraged the accessibility of this new topic, among others, by enabling narrow-bandwidth operation via seeding, multi-color schemes for FEL-pump FEL-probe methodology, isolated attosecond pulses, high repetition rates, and finally, undulator-based polarization control. Only by combining these technological capabilities, we will ultimately enable a new depth of observing and steering ultrafast dynamics in chiral systems. However, already the metrology of such complex pulse properties, in particular at SASE-FELs, remains a challenge for itself, yet being a prerequisite for this young field of science.

I will present the initial milestones of chirality science at FELs in the gas phase, the status of advanced metrology schemes for variably polarized, high-power (X)FEL pulses at the attosecond frontier, latest results from our angular-streaking campaign at the European XFEL, and the advent of related scientific prospects that are about to emerge at a variety of facilities worldwide. Exemplarily, the FLASH 2020+ agenda and the underlying exploitation strategy at DESY for this new field of interest will be sketched and discussed.

**Victor Kimberg**, KTH Royal Institute of Technology, Stockholm

### **Studying potentials and nuclear dynamics using dispersion relations in resonant x-ray scattering**

Resonant x-ray scattering made a sufficient contribution to understanding of femtosecond nuclear dynamics. It stands out for a distinctive capability to probe the ultrafast dynamics through the scattering duration control, enabled by energy detuning from x-ray absorption resonances and observed via variation in spectral dispersion relations. In this presentation I will discuss how intricate dynamic within the short-lived core-excited states is unveiled in resonant Auger spectroscopy (RAS) at S K-edge of the SF6 [1]. This example showcases diverse dispersion laws among spectral lines, capturing ultrafast nuclear dynamics in  $S1s^{-1}6t_{1u}^1$  core-excited state with the conspicuous absence of dynamics in  $S1s^{-1}7t_{1u}^1$  state of same character. The 2D spectral map emerges as a versatile tool for studying changes in molecular geometry upon decay. Employing a theoretical model, we demonstrate how the characteristics of the spectral dispersion laws (Raman, non-Raman, anti-Raman) mirror the relative gradients of intermediate and final states in RAS. A remarkably simple analytical expression, that captures correlation between gradients ratio and dispersion relations makes this approach a potent method for mapping molecular potentials.

[1] V. Kimberg et al., Phys Rev A, accepted (2024)

**Kateryna Korshynska**, TU & PTB, Braunschweig

**Finite temperature Josephson oscillations of an cold atom BEC in a double well**

Modern cooling and trapping techniques allow for a precise manipulation of cold boson gases that can be used in technology and fundamental physics. For instance, advances in the field of quantum sensors benefit from both theoretical and experimental investigation of interference phenomena in Bose gases. A typical way to study such phenomena is to place the gas in a double-well potential. There the population of the wells exhibits Josephson oscillations. In the fully coherent regime, when ultra-cold temperatures are achieved, the description of these oscillations is well established. However, it is hard to experimentally realize this ideal case. In this talk we discuss the experimentally more feasible case of cold but not ultra-cold gases where, in turn, various approximations have to be made on the theory side. Solving this problem in the non-interacting limit we show that the oscillations are largely affected by the temperature-dependent degree of coherence of the system. Moreover, we use the density matrix approach to include weak collisional interactions and explain thermalization and decoherence in the Josephson dynamics.

**Dr. Matthias Kübel**, Friedrich-Schiller-University, Jena

**Recoil momentum for dissociative strong-field ionization of molecules**

In photoionization of atoms, the remaining ion acquires a recoil momentum of equal magnitude but opposite sign as the emitted photoelectron. This fact holds for strong-field ionization. However, we can also adopt the common view of strong-field ionization as a two-step process, consisting of tunnelling and subsequent acceleration in the laser field. Because of their opposite charges, electron and ion are accelerated to the same final momentum with opposite sign. The situation is more interesting for a dissociating molecule: Once the molecular bond breaks, the mass of the charged ion changes, which should affect the sharing of the photoelectron momentum between charged and neutral fragments. In my talk, I will present measurements of strong-field dissociative ionization of hydrogen using a streaking technique. The experimental results will be discussed in the context of momentum sharing.

**Chunhai Lyu**, MPI for Nuclear Physics, Heidelberg

**Highly charged ions for next-generation clock applications**

As highly charged ions are less sensitive to external perturbations, they are attractive for the development of ultrastable atomic clocks. In this contribution, I will present our recent discovery of a new family of HCI clock candidates, covering 2/3 of the elements from the periodic table. Theoretical calculations show that the performance of these clock candidates could surpass state-of-the-art clocks by several orders of magnitude, rendering it possible to construct next-generation atomic clocks with a fractional accuracy  $\delta\nu/\nu < 10^{-20}$ . We expect that our findings will significantly enrich the applications of high-precision spectroscopies in searching for new physics beyond the standard model.

**Eloisa Manetti**, Paul Scherrer Institute, Switzerland

### **Highly charged ions for next-generation clock applications**

The formation of  $H_2^+$  and  $H_3^+$  has been observed for various organic molecules, such as ethanol and methanol, following double ionization by intense femtosecond laser pulses. However, the mechanisms underlying their formation are still actively studied. They are the result of proton transfer and roaming reactions (Ref 1).

We have investigated the formation time of  $H_2^+$  and  $H_3^+$  ions following double ionization of gas-phase ethanol molecules. The ethanol molecules were core ionized with soft X-ray pulses tuned above the oxygen K-edge and probed by fs NIR pulses. We detected the ion yield of  $H_2^+$  and  $H_3^+$  as a function of the X-ray – NIR pump-probe delay using an ion time-of-flight spectrometer at the Maloja endstation at SwissFEL.

Once an ethanol dication is embedded in an environment of other ethanol molecules, new intermolecular relaxation processes, such as H migration, open up (Ref.2). We have observed H migration to be a dominating relaxation process in doubly ionized ethanol clusters using the same experimental scheme as described above.

Ref 1: Ekanayake, N., Severt, T., Nairat, M. et al. H<sub>2</sub> roaming chemistry and the formation of H<sub>3</sub><sup>+</sup> from organic molecules in strong laser fields. Nat Commun 9, 5186 (2018). <https://doi.org/10.1038/s41467-018-07577-0>

Ref 2: Y. Tamenori, K. Okada, K. Tabayashi, A. Hiraya, T. Gejo, K. Honma. Formation of H<sub>3</sub>O<sup>+</sup> by the soft X-ray ionization of ethanol clusters. Chemical Physics Letters, Volume 433 (2006). <https://doi.org/10.1016/j.cplett.2006.11.038>

**Christian Medina**, MPI for Nuclear Physics, Heidelberg

### **Inter- and intramolecular proton transfer in ethanol molecules and clusters**

In this study, we present the preliminar momentum reconstruction for ion-neutral collisions involving molecular oxygen, using the TrapRemi apparatus. The Trap-REMI integrates an electrostatic ion beam trap (EBIT) where molecular oxygen beam at 2 keV is trapped and intersected with a molecular oxygen gas jet. The resultant recoil ions and neutral remnants are detected in coincidence by the reaction microscope (REMI), which is aligned longitudinally along the trap. Ion-neutral coincidence measurements enable the reconstruction of momentum from the collisions, and the calculation of Q factors.

**Wilko Middents**, Hemholtz Institute Jena

### **Polarization effects in the Compton scattering from atomically bound electrons**

Precise studies of the linear polarization for Compton scattered photons open the unique opportunity for a detailed test of the impulse approximation for energetic photon matter interaction. Compton scattering is the inelastic scattering of a photon from an electron, in which the scattered photon carries a lower energy than the incident photon. The energy of the scattered photon depends on the scattering angle. For scattering from bound electrons, the resulting Compton scattering peak is broadened due to the momentum distribution of the electrons leading to a Doppler shift of the incident and scattered photons. Additionally, we expect the electron momentum distribution to influence the scattered photon polarization such, that the linear polarization will vary across the Compton peak.

In an experiment performed at the synchrotron facility PETRA III at DESY in Hamburg, the highly linearly polarized synchrotron beam with a photon energy of 175 keV was scattered from a gold target. Using a state-of-the-art Compton polarimeter, the scattered radiation was analyzed under several scattering angles with a special interest to the linear polarization of the scattered radiation. Additionally, we developed a Monte-Carlo simulation of the Compton scattering from bound electrons based in the framework of the impulse approximation. From this simulation, we can determine the double-differential scattering cross-section as well as the linear polarization of the Compton scattered radiation for incident photon beams with an arbitrary linear polarization.

In my presentation, I will present both details of the experiment and the developed simulation and show the experimental results compared to the expected values provided by the simulation.



**Natalia S. Oreshkina**, MPI for Nuclear Physics, Heidelberg

### **QED corrections in unstable vacuum**

Self-energy and vacuum polarization effects in quantum electrodynamics (QED) are calculated for the supercritical Coulomb field, where Dirac energy levels become embedded in the negative energy continuum. In this regime, the quantum vacuum becomes unstable, resulting in spontaneous electron-positron pair creation. By calculating the imaginary part of the QED correction, we gain access to an unexplored channel of vacuum instability: radiative spontaneous pair creation. Our results show that this radiative channel is greatly enhanced in the vicinity of the threshold of the supercritical regime, providing evidence for nonperturbative effects with respect to the fine-structure constant  $\alpha$ . We therefore conjecture that the total probability of spontaneous pair creation could differ significantly from the predictions of Dirac theory, especially near the supercritical threshold.

**Tobias Over**, Hemholtz Institute Jena

### **A novel Compton telescope for polarimetry in the MeV range**

For photon energies from several tens of keV up to a few MeV, Compton polarimetry is an indispensable tool to gain insight into subtle details of fundamental radiative processes in atomic physics. Within the SPARC collaboration [1] several segmented semiconductor detectors have been developed that are well suited for application as efficient Compton polarimeters. For photon emission processes in the hard x-ray regime these kind of detectors enable revealing photon polarization effects in great detail [2]. In our presentation, a novel Compton telescope detector that will enable us to extend to photon energies up to the MeV range will be presented. In particular, we will discuss new experimental possibilities in the higher energy range.

[1] Th. Stöhlker et al. Nucl. Instrum. Methods Phys. Res. B 365 (2015) 680.

[2] K.H. Blumenhagen et al. New J. Phys. 18 (2016) 119601.

**Adisorn Panasawatwong**, MPI for the Physics of Complex Systems, Dresden

### **Complexity: chaos, regular, and complex**

We are developing a machine learning-based approach to quantify meaningful information from noisy physical observables. Distinguishing signal from noise in chaotic systems is a significant challenge. Our primary goal is to introduce a novel method for quantifying the inherent complexity of these signals, similar to resolution functions used in standard data analysis. A key aspect of our approach is to assign zero complexity to systems that exhibit either extreme regularity or extreme chaos. We designed a machine learning network specifically tailored to uncover hidden patterns within these noisy observables. This approach aims to enhance our ability to evaluate critical information from a wide range of applications, from classical noise to the complex quantum systems that produce noisy, intricate data sets.

**Luca Peisert**, Albert Ludwigs University, Freiburg

### **Entangled photon absorption efficiency in three-level systems**

Entangled photon absorption promises high absorption efficiency while maintaining the low photon flux density required for photosensitive systems. We investigate the effects of spectral entanglement on two-photon absorption in three-level systems and compare it with experimentally realizable photon distributions. Using Schmidt decomposition, we approximate the ideal entangled case with classical bichromatic pulses. Various three-level systems are evaluated for their potential yield and feasibility.

**Thomas Pfeifer**, MPI for Nuclear Physics, Heidelberg  
**Strong-field ionization physics in a laser cavity**

Confining, storing, and amplifying light inside a cavity has enabled major breakthroughs in fundamental research and technology, with quantum optics and the laser as prominent examples. This talk will highlight our experimental development of cavity optics towards strong-field light-matter interaction. The intra-cavity operation of a velocity-imaging spectrometer allows to observe spectra and angular distributions of electrons emitted in ultrashort pulsed standing waves. Asymmetric structures are observed, indicative of Kapitza-Dirac-like interactions of quasi-free electrons with intensity gradients in the cavity focus, controlled in space by timing the counter-propagating cavity-circulating laser pulses.

**Siddhartha Poddar**, MPI for the Physics of Complex Systems, Dresden  
**Reconstruction of three-dimensional molecular electronic density from coherent diffraction images using machine learning**

As the three-dimensional (3D) electron density profile recovery technique for a single macro-molecule from an ensemble of its 2D coherent diffraction images, generated using an X-ray free-electron laser (XFEL), I have applied an unsupervised machine learning algorithm namely Generative Adversarial Network (GAN). In this optimization procedure a constantly modifying three-dimensional structure is used to create diffraction images which have similar distribution to the given set of diffraction images. As the training procedure converges this structure followed by a 3D Phase Retrieval step should develop into an equivalent version of the target electronic density profile of the molecule under consideration.

**Jan Richter**, PTB, Braunschweig  
**King plot nonlinearity in calcium**

Precise isotope shift measurements serve as a powerful tool to investigate nuclear effects and to probe potential beyond-Standard-Model (BSM) interactions between electrons and neutrons. By combining recent isotope shift measurements of the  $^3P_0 \rightarrow ^3P_1$  transition in  $\text{Ca}^{14+}$  and the  $^2S_{1/2} \rightarrow ^2D_{5/2}$  transition in  $\text{Ca}^+$ , as well as precise nuclear mass measurements, a significant King plot nonlinearity with a  $900\sigma$  significance has been revealed. In this work, we analyze these experimental results to identify the dominant SM contributions, namely the second order mass shift and nuclear polarization. Furthermore, we use the data to constrain hypothetical BSM interactions, establishing the most stringent King plot-based bounds to date on a new scalar boson coupling to electrons and neutrons.

**Homar Rivera Rodríguez**, MPI for the Physics of Complex Systems, Dresden  
**Rydberg atoms in short-wavelength optical lattices**

In this work, we study a Rydberg atom subjected to the ponderomotive trapping potential of a short-wavelength optical lattice. Inspired by the *Rydberg composite*, where the Rydberg atom is immersed in a dense arrangement of atoms, we conceptualize the optical lattice light itself as a set of 1D *perturbers* located at the intensity maxima of the standing wave created by two counterpropagating lasers. The short-wavelength requirement ensures that there are multiple lattice periods and thus many perturbers within the extent of the Rydberg electron wave function. We analyze how the properties of this system depend on the interplay between the Rydberg excitation and the structure of the light, in particular the general scaling of energy shifts and electronic states.

**Nina Rohringer**, DESY-CFEL, Hamburg

**Perspective of nonlinear x-ray spectroscopy at FELs**

In this contribution I will give a critical review and personal outlook on the possibility of nonlinear x-ray spectroscopy at x-ray free-electron laser sources. Already a decade before the first light at the first operating short-wavelength free-electron laser FLASH, many different ideas of coherent nonlinear x-ray spectroscopy have been proposed (Shaul Mukamel and collaborators) that are based on the process of impulsive stimulated x-ray Raman scattering. These x-ray spectroscopies are analogues of multi-dimensional coherent femtosecond spectroscopy, where the key building block of impulsive vibrational Raman scattering is substituted with inelastic resonant x-ray Raman scattering stimulated by broad-band x-ray pulses), thereby getting access to measuring electronic coherences following a pump stimulus. I will give an overview of experimental achievements in this area and discuss the challenges ahead. A particular focus will be drawn to potential opportunities with new developments of COLTRIM reaction microscopes: I will discuss my personal ideas of nonlinear coherent x-ray photoelectron and resonant Auger spectroscopy and hope to spark a vivid discussion on a future evolution of this field.

**Prof. Jan-Michael Rost**, MPI for the Physics of Complex Systems, Dresden

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**Prof. Ulf Saalmann**, MPI for the Physics of Complex Systems, Dresden

**Zero-energy photoelectric effect**

We predict a near-threshold (“zero energy”) peak in multi-photon ionization for a dynamical regime where the photon frequency is large compared to the binding energy of the electron. The effect originates from the fact that bound-continuum dipole transitions are stronger than continuum-continuum ones.

**Riaan Philipp Schmidt**, PTB, Braunschweig

**Probing the isolated rotating magnetic field of structured light by atoms**

For more than 30 years, structured light has been one of the trends in optics, photonics, and related studies of light-matter interaction. In contrast to conventional plane waves, structured beams exhibit spatially dependent amplitude, phase, and polarization. Within this class of wave solutions, the azimuthally polarized beam is distinguished due to the zero electric and non-zero magnetic fields in its center. In the case of a single beam, this “isolated” magnetic field is oriented along the beam axis. On the other hand, the use of two azimuthally polarized beams makes it possible to generate a rotating magnetic field, while keeping the electric field still zero [1]. This configuration opens up new opportunities for studies of laser-induced ultrafast magnetization dynamics in solid matter, where suppression of electric field effects is important [2]. In the present contribution we explore the interaction of a single atom with different superpositions of azimuthally polarized beams. We perform calculations in the framework of the density matrix theory. For illustration purposes, we apply our general approach to the  $3s3p^3P_1-3s3p^1P_1$  transition in neutral Mg. Based on the results of our calculations, we show how the interaction of matter with the magnetic field of two azimuthally polarized beams can be enhanced. It is also demonstrated that observation of atomic population dynamics can be used as a sensor for the relative orientation and phase of the light field components.

[1] Sergio Martín-Domene et al., Appl. Phys. Lett. 124, 211101 (2024)

[2] Luis Sánchez-Tejerina et al., High Power Laser Science and Engineering, (2023), Vol. 11, e82, 8

**Julius Schwarz**, University of Hamburg

**Double core-hole spectroscopy on transition metal complexes**

Resonant double core-hole (DCH) spectroscopy allows for the observation of ultrafast dynamic processes in small  $3d$ -metal compounds in the gas phase with enhanced sensitivity. Using the intense X-Ray pulses of the European XFEL, electron and ion spectroscopy was used to reveal the signature of iron  $2p^2$  resonant DCH excitation in iron pentacarbonyl and ferrocene. Comparing the experimental results to theoretical calculations reconstructs single core-hole (SCH) and DCH photon-matter interactions in the two targets. The DCH Auger-Meitner electron signals offer insight to the electron dynamics during the core hole lifetime and their dependence on the chemical environment. The product ions show evidence for DCH processes in multiply charged iron cations.

**Armin Scrinzi**, LMU, Munich

**As good as it gets: photoabsorption and ionization of molecules**

On the example of recent results for accurate photoabsorption and photoelectron emission spectra I will discuss current techniques for molecules in strong and/or ultrafast fields. These methods fuse time-proven quantum chemistry with single- and multi-electron dynamics in strong fields. A few of the specific mathematical methods and computational advances that have pushed the limits for accurate ab-initio results to few-atomic molecules will be highlighted.

**Juliette Simonet**, University of Hamburg

**Ultrashort laser pulses: a new toolbox for ultracold quantum gases**

Ultrashort laser pulses provide new pathways to manipulate and probe ultracold quantum gases on femtosecond timescales. The strong light field of such pulses can photoionize a controlled number of atoms and enables the creation of hybrid quantum systems consisting of ultracold atoms and ions. In addition, the large bandwidth of the femtosecond laser pulse allows for ultrafast excitation of Rydberg states below the blockade radius in a dense quantum gas. We have developed a novel detection unit for charged particles consisting of a high-resolution ion microscope for tracing the position of ions with a high spatial resolution and a velocity map imaging electron spectrometer for measuring the momentum of the electrons. Coincidence detection of both species allows following the dynamics of interacting systems of charged particles as well as hybrid atom ion quantum systems. This work is funded by the Cluster of Excellence “CUI: Advanced Imaging of Matter” of the Deutsche Forschungsgemeinschaft (DFG) - EXC 2056 - project ID 390715994.

**Jonas Sommerfeldt**, Kastler Brossel Laboratory, Paris

**Lamb shift in antiprotonic atoms**

We present a theoretical study of the Lamb shift in antiprotonic atoms, i.e. atoms in which one electron in the atomic shell has been replaced by an antiproton. In these systems, QED effects are significantly increased as the antiproton experiences much stronger fields due to its smaller orbit. This fact will be used by the PAX experiment at CERN to make an almost isolated measurement of the Lamb shift between Rydberg states that is essentially unaffected by nuclear properties. We present accurate calculations of the QED effects in antiprotonic atoms that will be used with these upcoming measurements to perform tests of higher-order QED effects. A special emphasis is placed on the influence of the vacuum polarization as it is significantly increased compared to the self-energy in these systems.

**Julian Späthe**, Friedrich Schiller University, Jena

**Laser-driven high-flux source of coherent XUV radiation for coincidence spectroscopy – Part 2**

We have built a high flux XUV source driven by a 515 nm laser based on a gas nozzle scheme. In order to effectively monochromatize the generated high-harmonic light, we spectrally filter the 11th harmonic (26.4 eV) and focus it into a COLTRIMS setup, where we perform coincidence measurements. The XUV pulses can be overlapped with intense laser pulses to realize pump-probe experiments. In my talk I will focus on the technical realization and performance tuning of the XUV source. I will present several parameter scans and relate them to the theory of phase matching via numerical simulations. Among these, the position of the plasma relative to the focus has proved to be the most interesting. From the parameter scans we developed an operating scheme to obtain the maximum XUV flux, which allows us to measure the two-photon double ionization of argon (see talk by Sebastian Hell).

**Carolyn Stier**, Albert Ludwigs University, Freiburg

**Spectral structure and dynamics of partially distinguishable fermions on a lattice**

We study the fermionic many-body quantum dynamics generated by a Hubbard-like Hamiltonian with nearest neighbour interaction and a continuously tunable level of distinguishability of the particles. For not strictly indistinguishable fermions, distinct invariant symmetry sectors of the many-body Hilbert space are populated, with tangible impact on the many-body dynamics. We identify the regime of tunneling and interaction strengths where the many-body eigenstates acquire ergodic structure, and investigate how the interplay between dynamical instability and partial distinguishability affects the evolution of the many-body counting statistics.

**Sophia Strnat**, PTB, Braunschweig

**Vortex electron scattering by atomic targets**

Since their theoretical prediction in 2007 [1] and their first experimental realization in 2010 [2], vortex electron beams have been the focus of research in many areas of modern physics. In particular, vortex electrons have been found to be a powerful tool in electron microscopy, where they help to probe local properties of nanomaterials and biomolecules [3], determine magnetic states of materials [4], and the chirality of crystals [5, 6]. A deep theoretical understanding of the underlying fundamental processes and, in particular, of electron-atom scattering is therefore invaluable.

While most studies have focused so far on the elastic scattering of vortex electrons, much less is currently known about their inelastic scattering that leads to the excitation of target atoms. First theoretical investigations of the inelastic channel have been performed within the first-Born approximation, assuming that the (vortex) electrons move in free space rather than being influenced by the interaction with a target atom [9]. To extend this study and to analyze the effects of Coulomb distortion, which is known to play an important role in the elastic case [7,8], we develop a distorted-wave approach to the inelastic scattering. Detailed calculations have been performed for 20-100 eV vortex electrons with OAM projections  $m_\ell = 1, 2$  scattered by neutral hydrogen. The properties of the wave functions, i.e., probability densities and phases, are compared for free and distorted vortex electrons. Furthermore, squared scattering amplitudes for the  $1s \rightarrow 2p$  excitation are discussed. Based on the results of our calculations, we argue that Coulomb distortion has a remarkable effect in the low and intermediate energy regime and should be taken into account when comparing theoretical predictions with future experiments.

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**Andrey Surzhykov**, PTB, Braunschweig

### **Polarization transfer in bound-state Compton scattering**

Compton scattering of photons by target atoms (or molecules) is one of the fundamental processes of light-matter interaction. By providing access to the electron moment density (EMD) of a target, this process underlies various spectroscopic techniques. While in the past most investigations of the Compton scattering have focused mainly on differential cross sections, today the polarization of scattered light is of great interest. In this talk, therefore, we will review the recent theoretical advances in the description of polarization of Compton-scattered photons. Special emphasis will be placed to the further development of the relativistic S-matrix approach. Using this approach and density matrix theory, we will explore the polarization transfer from incident to scattered radiation.

**Sebastian Ulbricht**, PTB, Braunschweig

### **A gravitational analogue of the quantum metrological triangle**

In this talk, we consider a gravitational analogue of the quantum metrological triangle, giving rise to analoga of the Josephson effect and the quantum Hall effect for neutral quantum particles in a gravitational field. These parallels between electromagnetic and gravitational interaction can be drawn, since the weak field limit of General Relativity resembles the mathematical structure of electrodynamics. The gravitational metrological triangle provides a testing field for our understanding of quantum systems in gravity, proposing new quantum tests of the Weak Equivalence Principle and tests of the universality of quantum mechanics. Moreover, it opens a path towards new metrological applications such as alternative realizations of mechanical units [1].

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**Anne Weber**, King's College London

### **A rigorous and universal approach for highly-oscillatory integrals in attosecond science**

Light-matter interactions within the strong-field regime, such as high-harmonic generation, typically give rise to highly-oscillatory integrals, which are often solved using saddle-point methods. Not only do these methods promise a much faster computation, but they also inform a more intuitive understanding of the process in terms of quantum orbits, as the saddle points correspond to interfering quantum trajectories (think Feynman's path integral formalism). Despite these advantages, a sound understanding of how to apply saddle-point methods to highly-oscillatory integrals in high dimensionality, in a rigorous way, and with algorithms which work uniformly for arbitrary configurations and laser drivers, remains lacking. This hinders our ability to keep up with state-of-the-art experimental setups which increasingly rely on tightly-controlled laser waveforms. In this talk, I will introduce the key ideas of Picard-Lefschetz theory – the foundation of all saddle-point methods – and their implementation. Using high-harmonic generation and above-threshold ionisation as examples, I will show how those ideas provide a robust framework for fast computation of the integrals, as well as a widely-applicable algorithm to derive the relevant semiclassical quantum orbits that underlie the physical processes.

**Hans-Peter Weber**, Albert-Ludwigs University of Freiburg

### **Microscopic definitions of thermodynamic state variables**

Equilibrium thermodynamics is an effective theory coming up with stunningly reliable predictions on macroscopic state variables, despite the deliberate (and necessary) neglect of microscopic resolution. The success of this programme largely relies on – often rather implicit – assumptions which the theory's founders deduced from their intuition. We attempt to construct fundamental thermodynamic state and process variables from most elementary microscopic quantum dynamics (rather than from an already effective description within the formalism of open quantum systems), and to identify the necessary ingredients for their consistent definition. In a first step, we'll come up with a microscopic definition of pressure, which will also allow for a very instructive illustration of the often rather abstract concept of eigenstate thermalisation hypothesis<sup>4</sup>. In a second step, we'll try to microscopically simulate the phenomenon of irreversible energy transfer, as the fundamental dynamical process underlying the definition of heat and entropy.

**Matthias Wollenhaupt**, Carl von Ossietzky University, Oldenburg

**Non-perturbative control of multiphoton ionization by oppositely chirped counterrotating circularly polarized femtosecond laser pulses**

Recently, a new class of unusually shaped Free Electron Vortices (FEVs), termed ‘reversible electron spirals’, has been proposed theoretically [Strandquist et al., Phys. Rev. A 106, 043110 (2022)] for atomic single-photon ionization by two oppositely chirped and counterrotating circularly polarized (CRCP) attosecond pulses. Building on this concept, we present the first experimental demonstration of shaped FEVs created by atomic multiphoton ionization (MPI) using oppositely chirped CRCP femtosecond pulse pairs [Köhnke et al., Phys. Rev. A 110, 053109 (2024)]. In MPI by polarization-shaped pulses, several shaped FEVs of different rotational symmetry are superimposed resulting in the total photoelectron wave packet observed in the experiment. We employ velocity map imaging techniques to measure the photoelectron momentum distribution (PMD) and reconstruct the three-dimensional (3D) density by photoelectron tomography. 3D Fourier analysis is used to decompose the measured 3D PMD into the contributing FEVs with different rotational symmetries. We have extended the above scheme to non-perturbative REMPI. Using intense, oppositely chirped CRCP pulses gives rise to adiabatic excitation dynamics, which are mapped into the 3D-PMD and result in a significantly altered distribution of the symmetry components.

**Damian Włodzyński**, Jagiellonian University, Krakow

**Anderson complexes in Bose gas with periodically modulated disordered interactions**

It has been shown that for a two-body system on a ring, the disorder introduced via temporal modulation of interaction strength leads to Anderson localization for relative motion. As a result, particles form the so-called Anderson complex, and the relative distance between them is exponentially localized. We extend this analysis to the case of several bosons.

**Vladimir Yerokhin**, MPI for Nuclear Physics, Heidelberg

**Electron self-energy without expansion in binding field and Rydberg constant**

The electron self-energy is one of the most problematic effects in the hydrogen Lamb shift, whose theory is the cornerstone in the determination of the Rydberg constant [1]. Recently, we were able to achieve a breakthrough in calculations of the electron self-energy [2,3], basing on the method for improving the convergence of the partial-wave expansion suggested in [4]. I will discuss the recent progress in one- and two-loop self-energy calculations and the consequences for the improved determination of the Rydberg constant.

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