

TT 25: Nonequilibrium Quantum Systems I (joint session TT/DY)

Time: Tuesday 9:30–13:00

Location: H 3005

TT 25.1 Tue 9:30 H 3005

Periodically Driven Heavy-Fermion Systems — ●MICHAEL TURAEV¹ and JOHANN KROHA^{1,2} — ¹Physikalisches Institut, Universität Bonn, Germany — ²School of Physics & Astronomy, University of St. Andrews, UK

In this work we study the effects of terahertz (THz) light irradiation on heavy-fermion systems. A typical model for such systems is the periodic Anderson model where strongly repulsive, localized electrons in the 4f shell of rare-earth ions hybridize with a sea of conduction electrons. The Kondo effect induces a new flat band of heavy-fermions, near the Fermi energy. Applying a stationary THz light field induces a time-periodic hybridization between the conduction and the 4f electrons, rather than a modulation of the on-site 4f energy, due to the dipole selection rules. On one hand, the Floquet theorem predicts that the periodic driving produces replicas of the Kondo resonance, centered around multiples of the driving frequency. However, the THz light field could also break up the Kondo singlets, thereby destroying the heavy-fermion state altogether.

To analyze such a scenario we use the non-equilibrium dynamical mean field theory (DMFT), combined with the Floquet-Keldysh Green function method. We obtain that for weak driving compared to the bare hybridization, the Kondo effect is preserved and Floquet replicas of the heavy-fermion bands are observed. However, a strong driving can lead to an efficient suppression of the Kondo effect where the spectral weight of the flat band is reduced.

TT 25.2 Tue 9:45 H 3005

Stabilization of a parametrically driven BEC: an open quantum system approach — ●LARISSA SCHWARZ, SIMON B. JÄGER, and SEBASTIAN EGGERT — Physics Department and Research Center OPTIMAS, University of Kaiserslautern-Landau, Germany

We theoretically analyze the effects of periodically modulated repulsive interactions in a Bose-Einstein condensate (BEC) that features intrinsic damping mechanisms. We derive a master equation describing the dynamics of the momentum modes of the BEC in the parameter regime of weak driving strengths. Above a threshold for the modulation strength we find that the BEC becomes unstable. Below this threshold the combination of damping and periodic driving guides the system into a stationary state that shows an enhancement of fluctuations for specific momentum modes that can be controlled by the driving frequency. We analyze the stationary state of these fluctuations, quantify the condensate depletion and analyze the squeezed and anti-squeezed quadratures generated by the parametric driving, emphasizing the possibility to generate non-classical states of matter.

TT 25.3 Tue 10:00 H 3005

Charge density wave melting in higher dimensional Holstein models — ●EVA PAPROTZKI¹, ALEXANDER OSTERKORN², VIBHU MISHRA³, and STEFAN KEHREIN³ — ¹I. Institut für Theoretische Physik, Universität Hamburg — ²Institut "Jožef Stefan", Ljubljana, Slovenien — ³Institut für Theoretische Physik, Georg-August-Universität Göttingen

We study the Holstein model after a quench from the insulating charge density wave (CDW) state. Employing a semiclassical treatment of the phonons ("Truncated Wigner Approximation"), we are able to track the CDW order parameter in two- and three-dimensional systems. The number of dynamical variables increases only quadratically with system size. We pose the question whether the order parameter dynamics in higher-dimensional lattices can be connected to the dynamics of the one-dimensional case via factorization. Next to an analytical estimation for the time scale of such a relation, we provide numerical evidence for the weak and strong coupling regime based on our semiclassical methods. An additional semiclassical description of the electrons ("fermionic Truncated Wigner Approximation") yields better agreement with exact reference data in one spatial dimension for the order parameter and, in particular, for the phonon number than the approach with purely phononic semiclassical dynamics.

TT 25.4 Tue 10:15 H 3005

Quantum geometry and dynamics in in-homogeneous fields — ●CHEN XU^{1,2}, ANDREAS HALLER¹, SURAJ HEGDE², TOBIAS MENG², and THOMAS L. SCHMIDT¹ — ¹Department of Physics and Materi-

als Science, University of Luxembourg, Luxembourg — ²Faculty of Physics, TU Dresden, Germany

We revisit the problem of nonequilibrium semiclassical electron transport in the presence of inhomogeneous external perturbations. For this purpose, we study the quantum geometry of Bloch band structure beyond the Berry connection contribution. We provide a systematic way of obtaining semiclassical equations of motion in an N-band system and for higher order variations in inhomogeneities, we compute geometric corrections containing for example Berry phase and quantum geometric tensor. We also demonstrate how to derive the dynamics from a generic coupling between Bloch momentum and an inhomogeneous external field, thus generalizing previous studies.

TT 25.5 Tue 10:30 H 3005

Non-equilibrium Eliashberg theory for photon-mediated superconductivity — ●MICHELE PINI¹, CHRISTIAN H. JOHANSEN^{1,2}, and FRANCESCO PIAZZA^{3,1} — ¹Max-Planck-Institut für Physik komplexer Systeme, 01187 Dresden, Germany — ²Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University in Toruń, Grudziądzka 5, 87-100 Toruń, Poland — ³Institute of Physics, Universität Augsburg, 86159 Augsburg, Germany

In the recent years, new mechanisms have been proposed to induce photon-mediated superconductivity in a non-thermal steady-state. Within these settings, the photon-electron interaction which generates the pairing can assume a form analogous to an electron-phonon interaction. This suggests a description of the superconducting phase transition within Eliashberg theory, similarly to phonon-mediated superconductivity. However, as soon as photons and electrons are pulled away from mutual equilibrium, a standard Matsubara formulation of Eliashberg theory becomes impossible. To tackle this issue, we derive a more general non-equilibrium version of Eliashberg theory. We then apply this theory to describe the superconducting phase transition in a generic non-thermal steady-state setting. We present a numerical solution of the non-equilibrium Eliashberg equations and show that bringing the system out of equilibrium can have dramatic effects on the superconducting phase transition.

Note: The authors M. Pini and C. H. Johansen contributed to this work equally.

TT 25.6 Tue 10:45 H 3005

Few-body purity as an arrow of time in the Lanczos picture — ●MERLIN FÜLLGRAF and JOCHEN GEMMER — Department of Mathematics/Computer Science/Physics, University of Osnabrück, D-49076 Osnabrück, Germany

The Lanczos method to compute autocorrelation functions in quantum mechanics gives rise to so-called Lanczos coefficients associated with operator growth in the respective systems. These coefficients can be interpreted as hopping amplitudes of a semi-infinite tight-binding model whose first site corresponds to the correlation function itself. In this picture we introduce a few-body purity and study it against the background of an arrow of time. Moreover, we investigate the influence of structures in the Lanczos coefficients on this quantity and propose a qualitative model solely based on these coefficients describing their influence on the systems' dynamics.

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

[2] V.S. Viswanath, G. Müller, The Recursion Method: Applications to Many-Body Dynamics, Springer, New York (2008).

TT 25.7 Tue 11:00 H 3005

Hilbert space fragmentation and slow dynamics in particle-conserving quantum East models — ●PIETRO BRIGHI¹, MARKO LJUBOTINA², and MAKSYM SERBYN² — ¹University of Vienna, Boltzmannngasse 5, 1090 Vienna Austria — ²ISTA, am Campus 1, 3400 Klosterneuburg Austria

Quantum kinetically constrained models have recently attracted significant attention due to their anomalous dynamics and thermalization. In this work, we introduce a hitherto unexplored family of kinetically constrained models featuring conserved particle number and strong inversion-symmetry breaking due to facilitated hopping. We demonstrate that these models provide a generic example of so-called quantum Hilbert space fragmentation, that is manifested in disconnected

sectors in the Hilbert space that are not apparent in the computational basis. Quantum Hilbert space fragmentation leads to an exponential in system size number of eigenstates with exactly zero entanglement entropy across several bipartite cuts. These eigenstates can be probed dynamically using quenches from simple initial product states. In addition, we study the particle spreading under unitary dynamics, and find faster than diffusive dynamics at high particle densities, crossing over into logarithmically slow relaxation at smaller densities. Our work suggests that particle conserving constrained models with inversion symmetry breaking realize so far unexplored dynamical behavior and invite their further theoretical and experimental studies.

15 min. break

TT 25.8 Tue 11:30 H 3005

Influence of low- and high-energy magnetic excitations on electron dynamics in the vicinity of the Mott transition: a non-equilibrium D-TRILEX study — ●NAGAMALLESWARA RAO DASARI¹, HUGO U. R. STRAND², MARTIN ECKSTEIN¹, ALEXANDER I. LICHTENSTEIN¹, and EVGENY A. STEPANOV³ — ¹Institut für Theoretische Physik, Universität Hamburg, Notkestraße 9, 22607 Hamburg, Germany — ²School of Science and Technology, Örebro University, SE-70182 Örebro, Sweden — ³CPHT, CNRS, École polytechnique, Institut Polytechnique de Paris, 91120 Palaiseau, France

We present a simplified real-time diagrammatic method based on the dual triply irreducible local expansion (D-TRILEX) formalism and apply it to the single-band extended Hubbard model. In the vicinity of Mott-transition, we observed signatures of “water-fall” structures at low-binding energies and sharp dispersive high-energy bands in the momentum-resolved electronic spectrum. In the photo-excitation dynamics, these spectral features melt very slowly on the electronic time scale, allowing us to measure these slow dynamics in the time-resolved photo-emission spectrum. In addition, the electron-magnon interaction in metals manifests through the fast relaxation of electronic kinetic energy due to the rapid thermalization of magnons much earlier than the electron’s thermalization time scale. However, in the Mott-insulators, the photo-excited charge carriers transfer their excess kinetic energy to low-energy magnons instead of low-energy electrons (expected for impact ionization), leading to a non-thermal magnon distribution on a typical electronic time scale.

TT 25.9 Tue 11:45 H 3005

Effective time-dependent temperature method for fermionic master-equations — ●LUKAS LITZBA, ERIC KLEINHERBERS, NIKODEM SZPAK, and JÜRGEN KÖNIG — Faculty of Physics and CENIDE, University of Duisburg-Essen, 47057 Duisburg, Germany

We consider a quantum system coupled to a fermionic environment at a fixed temperature. Using the Redfield equation with time-dependent coefficients, we analyze the reduced evolution of the system. We find that the time-dependence of these coefficients can be described by an effective time-dependent contact temperature. In this way, we obtain a method which includes non-Markovian effects and can be applied to various types of Gorini-Kossakowski-Sudarshan-Lindblad equations. With this, we discuss its application to a simple setup consisting of quantum dots which may be realized experimentally. At short times, the effective temperature appears to be much higher than the true temperature of the environment but asymptotically it settles down towards the true environment value. This behavior follows from the formation of coherences between the system and the environment for short times, which is related to a transfer of energy from the coupling term of the Hamiltonian into the system.

TT 25.10 Tue 12:00 H 3005

Mean-field Decoupling of Single Impurity Anderson Model through Auxiliary Majorana Fermions — ●IRAKLI TITVINIDZE¹, JULIAN STOBBE¹, ALEXEY N. RUBTSOV², and GEORG ROHRINGER¹ — ¹I. Institute of Theoretical Physics, University of Hamburg, 20355 Hamburg, Germany — ²Moscow

We present a new method to study the time evolution of the single impurity Anderson model. We perform a mean-field decoupling of the impurity and the chain. This is achieved by introducing a pair of auxiliary Majorana fermions between the impurity and the chain. We obtain a self-consistent set of equations for the impurity and the chain. By solving them in equilibrium we obtain a phase transition between phases in which the mean field parameters are zero and we have a well-defined spin on the impurity, and the regime in which the mean field

parameters take finite values and there is no well-defined spin. Once we know the equilibrium properties of the system, we quench one or more model parameters and study the time evolution of the impurity and the chain. Within our mean-field treatment, we obtain a coupled set of differential equations for the impurity and chain and find that the results converge to their equilibrium values for most quenches. For very strong interactions, the excitations are trapped and the oscillations never persist.

TT 25.11 Tue 12:15 H 3005

Emergence of unitary symmetry of microcanonically truncated operators in chaotic quantum systems — ●JIAOZI WANG¹, JONAS RICHTER^{2,3}, MATS LAMANN¹, ROBIN STEINIGEWEG¹, JOCHEN GEMMER¹, and ANATOLY DYMARSKY⁴ — ¹U Osnabrück, Germany — ²U Stanford, USA — ³LU Hannover, Germany — ⁴U Kentucky, USA

We study statistical properties of matrix elements entering the eigenstate thermalization hypothesis by studying the observables written in the energy eigenbasis and truncated to small micro-canonical windows. We put forward a picture, that below certain energy scale collective statistical properties of matrix elements exhibit emergent unitary symmetry. In particular, below this scale the spectrum of the microcanonically truncated operator exhibits universal behavior for which we introduce readily testable criteria. We support this picture by numerical simulations and demonstrate existence of emergent unitary symmetry scale for all considered operators in chaotic many-body quantum systems. We discuss operator and system-size dependence of this energy scale and put our findings into context of previous works exploring emergence of random-matrix behavior in narrow energy windows.

[1] J. Wang, M. Lamann, J. Richter, R. Steinigeweg, A. Dymarsky, J. Gemmer, Phys. Rev. Lett. 128 (2022) 180601

[2] J. Wang, J. Richter, M. H. Lamann, R. Steinigeweg, J. Gemmer, A. Dymarsky, arXiv: 2310.20264 (2023)

TT 25.12 Tue 12:30 H 3005

Periodically Driven Spin-1/2 XXZ Antiferromagnetic Chains — ●DOMINIC WINDECKER¹, ASLAM PARVEJ², and SEBASTIAN EGGERT¹ — ¹University of Kaiserslautern-Landau, Landesforschungszentrum OPTIMAS — ²Universität Hamburg

Time-periodically driven quantum systems are of great interest due the possibility of unconventional states of matter and Floquet engineering. The interplay of many-body interactions and time-periodic manipulations facilitate new phenomena in the steady state. We analyze the Floquet steady states of finite spin-1/2 XXZ antiferromagnetic chains with periodically driven anisotropy parameter at frequencies below the band width, so that resonances are in principle possible. We use three different numerical real-time approaches (TS1, TS2 and RK4) with an adiabatic time-evolution protocol by ramping up the driving amplitude of the external periodic drive to prepare a non-equilibrium Floquet steady state. Stability, accessibility, preparation and characteristics of parametric resonance states in finite systems are discussed.

TT 25.13 Tue 12:45 H 3005

Tuning the switching behavior of oligophenyls in metal-molecule-metal junctions by fluorine substituents — ●SHENGMING ZHANG¹, ZHIQIANG LI², JOACHIM REICHERT¹, HAI BI², and JOHANNES BARTH¹ — ¹Physics Department E20, Technical University of Munich, Germany — ²Jihua Laboratory, Foshan, China

Single-molecule junctions represent a promising avenue in the realm of nanometer-scale electronic device development. Numerous investigations have concentrated on the I-V relationship, which often falls short in fully characterizing a single-molecule junction. In our study, we use Raman spectroscopy as a complementary tool to explore the vibrational states of individual, covalently bound molecules while sweeping the bias. Our focus is on a series of three terphenyl species. The first molecule incorporates four methyl side groups which aim to hinder the planarization of the neutral molecules. The molecules get transiently charged above a certain threshold voltage and coplanarize their phenyl rings. This conformational change goes along with an extension of the π -electron system, increases the polarizability and thus the Raman activity of the molecules significantly. In the second and third molecule, one resp. two methyl groups where fluorine substituted in order to tune the alignment of the HOMO to the Fermi level of the electrodes upon junction formation. This way, we can steer the threshold voltage where transient charging is planarizing the molecule. This approach underscores the tunability of characteristic transport properties in a molecular model system by intricate changes in its molecular structure.