DY 30: Nonequilibrium Quantum Systems I (joint session TT/DY)

Time: Wednesday 9:30–12:45 Location: CHE/0091

DY 30.1 Wed 9:30 CHE/0091

Quantum geometric force in nonlinear phononics — •Sota Kitamura and Takahiro Morimoto — University of Tokyo, Tokyo, Japan

When phonons are resonantly excited by intense laser fields, nonlinear effects can dynamically alter the crystal structure. The field of controlling material properties through such processes is referred to as nonlinear phononics. In conventional theoretical frameworks of nonlinear phononics, the electron dynamics are typically assumed to be adiabatic. However, this assumption generally breaks down under strong driving, and nonadiabatic corrections become essential.

Using nonequilibrium Green function methods, we investigate the electron dynamics under resonant phonon excitation beyond the adiabatic approximation, thereby exploring nonadiabatic effects appearing in the phonon equations of motion. Our analysis reveals that quantum geometric contributions originating from the electronic Berry curvature give rise to unconventional forces on phonons. These quantum geometric corrections are then applied to the dynamical control of crystal chirality, i.e., right- or left-handedness of chiral crystals, using a minimal tight-binding model coupled to the Peierls phonon.

DY 30.2 Wed 9:45 CHE/0091

Macroscopic mechanical torque for lattice and electronic chirality measurement — •Nikolai Peshcherenko[1], Ning Mao[1], Claudia Felser[1], and Yang Zhang[2,3] — [1]Max Planck Institute for Chemical Physics of Solids, 01187, Dresden, Germany — [2]Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee 37996, USA — [3]Min H. Kao Department of Electrical Engineering and Computer Science, University of Tennessee, Knoxville, Tennessee 37996, USA

The concept of chirality is known to be critical for a number of phenomena related either to a structural asymmetry or topological electronic band crossings. In the present work we develop a robust chirality probe of TR-symmetric systems with mechanical torque measurement. Namely, we show that driving a system out of equilibrium with temperature gradient (or electric field to excite electrons) would result in uncompensated angular momentum and mechanical torque. Calculations are made for both phonons (insulating case) and electrons (metallic case) carrying angular momentum. For phonons, our theoretical findings stand in reasonable agreement with a recent experiment [1]. For electronic subsystem, we discuss both cases of structural and topological electronic chirality probe.

[1] H. Zhang, N. Peshcherenko, F. Yang, T. Ward, P.Raghuvanshi, L.Lindsay, C.Felser, Y.Zhang, J.-Q. Yan, H.Miao, Nat.Phys.1 (2025)

DY 30.3 Wed 10:00 CHE/0091

Hybrid quantum–classical matrix-product state and Lanczos methods for electron–phonon systems with strong electronic correlations: Application to disordered systems coupled to Einstein phonons — •Heiko Georg Menzler[1], Suman Mondal[2], and Fabian Heidrich-Meisner[1] — [1]Institut für Theoretische Physik, Georg-August-Universität Göttingen, D-37077 Göttingen, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Dresden

We present two quantum-classical hybrid methods for simulating the time-dependence of electron-phonon systems that treat electronic correlations numerically exactly and optical-phonon degrees of freedom classically. These are a time-dependent Lanczos and a matrix-product state method, each combined with the multi-trajectory Ehrenfest approach. Due to the approximations, reliable results are expected for the adiabatic regime of small phonon frequencies. We discuss the convergence properties of both methods for a system of interacting spinless fermions in one dimension and provide a benchmark for the Holstein chain. As a first application, we study the decay of charge density wave order in a system of interacting spinless fermions coupled to Einstein oscillators and in the presence of quenched disorder. We investigate the dependence of the relaxation dynamics on the electron-phonon coupling strength and provide numerical evidence that the coupling of strongly disordered systems to classical oscillators leads to delocalization, thus destabilizing the (finite-size) many-body localization in this system.

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DY 30.4 Wed 10:15 CHE/0091

Frozen non-equilibrium dynamics of exciton Mott insulators in moiré superlattices — Shibin Deng[1], •Jonas Reimann[2], Heonjoon Park[3], Jonas M. Peterson[1], Ammon Fischer[2], Xiaodong Xu[3], Dante M. Kennes[2,4], and Libai Huang[1] — [1]Department of Chemistry, Purdue University, West Lafayette, IN 47907, USA — [2]Max Planck Institute for the Structure and Dynamics of Matter, Center for Free Electron Laser Science, 22761 Hamburg, Germany — [3]Department of Physics, University of Washington, Seattle, WA 98195, USA — [4]Institut für Theorie der Statistischen Physik, RWTH Aachen University, 52056 Aachen, Germany

Moiré superlattices, such as those formed from transition metal dichalcogenide heterostructures, have emerged as an exciting platform for exploring quantum many-body physics. A key open question is the coherence and dynamics of the quantum phases arising from photoexcited moiré excitons, particularly amid dissipation. Here we use transient photoluminescence and ultrafast reflectance microscopy to image non-equilibrium exciton phase transitions. Counterintuitively, experimental results and theoretical simulations indicate that strong long-range dipolar repulsion freezes the motion of the Mott insulator phase for over 70 ns. In mixed electron-exciton lattices, reduced dipolar interactions lead to diminished freezing dynamics. These findings challenge the prevailing notion that repulsion disperses particles, whereas attraction binds them. This talk focuses on the theoretical efforts that support the experimental data.

DY 30.5 Wed 10:30 CHE/0091

Cavity-induced Eliashberg effect: superconductivity vs charge density wave — •Md Mursalin Islam[1,2], Michele Pini[1,2], Rafael Flores- Calderón[2], and Francesco Piazza[1,2] — [1]Theoretical Physics III, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Nothnitzer Straße 38, 01187 Dresden, Germany

Recent experiments have shown that non-equilibrium effects can play a key role in cavity-based control of material phases, notably in systems with charge-density-wave order. Motivated by this, we extend the theory of the Eliashberg effect, originally developed for superconducting phases, to charge-density-wave phases. Starting from a minimal electronic model where superconductivity and charge-density-wave order are equivalent at equilibrium, we introduce coupling to cavity photons, which are in turn coupled to an environment at a temperature different from the one of the electronic environment. This drives the system into a non-thermal steady state, which breaks the equivalence between superconductivity and charge-density-wave order. In the superconducting case, we recover the known behavior: a shift from continuous to discontinuous phase transitions with bistability. In contrast, the charge-density-wave case displays richer behavior: tuning the cavity frequency induces both continuous and discontinuous transitions, two distinct ordered phases, and a bistable regime ending at a critical point. These findings demonstrate that the scope of cavity-based non-thermal control of quantum materials is broader than at thermal equilibrium, and strongly depends on the targeted phases.

DY 30.6 Wed 10:45 CHE/0091

Quantum Monte Carlo Nonequilibrium work estimator of Rényi negativites — •Jannis Kastell and David Luitz — Universität Bonn, Bonn, Germany

We develop a Quantum Monte Carlo method for the calculation of Rényi generalizations of the logarithmic negativity, an entanglement measure for mixed states. Extending previous works using the replica trick and nonequilibrium-work-based estimators of Rényi entanglement entropy, we adapt this framework to the moments of the partially transposed reduced density matrix at finite temperature. Using the stochastic series expansion (SSE) method, we compute these moments in bi- and tri-partitioned systems. We apply this approach to the spin-1/2 isotropic Heisenberg antiferromagnet on a 3D simple cubic lattice, analysing the scaling of the higher order moments with subsystem size for both contiguous and disjoint partitions. Our results demonstrate that this approach provides an efficient and scalable method for estimating mixed-state entanglement measures in large quantum many-body systems.

15 min. break

DY 30.7 Wed 11:15 CHE/0091

Enhancing quantum metric using periodic driving — •Dhruv Tiwari, Roderich Moessner, and Johannes S. Hofmann — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

The advent of periodically driven systems has revolutionized modern condensed matter physics by offering two transformative opportunities. First, they enable the realization of nonequilibrium analogs of well-established equilibrium phases under highly tunable conditions. Second, they facilitate the emergence of novel phases with no equilibrium counterparts. In this work, we focus on the former, leveraging the tunable parameters of periodically driven systems to enhance the quantum metric in flat-band models. The quantum metric, a fundamental geometric property of the band structure, plays a crucial role in stabilizing various correlated phases. Here, we present results demonstrating that an appropriately chosen periodic drive can amplify the quantum metric and modify density-density interactions. Using both numerical and analytical techniques, we map out the phase diagram of the resulting model.

DY 30.8 Wed 11:30 CHE/0091

Scattering in periodic fields: Floquet resonances — •Sebastian Eggert, Christoph Dauer, and Axel Pelster — University of Kaiserslautern-Landau (RPTU)

An alternative mechanism of tuning many-body interactions in atomic systems is proposed, which is based on dynamically creating Floquet bound states using time-periodic fields. By developing a Floquet-scattering theory we show that sharp Floquet resonances occur at which the effective interaction can be tuned to very large attractive or repulsive values. The resulting predictions explain recent experimental data and provide additional tuning possibilities. Analytic predictions are given for adjusting amplitude, frequency and mean of the applied oscillating field in order to to accurately choose location and width of scattering resonances over a wide range. This paves the road to a versatile toolbox of tailored interactions in setups with multiple atomic species.

DY 30.9 Wed 11:45 CHE/0091

A comparative study of perturbative and nonequilibrium Green's function approaches for Floquet sidebands in periodically driven quantum systems — •Karun Gadge[1], Marco Merboldt[2], Wiebke Bennecke[2], Jan Philipp Bange[2], Marcel Reutzel[3], Stefan Mathias[2], Michael A Sentef[4], Michael Schüler[5], and Salvatore R Manmana[1] — [1]Institute for Theoretical Physics, Georg-August-University Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen, Germany — [2]I. Physikalisches Institut, Georg-August-University Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen, Germany — [3]Fachbereich Physik, Philipps-University Marburg, Marburg, Germany — [4]Institute for Theoretical Physics and Bremen Center for Computational Materials Science, University of Bremen, 28359 Bremen, Germany — [5]Laboratory for Materials Simulations, Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland

We compare two complementary theoretical approaches to compute and interpret Floquet sidebands in periodically driven quantum materials: a first-order perturbative approach (PB1) and time-dependent nonequilibrium Green's functions (tdNEGF). Using graphene as a model Dirac system, we disentangle in pump-probe setups Floquet-dressed initial states, Volkov-dressed final states (also known as laser-assisted photoelectric effect, LAPE), and their interference. We quantify how photoemission matrix elements, polarization, incidence angle, and near-surface screening shape the momentum-resolved sideband intensity observed in tr-ARPES.

DY 30.10 Wed 12:00 CHE/0091

Towards Floquet-GW: interacting electrons in time-periodic potentials — •Ayan Pal[1,2], Erik G C P Van Loon[1,2], and Ferdi Aryasetiawan[1,3] — [1]Division of Mathematical Physics, Lund University, Professorsgatan 1, 223 63, Lund, Sweden — [2]NanoLund, Lund University, Professorsgatan 1, 223 63, Lund, Sweden — [3]LINXS Institute of advanced Neutron and X-ray Science, Lund, Sweden

The Floquet theory of time-periodic systems provides a middle ground between equilibrium and far-from-equilibrium physics, making it ideal for studying non-equilibrium steady states. We employ this framework to interacting electrons exposed to spatially and time-periodic potentials by combining Floquet theory with RPA and GW. This is applied to both the homogeneous electron gas and lattice Hamiltonians, allowing us to resolve the interplay between periodic driving, electronic correlations, and collective charge excitations. We compute Floquet-induced Greens function, dielectric function, and screened interaction; and demonstrate the formation of Bloch-Floquet sidebands in the electronic spectral function and in direct and inverse photoemission spectra. The periodic modulation further induces plasmonic sidebands and generates additional Floquet-umklapp regions for the electron-hole continuum. Our analysis highlights how the structure of the travelling drive - frequency, amplitude, and momentum controls the redistribution of spectral weight and the renormalisation of collective modes. This framework provides a route for predicting the plasmonic, dielectric, and optical response properties of weakly to moderately correlated materials under periodic laser driving.

DY 30.11 Wed 12:15 CHE/0091

Emergent Floquet Fermi Surfaces from Disorder — Inti Sodemann Villadiego, Akihiro Ozawa, and •Felix Frederking — Institut für Theoretische Physik, Universität Leipzig, Brüderstraße 16, 04103 Leipzig, Germany

We investigate the non-equilibrium steady states of periodically driven fermions coupled to a fermionic heat bath and in the presence of disorder (i.e. random impurities). In the absence of disorder, the steady state occupation would be a "stair-case" version of the Fermi-Dirac distribution, which is smooth at finite temperatures. Remarkably, however, we have found that disorder induces non-analyticities in the occupation of states that behave as emergent Fermi surfaces. We will discuss the physical phenomena arising from these non-equilibrium emergent Fermi surfaces and make the case for the feasibility of their detection in ulta-clean 2D materials subjected to low frequency radiation.

DY 30.12 Wed 12:30 CHE/0091

Emergent Fermi surfaces from non-equilibrium heat baths: exact results from Keldysh formalism — •Akihiro Ozawa and Inti Sodemann Villadiego — Institut für Theoretische Physik, Universität Leipzig, 04103, Leipzig, Germany

Recent studies have shown that periodically driven fermions coupled to a boson bath display non-analyticities in their occupation functions of momentum that behave like emergent Fermi surfaces. Remarkably, we have found that analogous non-equilibrium emergent Fermi surfaces can arise when the system is coupled to two baths at different temperatures, even without external periodic driving. The mechanism driving the formation of these non-equilibrium Fermi surfaces, is a kind of transfer from non-analyticities from the density of states into the occupation of states which is only allowed away from equilibrium, in the absence of detailed balance in the scattering rates. We demonstrate that this result is exact at weak coupling using the Keldysh formalism and propose a numerical scheme to investigate the fate of these non-analyticities at finite coupling.