Driven Mott insulators out of equilibrium: photovoltaics, phonons and heat dissipation.

Enrico Arrigoni, Graz University of Technology, Austria

I will present recent results for correlated Mott systems driven out of equilibrium.
We use steady-state Dynamical Mean Field Theory with an impurity solver based upon a combination of nonequilibrium Green's functions and Lindblad quantum master equations for open quantum systems [1].
I will talk about new improvements based upon a Configuration Interaction treatment of the many body Lindblad equation allowing for an efficient solution of the impurity problem deep in the Kondo regime [2].

In particular, I will discuss the interplay of strong correlation and Joule dissipation by phonons near the Mott dielectric breakdown [3] and in photoexcitation induced transport across a Mott insulating gap [4].

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Configuration interaction based nonequilibrium steady state impurity solver

Daniel Werner, TU Graz, Austria

We present a solver for correlated impurity problems out of equilibrium based on a combination of the so-called auxiliary master equation approach (AMEA) and the configuration interaction expansion. Within AMEA one maps the original impurity model onto an auxiliary open quantum system with a restricted number of bath sites which can be addressed by numerical many-body approaches such as Lanczos/Arnoldi exact diagonalization (ED) or matrix product states (MPS). While the mapping becomes exponentially more accurate with increasing number of bath sites, ED implementations are severely limited due to the fast increase of the Hilbert space dimension for open systems, and the MPS solver typically requires rather long runtimes. Here, we propose to adopt a configuration interaction approach augmented by active space extension to solve numerically the correlated auxiliary open quantum system. This allows access to a larger number of bath sites at lower computational costs than for plain ED. We benchmark the approach with numerical renormalization group results in equilibrium and with MPS out of equilibrium. In particular, we evaluate the current, the conductance as well as the Kondo peak and its splitting as a function of increasing bias voltage below the Kondo temperature TK. We obtain a rather accurate scaling of the conductance as a function of the bias voltage and temperature rescaled by TK for moderate to strong interactions in a wide range of parameters. The approach combines the fast runtime of ED with an accuracy close to the one achieved by MPS making it an attractive solver for nonequilibrium dynamical mean field theory.

Accelerating Nonequilibrium Green functions simulations: the G1-G2 scheme and beyond

M. Bonitz, J.P. Joost, K. Balzer, H. Ohldag, C. Makait, and E.Schroedter
Institute for Theoretical Physics and Astrophysics, Kiel University, Germany

Full two-time NEGF simulations suffer from a cubic scaling of the CPU time with the simulation duration. Recently we have introduced the G1-G2 scheme that exactly reformulates the Hartree-Fock-GKBA into time-local equations, allowing for a dramatic reduction to time-linear scaling [1]. Remarkably, this scaling is achieved quickly, and also for high-level selfenergies, including nonequilibrium GW and T-matrix approximation [2]. Even the dynamically screened ladder approximation is now feasible [3], and applications to electron-boson systems were demonstrated [4]. I will present applications to nonequilibrium situations including laser excitation of graphene nanoribbons [5] and ion stopping and neutralization by graphene and TMDC monolayers [6].

The scaling advantage of the G1-G2 scheme comes at a price, and I will discuss how these problems can be solved: i) for strong coupling situations and long si-mulations, the scheme becomes unstable. Possible solutions include purification schemes [3,5] or the use of the GKBA with correlated propagators [7]. ii) It is necessary to store the time-diagonal two-particle Green function which rapidly grows with system size. This can be overcome for the GW approximation using a recently developed quantum fluctuations approach [8]. Another promising concept to reduce the simulation size is the use of embedding selfenergies. Here, we demonstrate how the embedding concept can be introduced into the G1-G2 scheme, allowing us to drastically accelerate NEGF embedding simulations [9].

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Time-linear scaling nonequilibrium Green’s function methods for real-time simulations of interacting electrons and bosons

Yaroslav Pavlyukh, Wrocław University of Science and Technology , Poland

Simulations of interacting electrons and bosons out of equilibrium, starting from first principles and aiming at realistic multiscale scenarios, is a grand theoretical challenge. Here, using the formalism of nonequilibrium Green’s functions and relying in a crucial way on the recently discovered time-linear formulation of the Kadanoff-Baym equations, a versatile toolbox for the simulation of correlated electron-boson dynamics is presented [1].

As an illustration of the formalism, nonequilibrium dynamics of the open chain Holstein-Hubbard model is demonstrated for a set of parameters relevant for photovoltaic materials, i.e., a pair of electrons interacting with phonons at the crossover between the adiabatic and antiadiabatic regimes and at moderately large electron-electron interaction [2].

Under some physical scenarios, dressing of electronic states by bosons needs to be treated nonperturbatively. A substantial advance in the treatment of correlations, requiring no extra computational cost and preserving all conserving properties can be obtained by including the effects of dynamical screening due to both e-e and e-b interactions—the so-called doubly screened GW approximation. I demonstrate the application of the method to the correlation-induced charge migration of the glycine molecule in an optical cavity [3].

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Motion-induced spin transfer

Daigo Oue, University of Lisbon, Portugal

We propose a spin transport induced by inertial motion. Our system is composed of two host media and a narrow vacuum gap in between. Magnons reside in and are exchanged between the two media, carrying angular momenta (spins). One of the hosts is sliding at a constant speed relative to the other. This mechanical motion causes the Doppler effect, which shifts the density of states and the nonequilibrium distribution function in the moving medium. Those shifts induce the difference in the distribution function between the two media, and they result in tunnelling spin currents. The spin current is perturbatively evaluated with the nonequilibrium Green's function technique and a spin tunnelling Hamiltonian. The spin current will be of the order of nA, which could be detected by measuring the inverse spin Hall voltage. This scheme does not require temperature difference, voltage, or chemical potential and Our proposal will open a new door to spin manipulation by inertial motion.

In- and out-of-equilibrium ab initio theory of electrons and phonons

Gianluca Stefanucci, University of Rome Tor Vergata, Italy

We lay down the *ab initio* many-body quantum theory of electrons and phonons in- and out-of-equilibrium at any temperature. We begin by addressing a fundamental issue concerning the *ab initio* Hamiltonian in the harmonic approximation, which we show must be determined {\em self-consistently} to avoid inconsistencies. After identifying the most suitable partitioning into a ``noninteracting'' and an ``interacting'' part we embark on the Green's function diagrammatic analysis. We single out key diagrammatic structures to carry on the expansion in terms of dressed propagators and screened interaction. The final outcome is the finite-temperature nonequilibrium extension of the Hedin equations, featuring the appearance of the time-local Ehrenfest diagram in the electronic self-energy. We also derive the Kadanoff-Baym equations for electrons and phonons, discuss the theory of conserving approximations and show how to recover the Born-Oppenheimer approximation. We conclude by pointing out a possible correlation-induced splitting of the phonon dispersion in materials with no time-reversal invariance.

Hydrodynamics of charged two-dimensional Dirac systems II: the role of collective modes

Kitinan Pongsangangan, TU Dresden, Germany

We study the hydrodynamic properties of ultraclean interacting two-dimensional Dirac electrons with Keldysh quantum field theory. We study it from a weak-coupling and a strong-coupling perspective. We demonstrate that long-range Coulomb interactions play two independent roles: (i) they provide the inelastic and momentum-conserving scattering mechanism that leads to fast local equilibration; (ii) they facilitate the emergence of collective excitations, for instance plasmons, that contribute to transport properties on equal footing with electrons. Our approach is based on an effective field theory of the collective field coupled to electrons. Within a conserving approximation for the coupled system we derive a set of coupled quantum-kinetic equations. This builds the foundation of the derivation of the Boltzmann equations for the interacting system of electrons and plasmons. From this, we explicitly derive all the conservation laws and identify the extra contributions of energy density and pressure from the plasmons. We demonstrate that plasmons show up in thermo-electric transport properties as well as in quantities that enter the energy-momentum tensor, such as the viscosity. In a parallel paper we discuss some of the phenomenology of the corresponding hydrodynamic equations with an eye on thermo-electric transport properties.

From non-equilibrium Green's function to nonlinear optical properties of materials

Myrta Grüning, Queen's University Belfast, United Kingdom

In the past decades, many-body approaches based on the GW approximation and the Bethe-Salpeter equation have become state-of-the-art for calculating optical absorption in solids and nanostructures. In this talk, I'll present a real-time approach derived from the non-equilibrium Green's function, that allows extending the GW+BSE approach beyond the linear regime. [1,2] Using this approach, I'll address the importance of many-body effects and in particular of excitonic effects for nonlinear optical properties.[3] For example, I'll look at the case of single-layer monochalcogenide whose strong Second Harmonic Generation cannot be reproduced within the independent-particle approximation.[4]

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Magnetic dynamics driven ultrahigh harmonic generation in spin-orbit coupled systems

Ousmane Ly, Université de Nouakchott, Mauritania

It has been predicted 20 years ago [1], that when a normal metal is subjected to magnetic dynamics, a pure spin current is pumped toward the adjacent paramagnet. The resulting pumped carrier dynamics is found to operate at the same frequency underlying the magnetic drive. In the actual work, we predict that in the presence of spin-orbit coupling, the interplay between the s-d exchange coupling and the relativistic interaction leads to the emergence of ultrahigh harmonics in the carrier pumping [2, 3]. We demonstrate that an enhancement of the initial dynamics by orders of magnitude can be achieved upon properly tuning the parameters of the drive and the spin-orbit strength.

Using the non-equilibrium quantum transport framework TKwant [4], we investigate the scaling laws of the proposed effect. Furthermore, we establish the universality of the effect and demonstrate that it could be triggered in systems hosting non-collinear topological textures or magnetic impurities [5].

In the actual proposal magnetism is proposed as an alternative to laser pulses for the purpose of exciting highly nonlinear emission in solid state systems driven out of equilibrium.

Our proposal opens up an interesting perspective in utilising adiabatic magnetic precession to trigger ultrafast carrier dynamics deep in the THz regime and beyond.

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High-harmonic generation in strongly correlated systems

Yuta Murakami, RIKEN CEMS, Japan

The recent development of strong lasers enables us to study various nonlinear optical phenomena. One fundamental example is high-harmonic generation (HHG). HHG was first observed in gases, and its scope has been extended to condensed matter (CM). Although the major target of the HHG research in CM so far has been semiconductors and band insulators, HHG in strongly correlated systems (SCESs) also attracts attentions. SCESs are a potentially interesting playground for the HHG research since i) the excitation structures cannot be described by independent electrons and holes unlike conventional semiconductors and ii) various degrees of freedom (charge, spin and orbitals) can be strongly intertwined. In this talk, we reveal the physics of HHG in the Mott insulator described by the single-band Hubbard model using complementary nonequilibrium theories such as nonequilibrium dynamical mean-field theory (DMFT) and infinite time-evolving block decimation based on the matrix product state (MPS) [1-3]. We reveal the relation between HHG in the Mott insulator and its elemental excitations, and demonstrate that correlations between different degrees of freedom can lead to peculiar HHG features as experimentally reported [4]. We also explain a potential way to extend the capability of NEGF methods using MPS, which shall allow us to study more realistic models [5].

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Shining light on solid-state chemistry - absorption and emission spectroscopy implying periodic boundary conditions at the large scale

Anna Hehn, Christian-Albrechts-University Kiel, Germany

Time-dependent density functional theory has proven as powerful tool set for the description of excited states in solid-state chemistry. Nevertheless, when exceeding the computation of static excitation spectra towards excited-state properties or dynamic modeling, large-scale simulations are most often restricted to density functionals within the generalized gradient approximation. To establish hybrid functional accuracy with reasonable cost for photochemistry implying periodic boundary conditions, we therefore present two approximate time-dependent density functional theory schemes in both the mixed Gaussian and plane waves (GPW) and the Gaussian and augmented plane waves (GAPW) environment of the CP2K program package [1,2]. Both approximated hybrid functional theory exploiting the auxiliary density matrix method (ADMM) as well as semi-empirical tight binding (sTDA) approaches and related benchmarks for the accurate description of fluorescence spectra of framework materials are discussed and we will motivate the use of the presented algorithms for non-adiabatic molecular dynamics simulations.

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Inducing, probing and exciting topological magnons in two-dimensional honeycomb magnets

Emil Vinas Boström, Max Planck Institute for the Structure and Dynamics of Matter, Germany

The study of topological states of matter has recently been extended to systems with bosonic quasi-particles, such as magnons, photons, excitons and polaritons. In particular, there is great hope to utilize topological magnon states for fault-tolerant information transfer and processing. However, in contrast to electronic systems where it is experimentally straightforward to verify the topology of a given phase via conductivity measurements, there has so far been no direct measurements protocols available to ascertain if a magnonic bandstructure is topological or not.

Here I will discuss some recent work demonstrating how light can be used to induce and probe a non-trivial magnon band topology in two-dimensional honeycomb magnets [1,2]. More specifically, I will show how driving a one-band Hubbard model on the honeycomb lattice gives rise to higher order interactions in the effective Floquet spin Hamiltonian resulting in a bosonic Haldane model for the magnons. I will also show that the circular dichroism of two-magnon Raman scattering in such systems is directly related to the Chern number of the magnon bands, and thereby constitutes an optical probe of the magnon topology. In addition, I will present both recent and on-going work where light is used to excite and control magnon bulk and edge currents [3]. In particular, I will discuss how recent developments of the non-equilibrium Green's function formalism might allow to access spectral and transport properties of topological magnon systems.

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Time-dependent density functional theory: Simulating dynamics far from the ground state with the adiabatic approximation

Neepa Maitra, Rutgers University at Newark, United States of America

Time-dependent density functional theory (TDDFT) with the adiabatic approximation has enjoyed much success in the prediction of excitation spectra of molecules and materials, as well as predictions of time-resolved dynamics driven by strong non-perturbative fields that are not computationally feasible with other methods. However, errors arising from making the adiabatic approximation lead to unreliability in some results especially in the non-perturbative regime, and TDDFT can even sometimes completely fail. In this talk we demonstrate that reformulating real-time TDDFT calculations in a way that uses only information from response calculations greatly reduces the error that adiabatic approximations make, because the exchange-correlation functional is evaluated on a domain close to the one they were derived from. Errors from the adiabatic approximation in the response domain appear simpler to get a reasonable correction to, and we show how to cure the divergences that an adiabatic quadratic response kernel causes by deriving a practical simple frequency-dependent kernel and derive a generalized dressed TDDFT for oscillator strengths of double excitations. Examples including coupled electron-ion dynamics within Ehrenfest dynamics, electron scattering, and electron dynamics in strong fields will be shown.

Electron Transfer in Non-Equilibrium Environments

Thorsten Hansen, University of Copenhagen, Denmark

Coherent multi-dimensional spectroscopy continues to probe the electronic and vibratio-nal dynamics in molecular systems in greater and greater detail. Especially, the details of exciton dynamics in photosynthetic antennas and other systems have been explored. But also, electron transfer dynamics is being investigated. Such modern experiments create a need for new levels of detail in out description of exciton and electron transfer and related processes.

A decade ago, we formulated non-linear response theory on the Keldysh contour. This included a straightforward microscopic derivation of the well-known Marcus equation for electron transfer [1]. Vibrations were later introduced into this formulation in full generality.

Recently, we obtained a new expression for the rate; this one in terms of vibrational auto-correlation functions. This connects electron transfer theory to Mukamel's formulation of four-wave mixing spectroscopy. We can now explore electron transfer processes within a non-equilibrium environment represented by a set of damped harmonic oscillators.

I will give an overview of ongoing work and discuss upcoming challenges and opportunities.

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Self-consistent treatment of leading collective electronic fluctuations and vertex corrections in diagrammatic extensions of a non-equilibrium dynamical mean-field theory

Evgeny Stepanov, CNRS, École Polytechnique, IP Paris, France

The non-equilibrium dynamical mean-field theory (DMFT) [RMP 86, 779 (2014)] is a *state-of-the-art* method for describing the time-evolution of a strongly correlated problem under an external time-dependent perturbation. However, this approach neglects non-local electronic correlations that may strongly affect physical properties of the system.

Going beyond the non-equilibrium DMFT is computationally challenging. Currently, the *GW*+DMFT [PRL 118, 246402 (2017); PRB 100, 041111(R) (2019), PRB 100, 235117 (2019)] method can be seen as the most advanced numerical approach that can be used for this purpose. Unfortunately, this theory is able to treat only charge fluctuations and thus misses important non-local magnetic effects. Moreover, already this simplest extension of DMFT makes the description of the time evolution of the driven system extremely expensive numerically, which, at first glance, does not give any room for a further improvement of the method.

In this talk, I will show that the diagrammatic structure of a recently developed dual triply irreducible local expansion (D-TRILEX) method [PRB 100, 205115 (2019); PRB 103, 245123 (2021); SciPost Phys. 13, 036 (2022)] suggests an inexpensive way of improving diagrammatic extensions of the non-equilibrium DMFT. Indeed, upon neglecting three-point vertex corrections in diagrams for the self-energy and polarization operator, the D-TRILEX method reduces to an analog of the *GW*+DMFT theory that, however, accounts for all leading channels of instability (including non-local magnetic fluctuations) simultaneously. In addition, I will demonstrate that the action-based formulation of the D-TRILEX method allows for introducing numerically tractable simplified vertex corrections. Results of the first applications of the non-equilibrium extension of the D-TRILEX method will also be discussed.

Stopping Power in dense quantum plasmas using NEGF with GW selfenergies

Christopher Makait, Univ. Kiel, Germany

Warm dense matter (WDM) is a state of matter at solid state densities and temperatures around 10^6K. WDM driven out of equilibrium is of growing interest in many experiments, e.g. due to its relevance to ICF. In particular, time-resolved predictions of dynamics far from equilibrium, such as the equilibration of the electronic distribution and the two-temperature relaxation of electrons and ions are pivotal to future advances in this field. We analyze the first stage of the relaxation on the example of the stopping power.

A reliable theoretical description requires the treatment of electronic quantum effects as well as dynamical screening. These high requirements are fulfilled by quantum kinetic approaches, including NEGF, which have successfully been applied to WDM by a variety of groups [1,2,3], however, in the Markov limit.

Here, we present improved results. We use NEGF with the GW selfenergy in combination with the generalized Kadanoff-Baym ansatz [4] on Hartree-Fock level (HF-GKBA). While such calculations have recently experienced a dramatic acceleration [5], the application of this approach to uniform plasmas has so far been restricted to quasi-1D models [6]. Here we study the dynamics of 3D plasmas in cylinder symmetry and apply our method to the stopping of proton projectiles in a dense plasma which we find to agree well with static results. On the other hand, non-Markovian effects and shared Pauli-blocking significantly change the outcome for electron projectiles.

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Cumulant Green's function approach for cool to warm dense matter*

John Rehr, University of Washington, United States of America

J.J. Rehr and J.J. Kas, *Department of Physics, University of Washington*

There has been considerable interest in first principles theories of material properties at extreme conditions, e.g., the warm dense matter regime where the temperature T is of order the Fermi-temperature T_F. A number of approaches have been introduced for this purpose, including path integral Monte Carlo (PIMC), dielectric function methods, and finite temperature (FT) density functional theory, as reviewed in [1]. While these methods can yield excellent results for correlation energies and thermodynamic properties, they are not directly applicable to excited state and spectral properties. Here we discuss a finite-temperature cumulant Green's function approach, which yields both thermodynamic properties and optical to x-ray spectra, including dynamic exchange-correlation effects. Thermodynamic properties including the equation of state are obtained using the Martin-Schwinger formalism and the Galitskii-Migdal-Koltun sum rules [2]. This approach also yields FT exchange-correlation potentials $v_{xc}(T,n)$ and the FT-TDDFT kernel $f_{xc}(T,n)$ [3], which are in good agreement with the PIMC fits of Kariase*v et al.* [4] over a broad range of temperatures and densities. Finally pump-probe x-ray spectra are obtained using a two-temperature model [5]. Extensions including local field effects which are important at low densities are briefly discussed.

*Supported by the Theory Institute for Materials and Energy Spectroscopies (TIMES) at SLAC under DOE FWP 100291, with computer support from the DOE National Energy Research Scientific Computer (NERSC).

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Cutting rules and positivity in finite temperature and non-equilibrium Green's function theory

Robert van Leeuwen , University of Jyväskylä, Finland

For a given diagrammatic approximation in many-body perturbation theory it is not guaranteed that positive observables, such as the density or the spectral function, retain their positivity. For zero-temperature systems we developed a method [Phys.Rev.B 90,115134 (2014)] based on so-called cutting rules for Feynman diagrams that enforces these properties diagrammatically, thus solving the problem of negative spectral densities observed for various vertex approximations. In this work [1] we extend this method to systems at finite temperature by formulating the cutting rules in terms of retarded N-point functions, thereby simplifying earlier approaches and simultaneously solving the issue of non-vanishing vacuum diagrams that has plagued finite temperature expansions. Our approach is moreover valid for nonequilibrium systems in initial equilibrium and allows us to show that important commonly used approximations, namely the GW, second Born and T-matrix approximation, retain positive spectral functions at finite temperature. Finally we derive an analytic continuation relation between the spectral forms of retarded N-point functions and their Matsubara counterparts and a set of Feynman rules to evaluate them.

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A NEGF-GKBA approach to skyrmions creation and transport in the presence of electronic reservoirs

Emil Östberg, Lund University, Sweden

Topologically protected magnetic excitations, originating from the interplay of exchange, spin-orbit interactions and external fields, hold great promise for sustainable nanodevices, with lower energy consumption, heating, and decoherence. In this work, we address within a quantum-classical NEGF-GKBA+Spin formalism the role of the environment on skyrmion creation and dynamics. Specifically we consider a finite lattice with itinerant electrons and classical localized spins, where the electronic subsystem is in contact with metallic leads.We use a non-interacting approximation to the collision integral which, for the purpose of simulating a large enough lattice to host magnetic skyrmions, offers a reasonable trade-off between computation time and accuracy.

Our NEGF-GKBA+Spin approach provides novel insight into different aspects of skyrmion dynamics, e.g. nonlinear skyrmion transport, electronic dissipation, and scattering due to sample inhomogeneities. Most importantly, it brings to the foreground the explicit and prominent role that itinerant electrons have to play in skyrmion behavior, and their usefulness as topological markers of magnetic textures from localized spins.

Authors: Emil Östberg, Emil Viñas Boström and Claudio Verdozzi

Nonequilibrium DMFT approach to RIXS and Raman scattering

Philipp Werner, University of Fribourg, Switzerland

Resonant inelastic X-ray scattering (RIXS) and Raman scattering are photon-in photon-out techniques which are used to probe low-energy excitations of solids. The standard diagrammatic calculation of the RIXS or Raman amplitude requires the evaluation of four-point correlation functions, which is numerically difficult, especially in out-of-equilibrium situations. I will show how the problem can be reduced, within the dynamical mean field theory (DMFT) approximation, to the evaluation of a two-point correlation function, if the incoming light pulse is simulated explicitly. This approach is directly applicable to nonequilibrium setups, such as those explored in pump-probe experiments. I will illustrate the method with results for photo-excited multi-orbital Hubbard and electron-phonon systems.

Ultrafast time-resolved photoemission:Floquet engineering and beyond

Michael Schüler, Paul-Scherrer Institute / University of Fribourg, Switzerland

The nonequilibrium Green's function formalism (NGF) is one of the most powerful tools to describe ultrafast phenomena in condensed matter. In particular, its direct link to time- and angle-resolved photoemission spectroscopy (trARPES) renders the NGF approach the tool of choice for connecting to experiments. In this talk, we discuss Floquet engineering in graphene and how the inherent difficulties due to scattering can be overcome [1]. As the field of trARPES progresses into the THz regime, the conventional NGF theory of trARPES encounters problems of gauge invariance. We discuss the fully gauge invariant theory of trARPES [2] with application to THz dynamics. Finally, we present joint experimental and theoretical results on the ultrafast THz dynamics in the topological insulator Bi_2Te_3 , where we explored the sub-cycle regime of trARPES. Despite the ultrashort probe pulse, clear signatures of Floquet-Bloch states are observed in real-time, allowing for tracing the birth an ultimately dephasing of the Floquet states [3].

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Extending NEGF simulations to long times: Memory truncation and a non-perturbative Quantum Boltzmann equation

Martin Eckstein, University of Hamburg, Germany

Collective orders and photo-induced phase transitions in quantum matter can evolve on timescales which are orders of magnitude slower than the femtosecond processes related to electronic motion in the solid. This separation of timescales poses a mayor challenge to non-equilibrium Green's functions simulations, because the Kadanoff-Baym equations for the two-time Keldysh Green's functions involve a memory kernel which results a cubic scaling of the computation time with the maximum simulation time. In the first part of my talk, I will discuss progress based on a truncation of the memory kernel, which can can reduce the computational cost to linear scaling. The truncation is particularly easy to control within dynamical mean-field solutions based on a purely local self-energy. Here, simulation times up to two orders of magnitude longer are accessible both in the weak and strong coupling regime, allowing for a study of long-time phenomena such as the crossover between pre-thermalization and thermalization dynamics. Another idea to potentially deal with the separation of timescales are quantum Boltzmann equations. Here I will present a quantum Boltzmann equation which is based on a non-perturbative scattering integral, and makes no assumption on the spectral function such as the quasiparticle approximation [2]. In particular, a scattering integral corresponding to non-equilibrium dynamical mean-field theory is evaluated in terms of an Anderson impurity model in a non-equilibrium steady state with prescribed distribution functions. This opens the possibility to investigate dynamical processes in correlated solids with quantum impurity solvers designed for the study of non-equilibrium steady states.

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Hierarchical low-rank matrix methods for the numerical solution of the Kadanoff-Baym equations

Jason Kaye, Flatiron Institute, Simons Foundation, United States of America

The Kadanoff-Baym equations (KBE) for the nonequilibrium Green's function suffer from an $\mathcal{O}(N^3)$ scaling in the number N of time steps, which can be a prohibitive cost for applications in which long-time propagation is required to extract well-resolved physical observables. Several approaches to reducing this computational complexity have been proposed, including the generalized Kadanoff-Baym ansatz, memory truncation methods, and dynamic mode decomposition. We have recently proposed an algorithm which uses on-the-fly hierarchical off-diagonal low-rank compression to reduce the computational complexity to $\mathcal{O}(N^2) \log N$ for a class of systems which appears to be quite general. The algorithm does not require memory truncation, and it computes the Green's function with a user-controllable accuracy with respect to the exact solution of the full KBE. I will describe the details of the algorithm, and give an update of progress in algorithmic improvements and extensions, applications, and a software implementation.

Learning Feynman diagrams with tensor networks

Xavier Waintal, Pheliqs, CEA Grenoble, France

I will discuss our recent efforts to calculate many-body effects within the Keldysh formalism. Our technique combines a systematic expansion in terms of Feynman diagrams with tensor network techniques to calculate the corresponding multi-dimensional integrals. compared to previous approaches based on (diagrammatic) quantum Monte-Carlo sampling, we obtain a convergence that is dramatically faster and also appears to be immune from the difficulties associated with the sign problem.

I will illustrate the technique with calculations for the out-of-equilibrium Anderson problem, showing the emergence of Kondo physics in an interaction quench as well as transport calculations.

Compressing quantum dynamics

Denis Golez, Jozef Stefan Institute, Slovenia

The nonequilibrium evolution in quantum many-body systems is accompanied by a complexity growth that prevents the exploration of long-time dynamics. We will present a numerical scheme based on nonequilibrium Greens functions, where we tackle the complexity problem by compressing the evolution on-the-fly. The advance is based on an empirical observation that nonequilibrium Greens functions have a hierarchical low-rank structure making it highly compressible. Moreover, we use the compressed representation to reduce the computational cost in the solution of the nonequilibrium Dyson equation from the previous cubic to near quadratic. In the second part, we will present several examples where this scheme provides practical advantages and can reveal new insights into the nonequilibrium dynamics. In particular, we will focus on the dynamics in symmetry-broken systems and show how compression structure can serve as a new measure for nonthermal phase transition. In the end, we will comment on the physical origins of compressibility and when we can expect such techniques to perform superiorly.

Hierarchical Decomposition Scheme for Non-Equilibrium Quantum Systems

Thomas Blommel, University of Michigan, United States of America

The Kadanoff Baym equations are a set of coupled non-linear differential equation that describe the time-dependence of non-equilibrium Green's functions. These Green's functions are important objects because they give us access to all one-body observables. Solving these equations in full scales cubically with the number of timesteps, which prohibits long time propagation of the equations. Many methods have been proposed for circumventing this cubic scaling, many of which rely on uncontrolled approximations to the equations of motion. Recently, there has been success in decreasing the scaling of these equations by utilizing hierarchical decomposition methods. This method compresses the Green's function away from the diagonal in order to drastically reduce the amount of memory used as well as the computation time. We have implemented this scheme for multi-orbital models as well as for high order integrators. We show results for the compressibility as well as the speed-up in computation time for realistic molecular systems.

Fluctuations Approach to the Nonequilibrium GW Approximation and its Application to Spectral Two-Particle Observables

Erik Schroedter, Kiel University, Germany

The dynamics of quantum many-body systems following external excitation can be successfully studied using nonequilibrium Green functions (NEGF) or reduced density matrix methods. Approximations are introduced via a proper choice of the many-particle selfenergy or decoupling of the BBGKY-hierarchy, respectively. These approximations are based on Feynman's diagram approaches or on cluster expansions into single-particle and correlation contributions. In a recent paper [1] we have presented a different approach where, instead of equations of motion for the many-particle NEGF (or density matrices), equations for the correlation functions of fluctuations are considered. In particular, this approach is characterized by its capability to be combined with stochastic methods [2], leading to the stochastic GW and polarization approximations that are closely related to the nonequilibrium GW approximation. Here, we extend this approach to allow for direct access to spectral two-particle observables depending on the specific ordering of the underlying operators. In particular, we apply this extension to the calculation of the density response function and dynamic structure factor of correlated Hubbard clusters.

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[2] D. Lacroix, S. Hermanns, C. M. Hinz, and M. Bonitz, Phys. Rev. B **90**, 125112 (2014)

Time-resolved quantum transport with correlated nonequilibrium Green's functions

Riku Tuovinen, University of Jyväskylä, Finland

The theory of quantum transport has been a mature field since the pioneering works by Meir, Wingreen, and Jauho [1,2], who provided a general formula for the time-resolved current through correlated junctions in terms of nonequilibrium Green's functions (NEGF). Given the solution to the underlying Kadanoff-Baym equations (KBE) [3], it is possible to simulate not only charge and energy currents but also higher-order moments such as current correlations and the associated noise spectra [4].

While the two-time structure of the Green's function brings about a significant computational challenge, especially for efficiently describing ultrafast transport phenomena, fully conserving and systematic solutions to the embedded KBE have been outlined [5]. A simplified, approximate scheme of reconstructing the two-time objects via the generalized Kadanoff-Baym ansatz (GKBA) [5] reduces the computational complexity of the KBE, enabling fast simulations of open quantum systems [6].

Following recent progress in casting the GKBA equations in time-linear form [7], here we express the Meir-Wingreen formula in terms of a single-time quantity, thus allowing to simulate the dynamics of any open system at a time-linear cost [8]. Furthermore, electronic correlations and decoherence mechanisms — previously unattainable in practice — are incorporated through state-of-the-art approximations.

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An exact stochastic approach for inelastic transport through a molecular junction

Matthew Lane, King's College London, United Kingdom

We propose a method of calculating electronic current in a molecular junction where the coupling between electrons and harmonic phonons in the central region is accounted for exactly, and apply it to a quantum wire. We derive an electronic (reduced) density matrix of the whole system by integrating out the phonons in the central region using the method of path integrals [1]. This results in a modified Liouville equation for the density matrix of the electronic subsystem corresponding to a stochastic non-Hermitian Hamiltonian [2] in which the phonons are replaced by coloured complex-valued noises whose correlation functions encode the properties of the phonon bath exactly. Based on this Liouville equation, we develop an extension of the NEGF formalism with several distinctive features: (i) since the noises are complex, the Hamiltonians on the upper/lower branches of the complex-time contour are different, and generalised Langreth rules are required [3]; (ii) the right-most time on the contour is introduced as a third time argument in the GF, making it explicitly a three-time object [4]; (iii) partitionless thermalization of the junction is similarly obtained via stochastic evolution in imaginary time, prior to any arbitrarily time-dependent external bias. Finally, we derive an expression for the current in the form of the Born series w.r.t the noises and the phonon-free NEGFs of the junction.

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[3] L Kantorovich. Generalized Langreth rules. PRB, 2020.

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Tackling time-dependent quantum many-body systems with the time-dependent two-particle reduced density matrix

Iva Brezinova, TU Wien, Austria

Solving the time-dependent Schrödinger equation sufficiently accurately for strongly non-equilibrium or strongly driven quantum many-body systems remains a major challenge to date. This is particularly true for systems where correlations are important and cannot be treated at any mean-field level. Such systems are at the forefront of current experimental research, triggered by the great experimental control over ultracold quantum simulators as well as by the availability of ultrafast and strong laser fields that allow pump-probe experiments of quantum systems in a controlled way. In my talk, I will present our approach to tackle time-dependent driven few- and many-body systems based on the two-particle reduced density matrix. By avoiding the wavefunction altogether, the intractable exponential scaling with particle number can be avoided, but other challenges have to be overcome. I will review the essential building blocks of our time-dependent two-particle reduced density matrix method and demonstrate applications ranging from laser-driven multi-electron atoms to quench dynamics in the Fermi-Hubbard model.

NEGFs approach to temperature driven two-level atom

Nicolino Lo Gullo, Università della Calabria, Italy

Recent experiments have shown that it is possible to perform time-resolved measurements of the temperature at nanoscale. This opens new possibilities in the field of thermotronics which aims to develop thermal circuits that operate with temperature biases and heat currents just as how electronic circuits are based on voltages and electric currents. Here, we investigate a thermal half-wave rectifier based on a quantum two-level system (a qubit) that is driven by a periodically modulated temperature difference across it. To this end we present a nonequilibrium Green's function technique, which we extend to the time domain to account for the time-dependent temperature in one of two thermal reservoirs connected to the qubit. We find that the qubit acts a thermal diode in parallel with a thermal capacitor, whose capacitance is controlled by the coupling to the reservoirs. These findings are important for the efforts to design nonlinear thermal components such as heat rectifiers and multipliers that operate with more than one diode.

Nuclear Applications of Nonequilibrium Green's Functions

Pawel Danielewicz, Michigan State University, United States of America

Application of Nonequilibrium Green's Functions (NGF) in a couple of nuclear projects will be discussed. In one project, the impact of short-range correlations is studied, on the thermalization of nuclear slabs initiated with collective oscillations. The short-range range correlations are incorporated in terms of nucleonic self-energies in the Born approximation. In the second project, still in progress, the problem of a freeze-out of deuterons in thinning nuclear matter is studied. Deuteron binding and nucleon-nucleon scattering are described in terms of the same separable interaction. The coupled equations for deuteron and nucleon NGF are solved self-consistently.