PROGRESS IN NON-EQUILIBRIUM GREEN'S FUNCTIONS VI (PNGF6)

Lund, 17-21 August 2015

Programme

Contents

1 General Information

International Advisory Board: M. Bonitz, P. Danielewicz, F. Jahnke, A.-P. Jahuo, R. van Leeuwen.

Organising Committee: C. Verdozzi (Chair), A. Wacker, C.-O. Almbladh.

Support: The organisers acknowledge support from the Swedish Research Council and from the "Christian-Albrechts-Universität Kiel via the Kiel nano and surface science center (KinSis)"

Workshop Venue: The Department of Physics, University of Lund
Postal address: Box 118, 221 00 LUND -Sweden
Visiting address (Conference Entrance): Professorsgatan 1
Phone (switchboard): +46-(0)46 2220000

Talks in: Rydberg Lecture Hall (a.k.a. Rydbergsalen), 4th floor, H-building at Fysicum, Professorsgatan 1 (map at the end of this booklet).

Conference Secretary: Katarina Lindqvist,
katarina.lindqvist@matfys.lth.se, Telephone: +46-(0)46 2229090.

Internet Access: wi-fi available in all Lund University areas via "eduroam".

Posters: to be displayed in room H421/22 (next to Rydbergsalen). Posters can be put up after 10:30 am Tuesday 18th and stay on display until the end of the day.

Breaks: There will be a 30 minute break after the second morning talk and and a 30 minute break in the afternoon. Coffee and tea will be available in front of Rydbergsalen.

Conference desk: located outside Rydbergsalen.

Transportation: From Botulfplatsen (or from near the Central Railway Station), take bus #1 in the direction of Östra Torn, and (after 5-7 minutes) get off at the bus stop "Fysiologen". The bus runs every 15 minutes.

Social Programme: Details at the conference desk.

2 Workshop Format

The workshop continues the tradition of the previous meetings held in Rostock (1999), Dresden (2002), Kiel (2005), Glasgow (2009), Jyväskylä (2012) [1].

A central objective of the meeting is to provide an interdisciplinary and informal gathering of theorists for discussion of theoretical concepts across many fields of non-equilibrium physics. Further, by having experimentalists among the speakers, the conference aims to establish a robust connection between emerging experimental techniques and the theoretical NGF community.

This will occur via a range of invited (I) talks addressing topics in specific fields (40 minutes plus 5 minutes discussion) and contributed talks (C), which are allocated 20 minutes plus 2 minutes discussion time. Discussions should be lively; interrupting speakers (in a friendly and polite way, of course) is encouraged.

Equally important are the posters (P) (with a maximum size A0, portrait orientation), for which an afternoon session is provided. There will be mini-talks (3 minutes each) for the poster contributors to advertise their work. These mini-talks will be given in the (alphabetical) order established in Sect. 5.

Facilities will be available for PowerPoint or similar presentations via Data Projector. Overhead projection facilities will also be available. There will be two social events (conference reception and excursion with social dinner).

As examples of subtopics of the conference, we mention A) Developments of NGF technique for quantum systems: General aspects, Relativistic field theories, Strongly correlated systems, Electron-boson systems; B) NGF and specific systems: Nanotransport, Solid state optics and kinetics, Superconductivity, Nuclear Matter; C) Areas of potential interest for NGF, other methods and experiment, e.g. Time-Dependent Spectroscopy; D) Efficient Implementations for simulations of realistic, large scale systems.

[1] for information about past events, see http://www.theo-physik.uni-kiel.de/bonitz

3 Workshop Programme at a Glance

	Mon 17 Aug (2015)	Tue18	Wed 19	Thu 20	Fri 21
9:00		Danielewicz	van Leeuwen	Werner	Wang
9:45		Thygesen	Lipavsky	Potthoff	Jahnke
10:30		*Break*	*Break*	*Break*	*Break*
11:00		Schüler	Winge	Arrigoni	Kaasbjerg
11:22		Sentef	Hopjan	Strand	Schlünzen
11:45	**REGISTRATION**	Sörensen	L'Huillier	Lindroth	Aeberhard
12:30	**REGISTRATION**	*Lunch*	*Lunch*	*Lunch*	*Lunch*
13:40	**Welcome and Opening**				
14:00	Jauho	Reining	Hermanns	Gross (13:40)	Pavlyukh
14:45	Galperin	Poster ads (13× 3 min ea.)	Balzer	Stefanucci (14:25)	**Closing Remarks/END**
15:30	*Break*	*Break*	*Break*	*Excursion*	
16:00	Kubis	Knezevic	Pereira		
16:45	Garny	Köhler Poster ads (4 × 3 min ea.)	Citro		
17:30		**Poster Session**			
18:30	**Reception at Hotel**	-		**18:00 Conf. Dinner**	

4 Workshop Programme: Day Calendar

Monday 17th, August 2015

Morning

11:00 - 13:40 Registration

Afternoon

13:40 - 14:00 Welcome and Opening

14:00 - 14:40 **A. P. Jauho**,
Green's function techniques applied to large scale nanostructuring of graphene

14:45 - 15:25 **M. Galperin**,
Transport and optical response in a nanoscale device

15:30 - 16:00 Coffee Break

16:00 - 16:40 **T. Kubis**,
Contact self-energies: More than simple boundary conditions

16:45 - 17:25 **M. Garny**,
Renormalization out of equilibrium in relativistic quantum field theory

18:30 - Reception at the Nordic Hotel

Tuesday 18th, August 2015

Morning

09:00 - 09:40 **P. Danielewicz**,
Progress in Application of Nonequilibrium Green's Functions to Nuclear Reactions

09:45 - 10:25 **K. Thygesen**,
Many-body GW calculations for molecular transport junctions

10:30 - 11:00 Coffee Break

11:00 - 11:20 **M. Schüler**,
Time propagation of coupled fermionic-bosonic Kadanoff-Baym equations for plasmon-assisted double photoemission

11:23 - 11:43 **M. Sentef**,
Theoretical investigations of laser-driven superconductivity

11:45 - 12:25 **S. Ristinmaa Sörensen**,
Double ionization: investigating mechanisms and time scales

Lunch (12:30 - 14:00)

Afternoon

14:00 - 14:40 **L. Reining**,
A direct approach to the calculation of many-body Green's functions

14:45 - 15:25 **Mini-talks** for posters P1-P13 (3 minutes each)

15:30 - 16:00 Coffee Break

16:00 - 16:40 **I. Knezevic**,
Coupling Electrons, Phonons, and Photons at the Nanoscale: Challenges in Nonequilibrium Transport Simulation

16:45 - 17:05 **H. S. Köhler**,
Nuclear Response Functions by two-time Green's functions

17:08 - 17:24 **Mini-talks** for posters P14-P17(3 minutes each)

17:30 - POSTER SESSION (Room H421/22, next to Rydbergsalen)

Wednesday 19th, August 2015

Morning

09:00 - 09:40 **R. van Leeuwen**,
Kadanoff-Baym equations for time-dependent coupled electron-boson systems

09:45 - 10:25 **P. Lipavský**,
Formation of superconducting condensate under non-equilibrium conditions

10:30 - 11:00 Coffee Break

11:00 - 11:20 **D. Winge**,
Second Harmonic Generation in Quantum Cascade Lasers Simulated using Green's Functions

11:23 - 11:43 **M. Hopjan**,
Real-time dynamics of Hubbard-type model systems via a combination of the Kadanoff-Baym formalism with adiabatic DFT

11:45 - 12:25 **A. L'Huillier**,
Ultrafast Atomic Physics using Attosecond Pulses

Lunch (12:30 - 14:00)

Afternoon

14:00 - 14:40: **S. Hermanns**,
Nonequilibrium Green functions - Going beyond standard approximations for extended systems with state-of-the-art computing

14:45 - 15:25 **K. Balzer**,
Solving the Kadanoff-Baym equations via the auxiliary Hamiltonian representation: method and applications

15:30 - 16:00 Coffee Break

16:00 - 16:40 **M. Pereira**,
Nonequilibrium Green's Functions Theory for Transport and Optics of TERA-MIR Materials and Devices

16:45 - 17:25 **R. Citro**,
Spin pumping through an interacting quantum dot

Thursday 20th, August 2015

Morning

09:00 - 09:40	**P. Werner**, *Nonequilibrium dynamics of electron-phonon systems*
09:45 - 10:25	**M. Potthoff**, *Non-equilibrium self-energy-functional theory*
10:30 - 11:00	Coffee Break
11:00 - 11:20	**E. Arrigoni**, *Steady-state dynamical mean-field theory within an auxiliary master equation approach*
11:23 - 11:43	**H. Strand**, *Real-time dynamics of lattice bosons in high dimensions from nonequilibrium dynamical mean-field theory*
11:45 - 12:25	**E. Lindroth**, *Study of attosecond dynamics in atomic many-body systems using complex scaling*

Lunch (12:30 - 13:45)

Afternoon

13:40 - 14:20	**E. K. U. Gross**, *Some thoughts on the electron-phonon interaction*
14:25 - 15:05	**G. Stefanucci**, *NEGF approach to pump-probe photoabsorption spectroscopy*
15:30 -	Excursion (Guided tour of Kulturen and visit to Lund Cathedral)
18:00 -	Conference dinner (Kulturen Restaurant)

Friday 21st, August 2015

Morning

09:00 - 09:40	**J. Wang**, *Current conserving theory on shot noise*
09:45 - 10:25	**F. Jahnke**, *Semiconductor nanolaser with superradiant light emission connecting carrier and photon correlations*
10:30 - 11:00	Coffee Break
11:00 - 11:20	**K. Kaasbjerg**, *Non-equilibrium Green's function approach to light emission from plasmonic contacts*
11:23 - 11:43	**N. Schlünzen**, *Nonequilibrium Green functions approach to transport and diffusion in strongly coupled finite quantum systems*
11:45 - 12:25	**U. Aeberhard**, *Nonequilibrium Green's function theory of nanostructure solar cells*

Lunch (12:30 - 14:00)

Afternoon

14:00 - 14:40	**Y. Pavlyukh**, *Non-equilibrium approach to scattering theory and to plasmon losses in photoemission*
14:45	Closing Remarks

5 List of Posters

P1 BAUCH, Sebastian
The time-dependent generalized-active-space configuration interaction approach to correlated ionization dynamics
P2 BONITZ, Michael
Path integral Monte Carlo for correlated fermions - ways around the sign problem
P3 BOSTRÖM, Emil
Time-Resolved Spectroscopy and Dissociation Dynamics of Atoms at Surfaces: Insight from a Model-System Approach
P4 DAMTIE, Fikeraddis Ahmed
Time dependent study of multiple exciton generation (MEG) in nanocrystal QDS
P5 DORDA, Antonius
Spectral and transport properties of the nonequilibrium Anderson impurity model: auxiliary master equation approach within matrix product states
P6 FRANCKIÉ, Martin
Non-Equilibrium Green's Functions as a Validation Tool for QCL Modeling
P7 HERRMANN, Andreas
Non-Equilibrium Dynamical Cluster Approximation of the Falicov-Kimball Model
P8 HINZ, Christopher
Towards a Unified Numerical Framework for Quantum Mechanical Simulations
P9 HYRKÄS, Markku
Computing Exact Self-Energies with Polynomial Expansion
P10 KARLSSON, Daniel
NEGF for studying strongly interacting systems in quantum transport
P11 LANI, Giovanna
The SCE functional in the time domain: insights into its formal properties
P12 RIDLEY, Michael
Generalised Theory of Current Noise for an Arbitrary Time-Dependent Bias
P13 SHAHID, Nazish
Different forms of the Kadanoff-Baym equations in quantum statistical mechanics
P14 TANG, Gaomin
Full-counting statistics of charge and spin transport in the transient regime
P15 TITVINIDZE, Irakli
Non-equilibrium inhomogeneous DMFT for correlated Heterostructures
P16 TUOVINEN, Riku
Extending the time-dependent Landauer-Büttiker formalism to superconducting junctions and arbitrary temperatures
P17 YANG, Kaike
Dynamical correction of thermoelectric coefficients for strongly interacting electrons in the Coulomb blockade regime

6 List of Abstracts

I=Invited talk, C= Contributed talk, P= Poster presentation.

AEBERHARD, Urs (I)

Nonequilibrium Green's function theory of nanostructure solar cells

Urs Aeberhard

Abstract: The last two decades have seen the emergence of a variety of novel photovoltaic device concepts aiming at a solar energy conversion efficiency beyond the limitations of conventional bulk semiconductor single junction technologies. The implementation of such concepts as, the solar cells relying on intermediate bands, hot carriers or multiple-exciton generation, are largely based on the exploitation of the peculiar and tunable optoelectronic properties of nanostructure device components. The resulting deviation from the bulk-like behaviour conventionally assumed in the description of photovoltaic devices prevents the use of the standard semiclassical theory for the investigation and simulation guided optimization of such solar cell architectures. In this talk, an advanced and comprehensive framework for the theoretical description of nanostructure solar cell operation is presented, which relies on a non-equilibrium quantum statistical mechanics formulation of the photovoltaic processes in open quantum systems, corresponding to a combination of the nonequilibrium Green's function formalisms for inelastic steady-state quantum transport and quantum optics. After an outline of the general theory framework with focus on the specifics of the photovoltaic device operation mode, applications to the simulation of different nanostructure solar cell types are discussed.

ARRIGONI, Enrico (C)

Steady-state dynamical mean-field theory within an auxiliary master equation approach

Enrico Arrigoni, Antonius Dorda, Martin Nuss, Michael Knap, Irakli Titvinidze, Wolfgang von der Linden

Abstract: We present a method to compute electronic steady state properties of strongly correlated quantum systems out of equilibrium within dynamical mean-field theory (DMFT) [1]. The DMFT correlated impurity problem is mapped onto an auxiliary open system consisting of a small number of bath orbitals coupled to the interacting impurity and to Markovian reservoirs described by a generalized Lindblad equation [2,3]. The parameters of the auxiliary open system are used to optimize the mapping, which becomes exponentially exact upon increasing the number of bath orbitals. The auxiliary system is then solved by exact diagonalisation of the corresponding many-body non-Hermitian Lindblad equation, which allows to evaluate Green's functions directly in steady state upon bypassing the initial transient dynamics [3]. The approach can be regarded as the non-equilibrium extension of the exact-diagonalization based DMFT, and introduces appropriate absorbing boundary conditions for a many-body system out of equilibrium.
[1] J.K. Freericks et al., Phys. Rev. Lett. 97, 266408 (2006) [2] E. Arrigoni et al.,

Phys. Rev. Lett. 110, 086403 (2013) [3] A. Dorda et al., Phys. Rev. B 89, 165105 (2014).

BALZER, Karsten (I)

Solving the Kadanoff-Baym equations via the auxiliary Hamiltonian representation: method and applications

Karsten Balzer

Abstract: The Kadanoff-Baym equations (KBE), which are equations of motions with a long-range memory kernel for real-time Green's functions, underlie many numerical approaches based on the Keldysh formalism. In this talk, we review the possibility that the problem of solving the KBE can be mapped onto a noninteracting auxiliary Hamiltonian with additional bath degrees of freedom [1]. The solution of the auxiliary model does not require the evaluation of a memory kernel and can thus be implemented in a very memory efficient way. The mapping is derived for a self-energy which is (sufficiently) local in space, and it is shown that different self-energy decomposition schemes can be applied to generate the bath parameters [2]. Concerning the latter, we particularly report on the use of the Cholesky decomposition in combination with a suitable coarse graining. As applications of the method, we (i) present results for an interaction quench in the Hubbard model for an optical lattice with a narrow confinement, finding signatures of a two-stage relaxation, and (ii) simulate the stopping dynamics for swift charged particles that penetrate through fragments of a Honeycomb lattice. In both cases electronic correlations are treated on the level of inhomogeneous dynamical mean-field theory using second-order weak-coupling perturbation theory.
[1] K. Balzer and M. Eckstein, Phys. Rev. B 89, 035148 (2014); [2] C. Gramsch, K. Balzer, M. Eckstein and M. Kollar, Phys. Rev. B 88, 235106 (2013)

BAUCH, Sebastian (P)

The time-dependent generalized-active-space configuration interaction approach to correlated ionization dynamics

S. Bauch, H.R. Larsson, C. Hinz, M. Bonitz

Abstract: The possibility to observe the motion and interaction of electrons in the time domain due to the availability of ultrashort and strong laser pulses demands for non-perturbative theories including a systematic approach to electron-electron correlation and external short and strong electromagnetic fields. In this contribution, we present an overview on the recently formulated time-dependent generalized-active-space formalism for atomic and molecular photoionization phenomena [1,2]. We show details of the implementation using a combination of localized and grid-like basis functions to allow for good descriptions of both, the bound and the scattering part of the problem. As an example, we address the correlated ionization dynamics and photoelectron angular distributions of diatomic molecules in strong fields and discuss correlation effects in the direction dependence of electron emission [3].
[1] D. Hochstuhl and M. Bonitz, Phys. Rev. A 86 053424 (2012) [2] S. Bauch, L.K. Srensen and L. B. Madsen, Phys. Rev. A 90 062508 (2014) [3] S. Bauch,

H.R. Larsson, B. Hartke, and M. Bonitz, in preparation (2015)

BONITZ, Michael (P)
Path integral Monte Carlo for correlated fermions - ways around the sign problem
T. Schoof, S. Groth, J. Vorberger, and M. Bonitz

Abstract: Correlated fermions at finite temperature are of interest in many fields, including condensed matter, ultracold atoms and dense plasmas. Path integral Monte Carlo (PIMC) has been the method of choice for an ab initio description of the thermodynamics. It is the natural extension of ground state methods such as diffusion Monte Carlo (DMC). Yet, as DMC, PIMC is hampered by the notorious sign problem that prevents simulations at strong degeneracy. Our way to "avoid" it consists in using two complementary approaches. I will first present configuration PIMC - a method that allows for ab initio simulations exactly at strong degeneracy [1,2]. Second, I discuss a novel approach - permutation blocking PIMC [3] - that is capable to dramatically improve the performance of coordinate space approaches.
[1] T. Schoof M. Bonitz, A. Filinov, D. Hochstuhl, and J.W. Dufty, Contrib. Plasma Phys. 51, 687 (2011) [2] T. Schoof, S. Groth, J. Vorberger, and M. Bonitz, submitted for Phys. Rev. Lett. (2015), arXiv:1502.04616 [3] T. Dornheim, S. Groth, A. Filinov and M. Bonitz, submitted for publication (2015)

BOSTRÖM, Emil (P)
Time-Resolved Spectroscopy and Dissociation Dynamics of Atoms at Surfaces: Insight from a Model-System Approach
E. Boström, A. Mikkelsen and C. Verdozzi

Abstract: We consider a finite-system approach to pump and probe real-time dynamics in adsorbates, which merges in the time domain elements from the Anderson-Newns-Grimley model of chemisorption, the charge-transfer model of core-hole photoemission, and the Shin-Metiu model of atomic desorption. For our finite system, an exact numerical solution is possible, and several competing time-scales (electron interactions, core-hole relaxation, plasmon screening and anharmonic nuclear dynamics) can be exactly and simultaneously taken into account. We find that the desorption rate is enhanced by the presence of a surface. Conversely, the electron correlations at the adsorbate decrease the desorption energy, but at the same time they quench the electron motion; this results in an overall reduced dissociation rate. We also address the role played by the structure of the external fields: namely, we observe a strong dependence of the desorption rate on the time structure of the perturbing pulse: a 6fs and 35fs pulse of equal integrated intensity give radically different yields, favoring dissociation by the shorter pulse. For two-pulse setups, we find an increase in desorption yield at pulse intervals which match the plasmon frequency, suggesting an avenue for coherent control and optimization (for this setup, the phase-envelope relation of the later pulse also is of importance). Finally, we briefly discuss the validity of the Ehrenfest approximation for nuclear dynamics, and possible directions for future work.

CITRO, Roberta (I)
Spin pumping through an interacting quantum dot
Roberta Citro

Abstract: Within the nonequilibrium Green's-function formalism we have studied the time-dependent transport of charge and spin through an interacting quantum dot in different situations: either when it is sequentially coupled to a ring-shaped region in the presence of spin-orbit interaction, or when it is subject to an elastic deformation (suspended deformable dot). In the first case, the time-dependent modulation of the spin-orbit interaction along with the modulation of the dot level, induces an electrically pumped spin current at zero bias even in the absence of a charge current. The results beyond the adiabatic regime show that an additional rectification current with an anomalous current-phase relation is generated. In the case of the deformable dot, instead, the current shows an undefined parity with respect to the pumping phase, due to a dynamical phase shift caused by the elastic deformations (classical phonons). Finally, for a strongly interacting dot we show the presence of parasitic pumping currents due to additional phases caused by the interaction constraints. We discuss the relevance of our study in connection with recent experiments on out-of-equilibrium quantum dots and molecular systems for spintronics applications.

DAMTIE, Fikeraddis Ahmed (P)
Time dependent study of multiple exciton generation (MEG) in nanocrystal QDS
Fikeraddis Damtie and Andreas Wacker

Abstract: We study the exciton dynamics in an optically excited nanocrystal quantum dot. MEG is more efficient in nanostructures compared to bulk semiconductors due to enhanced Coulomb interactions and the absence of conservation of momentum[1, 2]. In the model we optically excite the system by creating a single high energy exciton in resonance to a double exciton. With Coulomb electron-electron interaction, the population can be transferred from the single exciton to the double exciton state by impact ionization (inverse Auger process). At longer time, the system relaxes back to the ground state as a result of dissipation. The ratio between the power transferred to the system per pulse energy and the recombination rate is used as a measure of how many pairs have been formed at energy near the resonance of single high energy and double exciton. Counting the recombined electron hole pairs rates we identified parameter regimes for optimal double exciton formations in small nanocrystal quantum dots. The occupation of the bi-exciton state is studied for different excitation parameters and it has been found that for certain set of parameters the probability of forming bi-excitons from single exciton (MEG) is enhanced. The maximum occupation of bi-exciton state as a function of the detuning between single exciton and bi-exciton state is calculated and it is found that the double exciton formation is possible when the two resonances are very close.
[1] W. M. Witzel, A. Shabaev, C. S. Hellberg, V. L. Jacobs, and A. L. Efros,

Phys. Rev. Lett. 105, 137401 (Sep 2010). [2] M. C. Beard, A. G. Midgett, M. C. Hanna, J. M. Luther, B. K. Hughes, and A. J. Nozik, Nano Letters 10, 3019 (2010).

DANIELEWICZ, Pawel (I)

Progress in Application of Nonequilibrium Green's Functions to Nuclear Reactions

Pawel Danielewicz, Arnau Rios and Brent Barker

Abstract: Computational difficulties aside, nonequilibrium Green's functions seem ideally suited for investigating the dynamics of central nuclear reactions. Many particles actively participate in those reactions. At the two energy extremes for the collisions, the limiting cases of the Green's function approach were successful: the time-dependent Hartree-Fock theory at low energy and Boltzmann equation at high. The strategy for computational adaptation of the Green's function to central reactions is discussed. The strategy involves, in particular, progressing through one and two dimensions to develop and assess approximations, rotation to relative and average coordinates, discarding of far-away function elements, local expansion in anisotropy and preparation of initial states for the reactions through adiabatic switching on of the interactions.

DORDA, Antonius (P)

Spectral and transport properties of the nonequilibrium Anderson impurity model: auxiliary master equation approach within matrix product states

Antonius Dorda, Martin Ganahl, Hans Gerd Evertz, Wolfgang von der Linden, and Enrico Arrigoni

Abstract: The auxiliary master equation approach [1,2] allows for a direct and efficient calculation of steady state properties of correlated impurity problems out of equilibrium, as is needed e.g. for nonequilibrium dynamical mean field theory [3]. The basic idea is to replace the original impurity problem by an auxiliary one, consisting of a finite number of bath sites embedded in Markovian environments. The dynamics of this open quantum system is then described by a Lindblad equation, in which the different bath parameters are optimized by fitting the bath hybridization function in Keldysh space. Upon increasing the number of bath sites, the results can be systematically improved and the solution of the auxiliary system converges exponentially towards the exact one. A systematic study using a non-Hermitian Lanczos solver has been carried out [1] and a very good agreement with reference values was found already for rather small system sizes. Here, we present results obtained within a matrix product states based treatment of the interacting Lindblad problem [4], which turns out to be important in order to achieve an appropriate resolution of the Kondo scale for intermediate and large interactions.

[1] A. Dorda et al., Phys. Rev. B 89, 165105 (2014), [2] E. Arrigoni et al., Phys. Rev. Lett. 110, 086403 (2013), [3] J.K. Freericks et al., Phys. Rev. Lett. 97, 266408 (2006), [4] A. Dorda et al., in preparation.

FRANCKIÉ, Martin (P)
Non-Equilibrium Green's Functions as a Validation Tool for QCL Modeling
Martin Franckié, David O. Winge, and Andreas Wacker

Abstract: Quantum Cascade Lasers (QCLs) [1] are intersubband lasers emitting from the THz to mid-IR. Much effort is put into simulating these devices in order to improve their performance. The complicated many-body problem requires an efficient, yet sophisticated, model. In order to investigate the level of detail required, we have performed non-equilibrium Green's function (NEGF) simulations of a THz [2] and a mid-IR QCL [3], and compared our results to simpler models. For the THz structure, employing a scattering injection scheme, both a rate equation (RE) and the NEGF models agree excellently with the experimental results. In a detailed comparison between our NEGF and two density matrix (DM) models [4] using the mid-IR QCL, it was found that in order for the DM model to produce reliable results, so-called second order currents, naturally included in the NEGF model, have to be considered; for these tunnelling injection designs, a higher sophistication is needed. In conclusion, simple approaches can be used if the relevant features are properly accounted for. In this context a fully self-consistent model like NEGF is a good tool for validating different approximations.
[1] J. Faist et al., Science 264 (1994), [2] E. Dupont et al., J. Appl. Phys. 111 (2012), [3] A. Bismuto et al., Appl. Phys. Lett. 96 (2010), [4] M. Lindskog et al., Appl. Phys. Lett. 105 (2014)

GALPERIN, Michael (I)
Transport and optical response in a nanoscale device
Michael Galperin

Abstract: Theoretical tools employed in ab initio simulations in the field of molecular electronics combine methods of quantum chemistry and mesoscopic physics. Traditionally these methods are formulated in the language of effective single-particle orbitals. We argue that in many cases of practical importance a formulation in the language of many-body states is preferable. We review methods of the nonequilibrium atomic limit and our contributions to their development and applications. In particular, model and ab initio simulations of quantum transport and optical response in molecular junctions illustrate the convenience and importance of the methodology.

GARNY, Mathias (I)
Renormalization out of equilibrium in relativistic quantum field theory
Mathias Garny

Abstract: Relativistic quantum field theory provides an extremely successful framework for describing elementary particle physics processes at high energies. While most applications are based on scattering theory or equilibrium methods, a number of interesting questions can only be addressed based on nonequilibrium techniques, mostly in the context of particle cosmology as well as heavy ion colli-

sions. In this talk we report on some progress on implementing renormalization for relativistic quantum fields far from equilibrium. While non-equilibrium methods are well-established in various approximate descriptions, a formulation that leads to manifestly cutoff-independent and non-secular evolution across all time-scales is still to be constructed. For a simple scalar QFT model, we explicitly demonstrate how renormalized Kadanoff-Baym equations can be obtained by taking into account relevant initial correlations. We verify independence of the regulator both analytically and numerically, and at all times. Finally, we comment on potential applications in inflationary cosmology.

GROSS, Eberhard (I)
Some thoughts on the electron-phonon interaction
E.K.U. Gross

Abstract: Starting from the Hamiltonian of the complete interacting system of electrons and nuclei, and performing the exact factorization of the corresponding electron-nuclear wave function, we identify what should be called "exact phonons" and the "exact electron-phonon interaction". The results are compared with the standard expressions coming from the Born-Oppenheimer approximation.

HERMANNS, Sebastian (I)
Nonequilibrium Green functions - Going beyond standard approximations for extended systems with state-of-the-art computing
Sebastian Hermanns, Niclas Schlnzen and Michael Bonitz

Abstract: NEGF have been successfully used to describe time-dependent processes in almost any field of many-body physics, from dense plasmas to baryogenesis in cosmology to atoms in laser fields [1-4]. Though in principle universally applicable, NEGF approaches are often limited with respect to basis size or approximation level. In this talk, we show how to alleviate these restrictions by use of the large-scale performance of modern vector architectures for the solution of the Kadanoff-Baym equations. We study approximation schemes from a computational point of view and detail how to decrease the computational demands, e.g. by applying the Generalized Kadanoff-Baym ansatz [5] and higher order integration schemes. The increase in achievable system size and propagation time can be used to extract high-resolution spectra and enables extrapolation to macroscopic systems.
[1] H. Haberland, M. Bonitz, and D. Kremp, Phys. Rev. E 64 026405 (2001), [2] M. Garny, A. Kartavtsev, and A. Hohenegger, Ann. of Phys. 328 1274 (2011), [3] N. E. Dahlen, and R. van Leeuwen, Phys. Rev. Lett. 98 153004 (2007), [4] R. van Leeuwen, R. Tuovinen, and M. Bonitz, J. Phys.: Conf. Ser. 427 011001 (2013), [5] S. Hermanns, N. Schlnzen, and M. Bonitz, Phys. Rev. B 90 125111 (2014)

HERRMANN, Andreas (P)
Non-Equilibrium Dynamical Cluster Approximation of the Falicov-Kimball Model
Andreas J. Herrmann and Philipp Werner

Abstract: We simulate the time-evolution of the Falicov-Kimball model after an interaction quench using a non-equilibrium generalization of the dynamical cluster approximation (DCA). By considering clusters of up to eight sites, we study how non-local correlations affect the relaxation dynamics of local and non-local observables.

HINZ, Christopher (P)
Towards a Unified Numerical Framework for Quantum Mechanical Simulations
C. Hinz, S. Bauch, S. Hermanns, N. Schlnzen and M. Bonitz

Abstract: In recent years, more sophisticated wave function[1,2] and nonequilibrium Green function[3][4] based approaches have been developed in an attempt to overcome the limitations of preceding many-particle methods. To be feasible, these approaches have to be integrated with high–performance computing (HPC). However, the advent of more complex and diverse HPC architectures - combined with the intricacy of the methods - has made this an increasingly involved task. To tackle these difficulties, we have developed a framework of highly composable and reusable components in an attempt to facilitate - among other things - rapid prototyping of new methods, convenient exchange of data and increased reuse of existing code. This has proven to be crucial during the recent development of the time-dependent restricted-active-space (TD-RASCI) method[1,2] as it relies on Hartree-Fock or similar methods to calculate the basis functions. In addition, the framework can guide and assist users in parallelizing their code across a multitude of architectures. We will showcase the first results of porting our codes to the new framework and discuss the insights gained and the obstacles encountered. [1] D. Hochstuhl, and M. Bonitz, Phys. Rev. A 86, 053424 (2012), [2] S. Bauch, L. K. Sorensen, and L. B. Madsen, Phys. Rev. A 90, 062508 (2014), [3] S. Hermanns, N. Schlnzen, and M. Bonitz, Phys. Rev. B 90, 125111 (2014), [4] R. van Leeuwen, R. Tuovinen, and M. Bonitz, Journal of Physics: Conference Series, vol. 427 (2013)

HOPJAN, Miroslav (C)
Real-time dynamics of Hubbard-type model systems via a combination of the Kadanoff-Baym formalism with adiabatic DFT
M. Hopjan, D. Karlsson, S. Ydman, C. Verdozzi and C.-O. Almbladh

Abstract: In this work, we propose a way to combine the strengths of exchange-correlations potentials from TDDFT with diagrammatic self-energies from NEGF, in a protocol aimed to avoid double-counting of interactions. The approach is compared against exact numerical methods (Exact Diagonalization and time-dependent DMRG) in systems with Hubbard-type interactions. We test the capability of the combined approximation with respect to several features: strength of

the interaction, speed and space-inhomogenity of the perturbation, system dimensionality and the system size (finite vs extended). In most of the tested regimes we observe good agreement with the exact results, and an improvement over the pure adiabatic local TDDFT or the pure Second-Born NEGF approximations. We also address the reasons behind the residual discrepancies, and briefly discuss possible directions for future work.

HYRKÄS, Markku (P)
Computing Exact Self-Energies with Polynomial Expansion
M. Hyrkäs and R. van Leeuwen

Abstract: We compute exact Green's functions for small quantum systems efficiently using a GPU accelerated polynomial expansion algorithm. This method is here applied to solve the exact interaction self-energy of a spherically symmetric Anderson impurity system which exhibits the Kondo effect.

JAHNKE, Frank (I)
Semiconductor nanolaser with superradiant light emission connecting carrier and photon correlations
Frank Jahnke

Abstract: In thermal light sources and conventional lasers the radiation stems from independent emitters, while the phenomenon of superradiance originates from a correlated electronic state similar to Bose-Einstein condensates or superconductors. The recent interest in superradiance was driven by studying these electronic correlations in connection with radiation properties. So far, superradiance was only revealed in terms of altered recombination time and dynamics, i.e., using macroscopic/classical properties of the emitted radiation. Our investigations address the link between quantum correlations of the active material and photon correlations in the emitted radiation. We use the superradiance of quantum dots in a cavity-QED laser to show a direct connection between entanglement of the emitters, superradiant pulse emission, and distinctive changes in the photon correlation function in the form of a giant bunching effect connected with super-thermal radiation. Results of a collaboration between theory and experiment are obtained for semiconductor nanolasers consisting of optical resonators with highly efficient three-dimensional mode confinement and quantum dot (QD) emitters, in which the three-dimensional carrier confinement leads to an atom-like carrier density of states. Using a microscopic theory we can identify regimes, in which the exchange of cavity photons between the QD emitters leads to the establishment of a coherent phase of the active material in a way that the excitation energy is stored in a coherent (subradiant) matter state. The associated photon trapping reduces the below-threshold photon number and leads to giant photon bunching with a second-order photon correlation function.

JAUHO, Antti-Pekka (I)
Green's function techniques applied to large scale nanostructuring of graphene
Mikkel Settnes, Stephen R. Power, Thomas Aktor, and Antti-Pekka Jauh

Abstract: Pristine graphene has no band gap which restricts its use in practical electronic devices. A way to remedy this problem is to use nanostructuring, e.g., by cutting graphene sheets into nanoribbons, by introducing periodic perturbations, or by applying sublattice asymmetric doping. All these methods of nanostructuring involve thousands if not millions of atoms and significant disorder, and therefore present a serious challenge for microscopic theoretical modelling. We have developed efficient Green's function methods to attack these problems (e.g., "patched" Green's functions which use a generalized self-energy concept, or nonequilibrium vertex corrections), and in this talk recent progress in the area will be reviewed.

KAASBJERG, Kristen (C)
Non-equilibrium Green's function approach to light emission from plasmonic contacts
Kristen Kaasbjerg and Abraham Nitzan

Abstract: We develop a theoretical framework based on the nonequilibrium Green's function formalism for the description of light emission from atomic-scale contacts. Our theory establishes a fundamental link between the finite-frequency quantum noise and AC conductance of the contact and the light emission. Calculating the quantum noise to higher orders in the interaction between the tunnel current and localized surface plasmons supported by the contact, we identify a plasmon-mediated electron-electron interaction as the source of experimentally observed above-threshold light emission from biased STM contacts.

KARLSSON, Daniel (P)
NEGF for studying strongly interacting systems in quantum transport
D. Karlsson, M. Hyrks, A.-M. Uimonen, R. van Leeuwen and C. Verdozzi

Abstract: Non-Equilibrium Green Functions (NEGF) is a powerful method for studying quantum transport. It can treat strong interactions, and also exactly incorporate macroscopic contacts in the description, through the so-called embedding technique. Here, we will present two cases in which a good description of interactions is crucial. The first case regards quantum transport through disordered chains, where we investigate how disorder effects and strong interactions compete. It is known that in equilibrium, disorder is detrimental to the conductivity. Similarly, strong interactions often decrease the conductivity. However, the competition between these two effects is known to sometimes enhance it. The case of non-equilibrium, i.e. finite bias, is much less studied. We have studied disordered and interacting short chains out of equilibrium. The chains are contacted to leads. Using the fully self-consistent second-Born approximation, we show that correlation effects in disordered chains can enhance the current through the chain,

also out of equilibrium. The second case regards quantum transport through a small number of quantum dots in the Kondo regime, where strong many-body effects open up fully transparent conductance channels. For a single dot, the equilibrium spectral function has a characteristic three-peak structure: Two Coulomb blockade peaks that are separated by the interaction strength U, and the Kondo peak that is situated at the chemical potential. Such a spectral function is difficult to obtain using standard self-consistent schemes in NEGF, as full self-consistency tends to smoothen the spectrum. At the same time, self-consistency guarantees that certain conservation laws, such as particle number conservation, are fulfilled. We here present some strategies, for example partial self-consistency, for obtaining qualitative features in the Kondo regime out of equilibrium.

KNEZEVIC, Irena (I)
Coupling Electrons, Phonons, and Photons at the Nanoscale: Challenges in Nonequilibrium Transport Simulation
I. Knezevic

Abstract: Semiconductor nanostructures find numerous applications in electronics, photonics, thermoelectrics, and phononics. Today, we understand a great deal about both semiclassical and quantum transport of the carriers of charge - electrons and holes - at the nanoscale, provided that the electrical or optical excitations are low in both frequency and intensity. However, under intense or fast excitation, interesting nanoscale phenomena emerge to reveal the intimate coupling of charge transport with the dynamics of the lattice and electromagnetic fields. Consequently, a general simulation approach to far-from-equilibrium and time-dependent transport must be a multiphysics one, requiring self-consistent coupling of the dynamics of charge carriers, phonons, and photons as they drive one another. Developing such three-pronged simulation tools is a complex endeavor. In this talk, I will discuss the associated challenges and present our recent work on the accurate simulation of (1) THz-frequency electronic transport in supported graphene with charged impurity clusters and (2) coupled electronic and thermal transport in quantum cascade lasers, including the effects of nonequlibrium phonons, coherent transport features, and going multiscale (bridging between a single stage and device-level simulation).

KUBIS, Tillmann (I)
Contact self-energies: More than simple boundary conditions
Yu He, Prasad Sarangapani, James Charles, Saima Sharmin, Junzhe Geng, Gerhard Klimeck and Tillmann Kubis

Abstract: A core feature of the nonequilibrium Green's function method (NEGF) is to separate the explicitly considered device from charge, heat, spin, etc. reservoirs. The connection between reservoirs and the device is maintained with contact self-energies. These self-energies usually represent leads that are semi-infinite, homogenous or periodic, ballistic and free of any irregularities such as defects or impurities. However, fabricated leads basically never meet these assumptions: Leads are often irregular, contain defects, have finite potential drops and host many

sources of incoherent scattering. This presentation discusses how to represent realistic, non-ideal and even irregular leads with appropriate contact self-energies. It is also shown how to include incoherent scattering in the lead to match the density of states at the device boundary and achieve reflectionless lead/device transitions. Contact self-energies can also be used to migrate the concept of reservoirs into device areas and thereby introduce efficient particle thermalization models. Even beyond NEGF, the contact self-energies can describe the impact of surface passivation and the saturation of dangling bonds. All these aspects will be discussed with results of the academic-open source nanodevice simulation tool NEMO5.

KÖHLER, H. Sigurd (C)
Nuclear Response Functions by two-time Green's functions
H.S. Köhler and N.H. Kwong

Abstract: Linear response functions are calculated for symmetric nuclear matter by time-evolving two-time Green's functions in real time. Of particular interest is the effect of correlations. The system is therefore initially time-evolved with a collision term calculated in a direct Born approximation as well as with full ring-(RPA) summation until fully correlated. An external time-dependent potential is then applied. The ensuing density fluctuations are recorded to calculate the density response. This method was previously used by Kwong and Bonitz for studying plasma oscillations in a correlated electron gas. The conserving self-energy insertions guarantees that the important energy sum-rule for the response functions is satisfied as our method generates the full vertex-functions.

L'HUILLIER, Anne (I)
Ultrafast Atomic Physics using Attosecond Pulses
Anne L'Huillier

Abstract: The interaction of atoms with intense laser radiation leads to the generation of high-order harmonics of the laser field. In the time domain, this corresponds to a train of pulses in the extreme ultraviolet range and with attosecond duration. We will describe applications of these attosecond pulses, and in particular recent results concerning single and double photoionization dynamics.

LANI, Giovanna (P)
The SCE functional in the time domain: insights into its formal properties
Giovanna Lani, Robert van Leeuwen and Paola Gori-Giorgi

Abstract: The strictly correlated electron limit (SCE) of the Hohenberg-Kohn energy functional, when employed in the DFT context, has recently shown [1] to be promising in tackling the difficult problem of strong electronic correlation. Whereas both its formal properties [2, 3] and its performance in the static case have been studied extensively, there are only a handful of studies in the time domain [4]. In this work we first investigate some properties of the adiabatic SCE (ASCE) functional, ranging from the compliance to constraints of exact many-body theo-

ries, such as the generalized translational invariance [5] and the zero-force theorem, to relations peculiar to the building blocks-so called co-motion functions- of the SCE functional. We then derive an analytical expression for the exact ASCE Hartree exchange-correlation kernel and we discuss its features in the context of long-range charge transfer excitations.
[1] F. Malet, A. Mirtschink, J. C. Cremon, S. M. Reimann, and P. Gori-Giorgi, Phys. Rev. B 87, 15146 (2013), [2] M. Seidl, P. Gori-Giorgi and A. Savin, Phys. Rev. A 75, 042511 (2007), [3] P. Gori-Giorgi, G. Vignale and M. Seidl, J. Chem. Theory Comput. 5, 743 (2009), [4] A. Mirtschink, PhD thesis, Energy Density Functionals from the Strong-Interaction Limit of Density Functional Theory (2014), [5] G. Vignale, Phys. Rev. Lett. 74, 3233 (1995)

LINDROTH, Eva (I)
Study of attosecond dynamics in atomic many-body systems using complex scaling
Eva Lindroth, Marcus Dahlström, Tor Kjellsson and Jimmy Vinbladh

Abstract: The possibility to produce light pulses in the attosecond domain has recently made it possible to explore the temporal aspects of atomic processes such as photoionization. Typically experiments use a pump and probe scenario where the delay between two phase-locked laser pulses of different colours serves as a "clock". Time is in quantum mechanics however encoded in the wave-function phase, and it is consequently phase differences which are directly accessible experimentally. Here I will discuss how we can calculate the scattering phase of the photo-electron after multi-photon absorption with the technique of (exterior) complex scaling. This technique is a way to impose outgoing boundary conditions and to obtain the analytic continuation of the Green's function. It has been used extensively on resonant phenomena, but is an important tool also in connection with short laser pulses and time-dependent processes.

LIPAVSKÝ, Pavel (I)
Formation of superconducting condensate under non-equilibrium conditions
Pavel Lipavský

Abstract: The formation of the condensate is studied using the two-particle T-matrix. An effect of a non-equilibrium distribution of electrons on the condensate is found, in particular, the normal current enters the gradient term of the Ginzburg-Landau theory leading to observable corrections in the near subgap linear response. The problem of selfconsistency in the T-matrix approach is discussed.

PAVLYUKH, Yaroslav (I)
Non-equilibrium approach to scattering theory and to plasmon losses in photoemission
Y. Pavlyukh

Abstract: The method on non-equilibrium Green's functions (NEGF) is a versa-

tile tool to treat processes evolving in time. At the same time this mathematical formalism also beneficial for the treatment of steady-state scenarios. We will consider two such examples: the double-photoemission and the ground state of a deep core-electron coupled to plasmonic excitations in a solid. The double-photoemission (DPE) is a process in which a system absorbs one photon and emits two electrons. They have to be measured in coincidence in order to be distinguished from the more probable sequential single photoemission which involves two independent electrons. As with any type of photoemission the major theoretical challenge is to account for the final state of the target, i.e., to exclude secondary and Auger electrons from the consideration. This is achieved with the Feshbach projection operator formalism. When translated to NEGF language it yields a set of rules allowing to construct the diagrammatic perturbation theory of DPE. Our approach allows in principle to treat intrinsic and extrinsic losses in photoemission on equal footing. For the photoemission from deep core levels the presence of satellites in the spectral function is a marked feature of the energy losses. They are caused by the generation of plasmons. We again use NEGF approach to perturbatively and self-consistently compute the satellite spectrum of a model system representing exactly this scenario.

PEREIRA, Mauro (I)

Nonequilibrium Green's Functions Theory for Transport and Optics of TERA-MIR Materials and Devices

Mauro Fernandes Pereira

Abstract: The predictive simulation of materials and devices for THz and Mid Infrared Radiation (TERA-MIR) is a fascinating topic of modern physics. The scattering and dephasing mechanisms in the THz range can be of the same order of magnitude as the transition energies and thus fully quantum mechanical approaches are required. In this talk, I review a predictive Nonequilibrium Green's Functions (NEGF) approach that has successfully described transport properties of Quantum Cascade Lasers (QCLs) in the THz range. Dynamically screened electron-electron, electron impurity and electron-phonon scattering in fully frequency and momentum dependent approach are included in the formalism. Most of the talk will be dedicated to describing the mathematical details of the approach for QCLs and comparisons with experimental data will be shown. QCLs are after all complex superlattices and in the final part of the talk, an extension of the approach including a Photon Green's Functions will be used to describe optical nonlinearities of superlattices within an anisotropic medium approach and in the end, the isotropic limit will be taken, describing mid infrared dilute semiconductor systems. The combined role of scattering and dephasing as well as many particle effects will be used to explain recent experimental data for luminescence with a complex evolution as a function of temperature. The author acknowledges support from MPNS COST ACTION MP1204 - TERA-MIR Radiation: Materials, Generation, Detection and Applications and BM1205 European Network for Skin Cancer Detection using Laser Imaging.

POTTHOFF, Michael (I)
Non-equilibrium self-energy-functional theory
Michael Potthoff

Abstract: Using perturbation theory to all orders, the grand potential of a system of strongly correlated electrons can be expressed as a functional of the self-energy such that the physical self-energy is a stationary point. Non-perturbative approximations may be constructed by restricting the domain of the self-energy functional to a subspace of trial self-energies spanned by an exactly solvable reference system [1]. This comprises powerful approximations such as the dynamical mean-field theory and the variational cluster approximation. Here we show how this concept can be extended to the non-equilibrium case. Even for simple reference systems, accessible to exact-diagonalization methods, the non-equilibrium self-energy-functional theory [2] should provide non-perturbative approximations which are conserving in the sense of Baym and Kadanoff. Several general and practical issues, results for parameter quenches in the single-band Hubbard model, and the prospects of the new approach are discussed.
[1] M. Potthoff, Eur. Phys. J. B 32, 429 (2003), [2] F. Hofmann, M. Eckstein, E. Arrigoni and M. Potthoff, Phys. Rev. B 88, 165124 (2013)

REINING, Lucia (I)
A direct approach to the calculation of many-body Green's functions
Lucia Reining

Abstract: Many-body perturbation theory is a powerful approach to describe many properties of materials. Most often one uses Dyson equations with self-energy kernels that are approximated to low order in the interaction. In Hedin's GW approximation, for example, the self-energy is a product of the one-body Green's function and the screened Coulomb interaction. This is the state-of-the art method for bandstructure calculations in a wide range of materials. However, sometimes the GW approximation and related approaches are not sufficient, for example when one is interested in satellite structure beyond the quasi-particle peaks in the spectral function, or in the case of strong coupling, where the quasi-particle picture is no longer adequate. We explore an alternative route to the calculation of interacting electron Green's functions. It is based on a set of functional differential equations relating the one-body Green's function to its functional derivative with respect to an external perturbing potential [1]. This set of equations can be used to generate the perturbation series. Here we will show that working directly with the differential equations yields precious insight concerning some fundamental questions, guidelines for practical calculations, and methods that lead to an improved description of spectra. Results will be illustrated on various levels of approximation, ranging from simple models [2] to full ab initio calculations [3].
[1] L.P. Kadanoff and G. Baym, Quantum Statistical Mechanics (New York: Benjamin, 1962), [2] G. Lani, P. Romaniello, and L. Reining, New J. Phys. 14, 013056 (2012); J.A. Berger et al., New J. Phys. 16, 113025 (2014), [3] M. Guzzo et al., Phys. Rev. Lett. 107, 166401 (2011); Phys. Rev. B 89, 085425 (2014)

RIDLEY, Michael (P)

Generalised Theory of Current Noise for an Arbitrary Time-Dependent Bias

Michael Ridley, Angus MacKinnon and Lev Kantorovich

Abstract: The problem of explicit time-dependence in electron transport through molecular junctions is a problem of increasing importance, as the dynamical response properties of nanostructures following the switch-on of a time-dependent bias are now the subject of experimental investigation. Recent work in the application of the Nonequilibrium Green's Function (NEGF) formalism to the switch-on problem has lead to the development of an efficient scheme for calculating the electronic current through a multilead nanojunction. This method enables access to both the short-time transient response of the system to the switch-on event, and to the current at long times after the transient. In this approach, the Wide-Band Limit Approximation (WBLA) was employed to enable exact integration of the Kadanoff-Baym equations and arrive at a closed integral expression for the time-dependent current. We now extend this formalism to the calculation of the two-time current correlation function in a nanojunction subject to an arbitrary time-dependent bias. This requires the derivation of additional Green's Functions, both for the molecular region and for molecule-mediated lead-lead electron transfer processes. We go on to show that, in the limit where the bias becomes constant, and the switch-on time is relegated to the distant past then the correlation function depends on the time-difference only, corresponding to the condition of an ideally stationary current. This enables derivation of the frequency-dependent power spectrum, and, in the limit of zero frequency, well-known expressions from the Landauer-Buttiker formalism for the shot and thermal noise are recovered. Finally, we intend to present numerical calculations of the two frequency power spectrum in the case of a sinusoidal bias applied to the leads.

RISTINMAA SÖRENSEN, Stacey (I)

Double ionization: investigating mechanisms and time scales

S. L. Sörensen

Abstract: Access to many-particle dynamics in real time is important for understanding processes involving electron correlations in both model systems and realistic materials. The most fundamental multi-electron process is double ionization upon absorption of a single photon, and the prototype system is xenon. While strong-field two-electron emission was recently studied in xenon [1,2] our recent work provides the first experimental information on the time for the electron pair to leave the atom [3]. We study the temporal delay between the two electrons emitted in direct, indirect and sequential double ionization processes. We can account for the perturbation caused by the probing field and from the two-photon delay obtain the one-photon photoemission delay. We find a value of about 500 as, in agreement with calculations using the random-phase approximation for the conjugate shake-off (including 5s-5p correlation) and knockout mechanisms of direct double ionization. The development of attosecond light sources at higher repetition rate and photon energy will improve the precision, potentially allowing

discrimination between the two mechanisms.
[1] B. Bergues. et al. 2012 Nat. Commun. 3, 813, [2] A. N. Pfeiffer et al. 2011 Nat. Phys. 7, 428, [3] E. P. Månsson et al. 2014 Nat. Phys. 10, 207-211

SCHLÜNZEN, Niclas (C)
Nonequilibrium Green functions approach to transport and diffusion in strongly coupled finite quantum systems
Niclas Schlünzen, Sebastian Hermanns, and Michael Bonitz

Abstract: Transport properties of strongly correlated quantum systems are of central interest in condensed matter, ultra-cold atoms and in dense plasmas [1-3]. There, the proper treatment of strong correlations is important. The nonequilibrium Green functions framework is well suited for this task. In this contribution, we study transport properties of finite spatially inhomogeneous Hubbard clusters of up to several hundred sites in one to three dimensions [4,5]. We analyze the diffusion process with respect to the particle number and interaction strength. Extrapolating to macroscopic particle numbers, we compare our results to experiments of Schneider et al. for ultra-cold atoms in a 2D lattice [1]. The very good agreement with our T-matrix calculations underlines the important role of correlations in these systems, which cannot be captured by Boltzmann equation or Hartree-Fock based methods.
[1] U. Schneider et al., Nature Phys. 8 213-218 (2012), [2] J. P. Ronzheimer et al., Phys. Rev. Lett. 110 205301 (2013), [3] H. Haberland, M. Bonitz, and D. Kremp, Phys. Rev. E 64 026405 (2001), [4] M. Bonitz, N. Schlnzen, and S. Hermanns, Contrib. Plasma Phys. 55 152-18 (2015), [5] N. Schlnzen, S. Hermanns, M. Bonitz, and C. Verdozzi, submitted for publication

SCHÜLER, Michael (C)
Time propagation of coupled fermionic-bosonic Kadanoff-Baym equations for plasmon-assisted double photoemission
Michael Schüler, Yaroslav Pavlyukh, Jamal Berakdar

Abstract: Coincidence measurements of double photoemission (DPE) represent a direct way of tracing various facets of electronic correlations in molecular as well as extended systems, such as dynamical screening and collective excitations. Motivated by recent experiments on C60 molecule, known its strongly pronounced plasmon resonances, we study non-equilibrium electron dynamics triggered by the interaction with the light pulse and involving electron emission and excitation of a quantized plasmon. The plasmon decays leading to the emission of a secondary electron which is observed in coincidence with the first electron. Such plasmon-mediated double photoemission is studied in terms of an effective fermion-boson model system. The model generalizes the s-model analyzed by Langreth for describing photoemission accompanied by plasmon excitation [1] and additionally accounts for the relaxation and dephasing caused by the interaction with a fermionic and bosonic bath. In addition to the electronic Green's functions the coordinate-coordinate bosonic correlators are propagated on GW level as functions of two time-arguments. Their second-order equation of motion leads to important modi-

fications to the standard Kadanoff-Baym propagation scheme [2,3]. The generalized Kadanoff-Baym ansatz [4] can be extended to the bosonic degrees of freedom in order to significantly reduce the computational cost of our method.
[1] D. C. Langreth, PRB 1, 471 (1970), [2] M. Puig von Friesen, C. Verdozzi, and C.-O. Almbladh, PRL 103, 176404 (2009), [3] A. Stan, N. E. Dahlen and R. van Leeuwen, JCP 130, 224101 (2009), [4] P. Lipavsky, V. Spicka, and B. Velicky, PRB 34, 6933 (1986)

SENTEF, Michael (C)
Theoretical investigations of laser-driven superconductivity
Michael A. Sentef

Abstract: The control of material properties with femtosecond laser pulses at tunable wavelengths is a tantalizing prospect of ultrafast materials science. Recent progress in pump-probe spectroscopies has lead to a host of intriguing results, such as the observation of amplitude mode oscillations in a BCS superconductor [1] or the proposal of light-induced superconducting-like states at high temperatures [2, 3, 4]. It is thus of high importance to develop theoretical frameworks and efficient numerical simulation codes in order to provide a theoretical understanding of dynamical effects in ultrafast materials science beyond quasi-equilibrium approximations. Kadanoff-Baym-Keldysh Green functions are a suitable tool for this endeavor. In this talk, I will present recent simulations of the nonequilibrium dynamics in laser-driven superconductors using the Nambu-Gor'kov formalism and the Migdal-Eliashberg approximation to phonon-mediated superconductivity. A rapid optical stimulation of an electron-phonon coupled superconductor creates electron-hole pairs and quenches the energy gap, which then relaxes showing clear spectroscopic signatures of renormalized Higgs amplitude mode oscillations, which we propose to be measured using time- and angle-resolved photoemission spectroscopy [5]. In a different setting, larger wavelength THz lasers directly couple to IR-active phonons, which were proposed to rectify a Raman phonon via nonlinear phonon-phonon coupling [6]. Such a rectification leads to a modified atomic structure, which in turn changes the electronic band structure. As a first step towards understanding the effects of such a real-time modification, we investigate the dynamics of a phonon-mediated superconductor after a ramp of its electronic bandwidth. The induced increase of the density of states near the Fermi level leads to an enhancement of superconductivity. We show how electron-phonon coupling stabilizes this rapid enhancement on short time scales [7].
[1] Matsunaga et al., Science 345, 1145 (2014), [2] Mankowsky et al., Nature 516, 71 (2014), [3] Kaiser et al., Phys. Rev. B 89, 184516 (2014), [4] Mitrano et al., arXiv:1505.04529, [5] Kemper et al., arXiv:1412.2762, [6] Subedi et al., Phys. Rev. B 89, 220301 (2014), [7] Sentef et al., arXiv:1505.07575

SHAHID, Nazish (P)
Different forms of the Kadanoff-Baym equations in quantum statistical mechanics
Alexander. S. Kondratyev and Nazish Shahid

Abstract: A new form of the Kadanoff Baym equations for a system of interacting particles is offered on the basis of the retarded and advanced quantum Greens functions. The comparison of the traditional and the offered forms of the equations allows to analyze the question to what extent Landau Silin kinetic equations for the neutral Fermi liquid and for the electron liquid of normal metals take into account quickly varying in space and time disturbances.

STEFANUCCI, Gianluca (I)
NEGF approach to pump-probe photoabsorption spectroscopy
G. Stefanucci, E. Perfetto, A.-M. Uimonen and R. van Leeuwen

Abstract: After revisiting the theory of pump-probe photoabsorption spectroscopy we propose a nonequilibrium Green's function (NEGF) approach to calculate the transient spectrum of nanoscale systems. We can deal with arbitrary shape, intensity, duration and relative delay of the pump and probe fields and we can include ionization processes as well as hybridization effects due to surfaces. We present numerical simulations of atomic systems using different approximate self-energies and, whenever possible or available, find good agreement with CI calculations and experiments. The NEGF approach offers a first-principle methodology to predict and interpret pump-probe photoabsorption spectra of systems that are out of reach with other methods. If time permits we will also discuss future challenges and reachable goals.

STRAND, Hugo (C)
Real-time dynamics of lattice bosons in high dimensions from nonequilibrium dynamical mean-field theory
Hugo U. R. Strand, Martin Eckstein and Philipp Werner

Abstract: We generalize the bosonic formulation of dynamical mean-field theory (BDMFT) [1] to out-of-equilibrium situations, and develop a Nambu strong coupling real-time impurity solver. The impurity solver, being a pure Luttinger-Ward based diagrammatic expansion, is conserving and relies on solving the real-time Dyson equation on the three legged Kadanoff-Baym real-time contour, in combination with a self-energy self-consistency [2]. In this framework we study the out-of-equilibrium properties of the Bose-Hubbard model at finite temperatures. As a first test we mimic the pioneering superfluid quench experiments of Greiner et al. [3]. Accounting for quantum fluctuations using BDMFT qualitatively changes the superfluid collapse-revival oscillations, and introduces significant damping, which is absent on the mean-field level [4]. We also perform modulation spectroscopy and observe linear high order resonances of the boson occupation and non-linear multi-photon absorption processes, results that have direct bearing on cold-atom spectroscopy [5]. The out of equilibrium spectroscopy is analyzed and explained

using the equilibrium spectral function and structure factor in the strong coupling limit. In particular, we discuss the nontrivial temperature dependence of the resonances.
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TANG, Gaomin (P)
Full-counting statistics of charge and spin transport in the transient regime
Gaomin Tang and Jian Wang

Abstract: A stochastic process can be characterized by the distribution function. The full-counting statistics (FCS) is an elegant way to study the current correlations in mesoscopic systems and yield not only the noise but all higher order cumulants. It calculates the probability distribution function of the number of electrons transferred through a particular terminal during given period of time that contains fundamental information about the current fluctuation in the system. We report the investigation of FCS of transferred charge and spin in the transient regime where the connection between central scattering region (quantum dot) and leads are turned on at t = 0. A general theoretical formulation for the generating function (GF) is presented using a nonequilibrium Green's function (NEGF) approach for the quantum dot system. The GF of FCS in electron transport systems is obtained using the method of path integral together with NEGF technique based on the two-time quantum measurement scheme. This formalism can also be generalized to account for spin transport for the system with noncollinear spin as well as spin-orbit interaction. We can use it to get the GF of spin-polarized transferred charge, transferred spin, as well as the spin transferred torque for a magnetic tunneling junction in the transient regime. The GF is compactly expressed by a functional determinant represented by Green's function and self-energy in the time domain. With this formalism, FCS in spintronics in the transient regime and long time limit can be studied.

THYGESEN, Kristian (I)
Many-body GW calculations for molecular transport junctions
Kristian S. Thygesen

Abstract: The failure of standard density functional theory (DFT) to provide a reliable description of the conductance of molecular junctions is well known. Going beyond the single-particle approximation we show that the GW self-energy yields conductance and thermopower of simple molecular junctions in significantly better agreement with experiments[1,2]. The main improvement, compared to conventional DFT, originates from a better energy level alignment at the metal-molecule interface. However, the GW self-energy can also affect the shape of the molecular orbitals[3] and furthermore accounts for the finite response time associ-

ated with the formation of the image charge in the electrodes which can affect the conductance significantly[4].
[1] C. Jin et al., J. Chem. Phys. 139, 184307 (2013), [2] C. Jin, T. Markussen, and K. S. Thygesen, Phys. Rev. B 90, 075115 (2014), [3] M. Strange et al., Phys. Rev. B 86, 195121 (2012), [4] C. Jin et al., Phys. Rev. B 89, 041102(R) (2014)

TITVINIDZE, Irakli (P)
Non-equilibrium inhomogeneous DMFT for correlated Heterostructures
I. Titvinidze, A. Dorda, W. von der Linden, E. Arrigoni

Abstract: In this talk we present new developments of a recently introduced [1] theoretical scheme to deal with correlated system out of equilibrium. This approach allows to efficiently investigate steady-state behavior of the system based upon dynamical-mean-field theory (DMFT) within the nonequilibrium (Keldysh) Green's functions formalism [2]. The main novelty of the method is in the solution of the impurity problem. Here the idea is that the baths coupled to the interacting impurity are replaced by a finite number of bath sites coupled to Markovian reservoirs [1, 3]. Up to now the method has been applied to a single correlated layer sandwiched between two metallic leads at different chemical potentials. Here we show how to extend it to more complex geometries to treat more physically relevant heterostructures. In particular we present results for the steady-state current, spectral function and self-energy. First, we will review the case of a single correlated layer and show the effect of the local Hubbard interaction and bias voltage for weak and the intermediate hybridization strength to the leads. Afterwards we present results for systems of particular interest, such as charge modulated superlattices, modulated doping close to the Mott insulator, and resonance effects.
[1] E. Arrigoni et al, Phys. Rev. Lett. 110, 086403 (2013). [2] J.K. Freericks, V. M. Turkowski, and V. Zlatic, Phys. Rev. Lett. 97, 266408 (2006) [3] A. Dorda et al, Phys. Rev. B. 89, 165105 (2014).

TUOVINEN, Riku (P)
Extending the time-dependent Landauer-Büttiker formalism to superconducting junctions and arbitrary temperatures
Riku Tuovinen, Gianluca Stefanucci and Robert van Leeuwen

Abstract: Recently introduced time-dependent Landauer-Büttiker formalism deals with a general electronic transport setup for a noninteracting lattice coupled to infinite wide bandwidth leads [1-3]. The generality in the setup comes from the arbitrary shape and size of the central region and the leads. For the Green's function in this setup it is possible to solve the Kadanoff-Baym equations analytically and derive a closed-form expression for the time-dependent one-particle density matrix. In the present study, we present an extension to this formalism for superconducting junctions by interpreting the Hamiltonians and Green's functions as Nambu matrices [4,5]. We also extend the earlier analytic results in Refs.[2,3] for arbitrary temperatures by contour integration techniques similar to those discussed in Ref.[6] Results for time-dependent responses in specific applications are shown together with a discussion about work in progress.

[1] G. Stefanucci and R. van Leeuwen. Nonequilibrium Many-Body Theory of Quantum systems. Cambridge Univerisity Press (2013), [2] R. Tuovinen, R. van Leeuwen, E. Perfetto and G. Stefanucci. J. Phys.: Conf. Ser. 427, 012014 (2013), [3] R. Tuovinen, E. Perfetto, G. Stefanucci and R. van Leeuwen. Phys. Rev. B 89, 085131 (2014), [4] G. Stefanucci, E. Perfetto and M. Cini. Phys. Rev. B 81, 115446 (2010), [5] J. C. Cuevas, A. Martn-Rodero and A. Levy Yeyati. Phys. Rev. B 54, 7366 (1996), [6] A. P. Jauho, N. S. Wingreen and Y. Meir. Phys. Rev. B 50, 5528 (1994)

VAN LEEUWEN, Robert (I)

Kadanoff-Baym equations for time-dependent coupled electron-boson systems

Robert van Leeuwen

Abstract: In this presentation I will discuss the application of the non-equilibrium many-body Green's function formalism for the description of coupled electron-boson systems out of equilibrium. Within this formalism the system is described by electronic and bosonic propagators which satisfy a coupled system of integro-differential equations, known as the Kadanoff-Baym equations. The formalism is very general and can deal with a wide variety of physical systems, such as electrons coupled to quantised photons or to phonons. We illustrate the formalism and some simple model systems that allow for comparison to exact results. We further give an outlook how to deal with more realistic systems in a simplified version of the formalism.

WANG, Jian (I)

Current conserving theory on shot noise

J.T. Yuan, Y. Wang, and Jian Wang

Abstract: In scattering problems, the starting point is to assume that the potential in the electrode is completely screened which means that the total charge in the scattering region is zero at any time. This in turn ensures the current conservation, an important requirement for quantum transport theory. Currently, the current conserving ac transport theory has been well established in terms of scattering matrix theory or non-equilibrium Green's function which can be applied to investigate ac current. However, since the displacement current is not considered on the operator level, the correlation of current does not satisfy the conservation law. Recently, a current conserving ac transport theory has been developed by us at the operator level using non-equilibrium Green's function theory. The displacement current operator has been defined. This enables us to investigate correlation of displacement current.

WERNER, Philipp (I)
Nonequilibrium dynamics of electron-phonon systems
Philipp Werner, Martin Eckstein, Yuta Murakami, Naoto Tsuji, Hideo Aoki and Denis Golez

Abstract: Pump-probe experiments enable the study of relaxation processes in solids on the intrinsic timescale of the electrons. Here, we discuss how the coupling to optical phonons affects the nonequilibrium dynamics in the Mott insulating, metallic and superconducting state. Using nonequilibrium dynamical mean field theory in combination with strong-coupling or weak-coupling perturbative impurity solvers, we simulate the time-evolution of the Holstein and Holstein-Hubbard model after a quench in the electron-phonon coupling strength or a photo-doping pulse and investigate how the feedback from the excited phonons on the electrons affects the relaxation process. We also discuss how the techniques developed for electron-phonon systems enable the study of dynamical screening phenomena in photo-excited electron systems with long-range Coulomb interactions.

WINGE, David (C)
Second Harmonic Generation in Quantum Cascade Lasers Simulated using Green's Functions
David Winge, Martin Lindskog and Andreas Wacker

Abstract: Quantum cascade lasers (QCLs) [1] structures have in addition to providing reliable sources in the mid-IR, been shown to exhibit giant second order susceptibility [2]. This makes them excellent for second harmonic generation as well as difference frequency generation which currently is used to build room temperature Terahertz sources [3]. In this work we solve the transport problem in a QCL using a non-equilibrium Green's function formalism [4]. A classical laser field is used to probe the system and the use of a second energy in the Green's functions, to account for exchange of quanta with the laser field, allows us to extract the polarization current at the second harmonic frequency (with respect to the fundamental laser frequency). The second harmonic signal generated in the waveguide can thus be estimated and related to experiments with good agreement [5].
[1] Faist, et al., Science 264, 553-556 (1994), [2] Capasso, et al., Quantum Electronics, IEEE Journal of, 30, 1313-1326 (1994), [3] Belkin, et al., Nature Photonics 1, 288-292 (2007), [4] Wacker, et al., Sel. Top. in Quantum Electronics, IEEE Journal of, 19, 1200611 (2013), [5] Winge, et al., Optics Express 22, 18389-18400 (2014)

YANG, Kaike (P)

Dynamical correction of thermoelectric coefficients for strongly interacting electrons in the Coulomb blockade regime

Kaike Yang, Gianluca Stefanucci, Stefan Kurth and Roberto D'Agosta

Abstract: For molecules weakly coupled to leads the exact zero-bias Kohn-Sham conductance can be orders of magnitude larger than the true conductance due to the lack of dynamical exchange-correlation effects. Recently, it has been shown [1] how these dynamical exchange-correlation corrections can be calculated using only quantities obtained from static density functional theory. Here we investigate thermoelectric transport and derive the exchange-correlation correction to the Seebeck coefficient. We show how the Coulomb blockade peaks in both the conductance and the Seebeck coefficient correspond to changes of the number of electrons on the molecule by an integer. Finally, we compare our results to some recent experiments.

[1] S. Kurth and G. Stefanucci, Phys. Rev. Lett. 111, 030601 (2013), Phys. Rev. Lett. 107, 216401 (2011)

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8 Maps

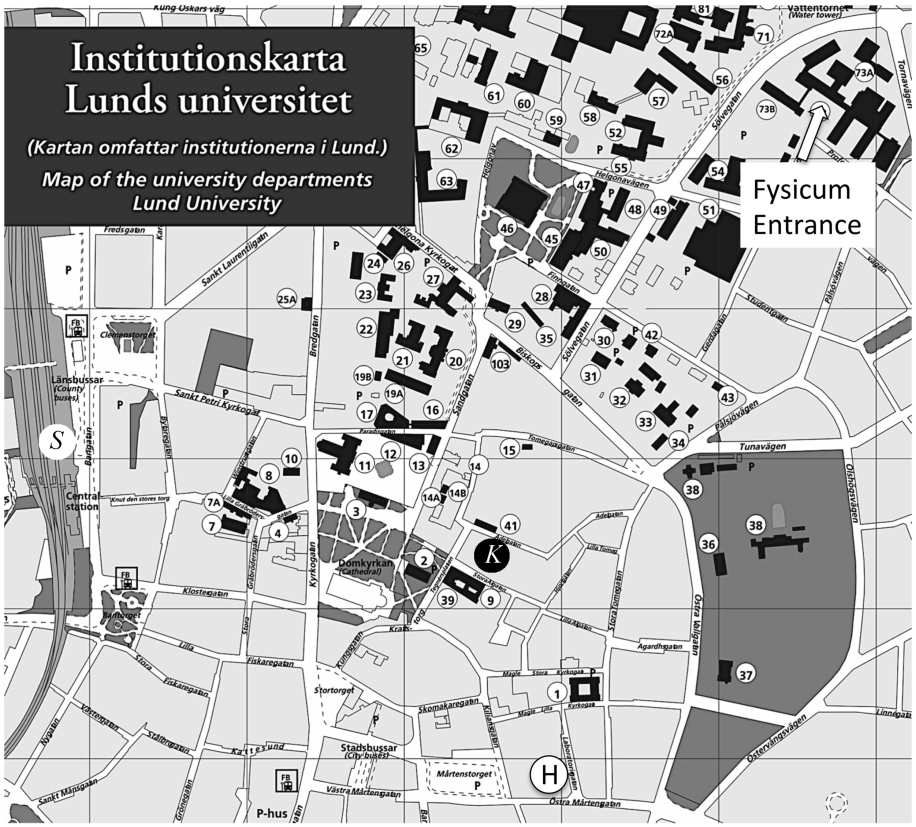

Figure 1: Map of Lund, where the Physics Department (Fysicum), the Nordic Hotel (H), the Central Railway (S) and the Kulturen museum (K) are shown *(adapted for PNGF6 with the kind permission of Stadsbyggnadskontoret in Lund).*

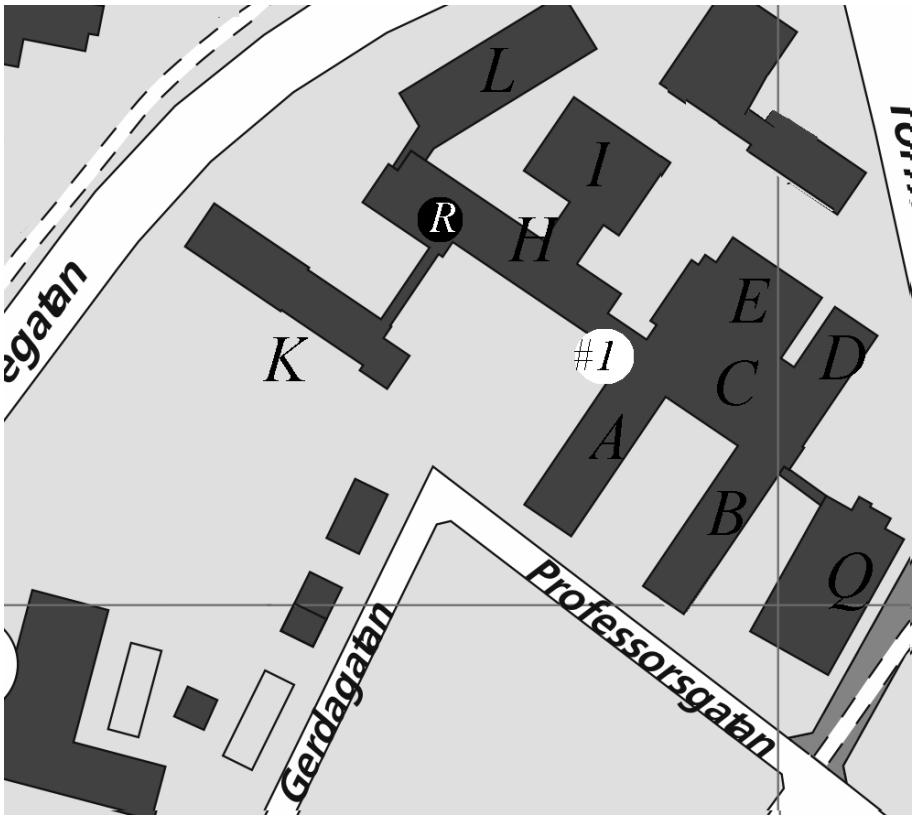

Figure 2: Map of Fysicum, where the main entrance (#1) and Rydbergsalen (R) are shown. The other capital letters denote different areas of the building. *(adapted for PNGF6 with the kind permission of Stadsbyggnadskontoret in Lund).*

9 Conference Proceedings

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10 Notes