DY 1: Quantum Dynamics, Decoherence and Quantum Information I

Time: Monday 9:30–12:15 Location: H39

DY 1.1 Mon 9:30 H39

Iterated Mori projector (IMoP) approach for driven dissipative quantum many body systems — •Peter Degenfeld-Schonburg and Michael J. Hartmann — Technische Universität München, Physik Department I, James Franck Str., 85748 Garching, Germany

We report on a pertubative method for driven dissipative quantum many body systems on a lattice that goes beyond Meanfield. Our approach is based on the Mori projection operator technique where we treat a single lattice site as the system of interest and trace out the dynamical many body environment comprised of all remaining lattice sites. The resulting on-site master equation describes the dynamics up to second order in the hopping. To account for a dynamical environment the master equation is solved iteratively. We apply our methods to arrays of coupled non-linear harmonic oscillators, i.e. to a Bose Hubbard model, in a driven and dissipative regime and numerically show the advantage of IMoP over Meanfield.

DY 1.2 Mon 9:45 H39

Counting statistics for Dicke-Superradiance — •Wassilij Kopylov, Clive Emary, and Tobias Brandes — TU Berlin, Institute of Theoretical Physics, Deutschland

We consider the Dicke-Hamiltonian valid in a rotating frame and couple it to a dissipative zero- temperature bath. We derive a cumulant generating function for emitted photons using the P - representation of the master equation with counting field for this model in the thermodynamic limit. The macroscopic occupation in the superradiant case is determined by the linear terms in the master equation.

DY 1.3 Mon 10:00 H39

Equation-of-motion method for full counting statistics: Steady-state superradiance — •Malte Vogl, Gernot Schaller, Eckehard Schöll, and Tobias Brandes — Institut für Theoretische Physik, TU Berlin, Berlin, Germany

For the multimode Dicke model in a transport setting that exhibits collective boson transmissions, we construct the equation of motion for the cumulant-generating function. Approximating the exact system of equations at the level of the cumulant-generating function and system operators at lowest order allows us to recover master equation results of the full counting statistics for certain parameter regimes at very low computational cost. The thermodynamic limit, which is not accessible with the master equation approach, can be derived analytically for different approximations.

Ref.: M.V., G. Schaller, E. Schöll, and T.Brandes, PRA **86**, 033820 (2012)

DY 1.4 Mon 10:15 H39

General Decoupling Procedure for Expectation Values of Four-Operator Products in Electron-Phonon Quantum Kinetics — •Nicolas Teeny and Manfred Fähnle — Max Planck Institute for Intelligent Systems, 70569 Stuttgart, Heisenbergstr.3,Germany

Electron-phonon quantum kinetic effects are important for studying the coherent ultrafast dynamics on time scales shorter than about a picosecond after exciting the electrons of a solid with a short laser pulse of duration smaller than 100 femtoseconds. An example is the femtosecond-demagnetization of a ferromagnetic film after exposure to a strong optical laser pulse. In the density-matrix formalism of electron phonon quantum kinetics the hierarchy of infinitely many coupled equations of motion for the expectation values of products of electron and phonon creation and annihilation operators of arbitrary order is usually terminated on the level of equations of motion for the expectation vales of three-operator products by using decoupling procedures for the four-operator products occurring in these equations. In the literature decoupling procedures are discussed for special types of electron and phonon states. In the talk generalized decoupling procedures are derived for arbitrary electron and phonon states.

DY 1.5 Mon 10:30 H39

The role of non-linear second-order coupling Hamiltonians in photoemission and Raman spectroscopy — Johannes Flick[1], Heiko Appel[1], and •Angel Rubio[1,2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]NanoBio Spectroscopy group and ETSF, Universidad del País Vasco, San Sebastián, Spain

In this talk we employ an exact Fock space representation to study Holstein-Su-Schrieffer-Hamiltonian systems[1,2] coupled to quantized photon modes. In particular, we include non-linear electron-phonon couplings, which originate from an expansion to second order in the nuclear displacement[3]. We perform exact diagonalizations and real-time propagations for the model in Fock space and investigate the effect of the nonlinear couplings on photoemission (PE), inverse photoemission (IPE) and Raman spectra.

[1] W.P. Su, J.R. Schrieffer, A.J. Heeger Phys. Rev. Lett., **42** (1979), pp. 1698−1701
[2] T. Holstein, Ann. Phys. (N.Y.) **8**, 325 (1959)
[3] L. Cederbaum and W. Domcke, J. Chem. Phys. **60**, 7 (1974). **80**, 212303 (2009).

15 min. break.

DY 1.6 Mon 11:00 H39

Linear and non-linear responses in pump-probe spectroscopy — •Tanja Dimitrov[1], Heiko Appel[1], and Angel Rubio[1,2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]NanoBio Spectroscopy group and ETSF, Universidad del País Vasco, San Sebastián, Spain

In this work, we investigate the time-dependent dipole response of molecular systems for pump probe laser experiments. We compare the response of widely used approximate adiabatic functionals in time-dependent density functional theory to the exact solution of the time-dependent Schrödinger equation for realistic model systems. In particular, we focus on the role of memory effects and the corresponding signature in the optical absorption spectra.

DY 1.7 Mon 11:15 H39

Efficiency scaling of non-coherent upconversion — •Jochen Zimmermann[1], Roberto Mulet[1,2], Thomas Wellens[1], Greg D. Scholes[1,3], and Andreas Buchleitner[1] — [1]Albert-Ludwigs-Universität Freiburg — [2]University of Havana, Cuba — [3]University of Toronto, Canada

A very promising approach to obtain efficient upconversion of light is the use of triplet-triplet annihilation of excitations in molecular systems. In real materials, besides upconversion, many other physical processes take place - fluorescence, non-radiative decay, annihilation, diffusion - and compete with upconversion. The main objective of the presented work [1] is to design a proof of principle model that can be used to shed light on the relevance of the interaction between the different physical processes that take part in these kinds of systems. Ultimately, we want to establish general principles that may guide experimentalists toward the design of materials with maximum efficiency. Here we show, in a 1D model system, that even in the presence of these processes upconversion can be optimized by varying the ratio between the two molecular species present in this kind of materials. We derive scaling laws for this ratio and for the maximum efficiency of upconversion, as a function of the diffusion rate J, as well as of the creation and of the decay rate of the excitations.

[1] J. Zimmermann, R. Mulet, T. Wellens, G.D. Scholes and A. Buchleitner. arXiv:1211.5004 [cond-mat.mtrl-sci]

DY 1.8 Mon 11:30 H39

Wave-packet revivals and decoherence in vibronically coupled systems — •Heiko Appel — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Electronic decoherence is central for our understanding of physical processes that are prevailing in a large variety of phenomena such as photosynthesis, vision or solar-cell applications. In this work, we investigate the coupled vibronic dynamics in short trans-polyacetylene oligomers which are described in terms of a Su-Schrieffer-Heeger (SSH) Hamiltonian. Using explicit matrix representations of Fock space operators, we illustrate how to construct a numerically exact solution for the coupled system of electrons, phonons and photons. From the exact solution of the model, we extract time scales for electronic decoherence and relate this to the decay of wave-packet revivals.

DY 1.9 Mon 11:45 H39

Influence of Vibrations on Energy Transfer and Optical Properties of Light-Harvesting Systems — •Gerhard Ritschel[1], Jan Roden[1,3], Walter T. Strunz[2], and Alexander Eisfeld[1,4] — [1]Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany — [2]Technische Universität Dresden, Germany — [3]University of California, Berkeley, USA — [4]Harvard University, Cambridge, USA

The transfer of electronic excitation energy as well as optical properties of complexes of interacting chromophores, e.g. the FMO complex or the LH2 antennae in biological photosynthetic systems, are strongly influenced by an environment. For a proper theoretical description it is essential to include non-Markovian effects resulting from an electron-environment coupling that is a rather structured function of energy leading to a complicated retroaction on the excitation dynamics. Based on the non-Markovian quantum state diffusion an approximate non-perturbative master equation can be derived that captures the whole range from coherent dynamics to incoherent diffusion. Especially situations where environment-assisted transfer occurs can be investigated. Using that approach we calculated energy transfer in one FMO subunit as well as in the full FMO trimer and calculated linear spectra at various temperatures employing the thermofield description.

DY 1.10 Mon 12:00 H39

Concersvative Brownian motion simulation of a hard-boson gas — •Wolfgang Paul — Institut für Physik, Martin Luther Universität, 06120 Halle (Saale)

We present a simulation study of the properties of the Tonks-Girardeau gas, a system of N hard-core bosons confined in a one-dimensional harmonic trap. For this system the ground-state wave function is exactly known based on a Bose-Fermi mapping theorem. We employ Nelsons* interpretation of quantum mechanics in which this N-body wave function gives rise to a set of stochastic differential equations for the positions of the N particles, which can be simulated by standard methods. Particularly, real space densities and momentum distributions can simply be determined by time averages along particle trajectories. Employing this approach we are able to significantly extend the range of particle numbers N treated numerically compared to earlier approaches, while reproducing all exactly known results for this model. We also show that for the bosons in a harmonic trap, contrary to what has been assumed so far, the momentum distribution reflects the system size scaling of the occupation numbers of the natural orbitals, i.e., it can be used to decide on the presence of a Bose-Einstein condensate.