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Abstracts

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Talks

Electro-thermal transport in quantum point contact

Aly, Arafa

We have presented the Peltier coefficient and thermal transport in quantum point contact (QPC), under the influence of external fields and different temperatures. The Peltier effect has long been discovered several tens years ago. Young researches now are not quite familiar with this effect. We tried to combine this old effect with modern low dimensional quantum system materials, e.g. quantum point contact, open up a new research field. Also we obtained the oscillations of the Peltier coefficient in external fields. Numerical calculations of the Peltier coefficient have been performed at different applied voltages, amplitudes and temperatures. The obtained results are concordant with the experimental results in the literature.

Superconducting Parameters of Photonic crystals

Aly, Arafa

We have investigated the transmission of one-dimensional superconducting photonic crystals. The superconducting state parameters such as, critical temperature and energy gap were estimated. We found the superconducting parameters control of the superconducting materials index under certain frequencies. The variance of the intensity and the bandwidth of the transmission are strongly dependent on the superconducting parameters. Such a photonic crystal can be used as temperature-controlled optical shutter. Moreover, the feasibility of realizing this kind of photonic crystal is also discussed.

Physics in Doha. Joys and Challenges in International Education

Ameduri, Marco

Kondo physics in chaotic mesoscopic systems

Bedrich, Rainer

We study the Kondo effect induced by a magnetic impurity interacting with a small metallic grain. Here, in contrast with the Kondo effect occurring in a bulk material, the metallic host is characterised by a finite mean level spacing. This low energy scale can generate deviations from the universal behavior which would be expected for a bulk system. The physical properties of the system are computed within a mean-field approximation for the Kondo interaction. In particular, we study the local magnetic susceptibility, the conductance, and the local density of electronic states as a function of the temperature, the mean level spacing, the Kondo coupling, and the chemical potential. The latter can be experimentally tuned by varying a gate voltage applied to the metallic grain. As a first step, we consider a constant distribution of the non-interacting energy levels. Our results are in agreement with the results obtained from different approaches, suggesting that the mean-field approximation is valid. A more realistic situation is then considered, for which the energy levels are distributed randomly. This is realised within the random matrix theory, which has been developed in the framework of chaotic systems studies.

Spin coherence and dynamic nuclear polarization in semiconductors

Beschoten, Bernd

Nuclear spins are a candidate for solid-state implementation of a quantum computer, since they are localized and exhibit spin relaxation times in the order of seconds. Electron spins can be used to address and control nuclear spins by the hyperfine interaction. Therefore, we investigated dynamic nuclear polarization in bulk n-GaAs in small magnetic fields using all-optical NMR. Electron spins are coherently pumped by a circularly polarized laser pulse. Their orientation is probed by time-resolved Faraday rotation. Two-color pump probe experiments in n-type GaAs yield the energy dependence of the coherency of electron spins near the Fermi level or of hot electron spins with excess kinetic energy. The resonant excitation of localized donor-like electron spin states was found to rive rise to large nuclear fields influencing the precession frequency of the spins in an external magnetic field. The origin of this dynamical nuclear polarization is assigned to the relaxation of the localized donor-like spin states. In contrast, delocalized electron spins with long spin lifetimes couple only weakly to the nuclear system. Those states might be used for fast readout of the nuclear fields by the Overhauser shift using resonant spin amplification. The dynamical nuclear polarization upon resonantly exciting electron spins yields the basis for an all-optical NMR technique and opens a link to alternative, NMR-based routes to quantum information processing.

All-optical coherent control of ballistic electrical currents in semiconductors and molecular wires

Betz, Markus

Traditionally, control over the charge motion in semiconductors is achieved electronically. Our approach to circumvent this limitation is the use of the coherence properties of harmonically related near-infrared pulses. In particular, we demonstrate all-optical coherent control of electrical currents in materials as diverse as bulk silicon and carbon nanotubes. For the generation of ballistic electrical currents in clean, unbiased silicon we use 150 femtosecond pulses with photon energies of 0.8 eV and their second harmonic. Current injection results from the quantum interference between oneand two-photon absorption pathways across the indirect bandgap and is detected by recording the emitted THz radiation. Most strikingly, the vector direction of the current as well as its amplitude can be controlled by varying the relative phase and the polarization of the two-color pump field. Using the same coherent control scheme we show that all-optical current injection is also possible in carbon nanotubes. THz emission spectroscopy of an aligned forest of single-walled nanotubes reveals peak electrical currents as large as 1 nA per molecular wire. These results open up new perspectives for optoelectronic functionalizations of carbon nanomaterials.

Ultrafast semiconductor quantum optics

Bratschitsch, Rudolf

Semiconductor quantum dots are promising solid-state systems for fundamental quantum optical experiments and quantum information processing. Ultrafast sequences of coherent quantum operations may be envisioned with femtosecond light pulses, if the involved energy levels are separated by at least tens of meV. We present the first femtosecond pump-probe experiment on a single self-assembled CdSe/ZnSe quantum dot. In this few-fermion system, Coulomb renormalization and single-photon gain are observed on an ultrafast timescale. The ability to add or remove single photons to and from photon bunches is explored. To not only reach single-electron but also single-photon sensitivity, we present two ideas to increase the light-quantum dot coupling via optical nanoantennas and dielectric microresonators.

DNA magnetism: A new paradigm in nano-bio-systems

Chakraborty, Tapash

In this talk, I shall address the fundamental role of electronic and vibrational interactions on the magnetic properties of homogeneous and randomly-sequenced DNA. I will discuss about several interesting magnetic properties of DNA. The intra-strand electron-electron interaction enhances magnetization while the inter-strand interaction suppresses it. Renormalization of the hopping integrals due to electron-vibron interactions results in a paramagnetic to diamagnetic transition as a function of temperature. Influence of inter-electron interactions is therefore to transform the diamagnetic system into a paramagnetic one, while the temperature can reverse that behavior. Being entirely intrinsic, these properties would not be influenced by the environment. In addition to being of fundamental importance, the magnetic behavior of DNA might also lead to novel developments on DNA-based devices. As an example, it would perhaps be possible to design a DNA molecule with given magnetic properties that would depend entirely on the composition and the operating temperature. This would usher in a new field, the magnetic nanodevices with DNA as a building block.

Entanglement perturbation theory for the quantum ground states in two dimensions

Chung, Sung

I will give an overview of the recently developed many-body method, the entanglement perturbation theory (EPT), to calculate partition functions in two and three dimensional classical systems and the quantum ground states in one and two dimensions [1-3]. The EPT does not use numerical renormalization group, free from the finite-size problem and simple, general and exact in numerical implementation. Moreover EPT can avoid the notorious negative sign problem in the two dimensional fermions.

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Plasmonic beam optics in metal nanoparticle arrays

Citrin, David S.

Controlling the conductance of pi-conjugated molecules

Crljen, Zeljko

We performed series of calculations of the conductance of certain classes of pi-conjugated molecules: phenyl ethylene oligomers (Tour wires), phenylene vinylene oligomers (OPV) and polyynes. The considered geometry consisted of the molecule between the gold electrodes. Keeping the contact geometry for all of molecules the same, optimizing it with respect to the adsorption site we obtained the functional dependence of the conductance on the intrinsic molecular properties. In the low bias regime we found that polyvnes, the one-dimensional chains of carbon atom with alternating single and triple bonds between carbon atoms, show the highest conductance with the value of 100 microS at zero bias. In Tour wires and OPV molecules, the conductivity shows the decrease proportional to the number of benzene rings in the molecule. We will show that the conductance of polyynes is stable with respect to the applied bias and the length of the molecule while in Tour wires and OPVn it exibits the nonlinear behaviour as a consequence of different electronic structure around the Fermi level of the system. The dependence of the conductance on the molecular length clearly shows that pi-conjugated molecules show good molecular wire properties, with the metalliclike conductance in polyynes, which controlably reduces down with the number of phenyl rings in phenyl type oligomers.

Charge-memory polaron effect in molecular junctions

D'Amico, Pino

The charge-memory effect, bistability and switching between charged and neutral states of a molecular junction, has been observed in recent STM [1, 2] and single-molecule [3] experiments, and also investigated theoretically [4, 5]. In this work we considered the problem within a polaron model describing the interaction between electronic and vibronic degrees of freedom. We show that upon applying gate or bias voltage, it is possible to observe charge-bistability and hysteretic behavior which can be the basis of a charge-memory element. Physical quantities like lifetimes, charge-voltage and current-voltage curves are calculated by the master equation method for weak coupling to the leads [6] and at stronger coupling by the equation-of-motion method for nonequilibrium Green functions [7]. In the latter case we further perform a systematic analysis of the bistability behaviour of the system for different internal parameters such as the electron-vibron and the lead-molecule coupling strength.

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Ultrafast spectroscopy of a single metal nanoparticle

Del Fatti, Natalia

The linear and nonlinear optical properties of a metal nano-object are dominated by apparition of a confinement induced resonance, namely the surface plasmon resonance. Its spectral characteristics are determined by the composition, size, shape, and environment of the object. These parameters fluctuate from particle to particle limiting the information that can be extracted from ensemble optical measurements and making difficult precise comparison between experiments and theoretical models. This is in particular the case in experiments based on time-resolved nonlinear optical spectroscopy, an efficient and quasi-unique tool to investigate the electronics and vibrational properties of nanoparticles. This limitation can be circumvented by investigating a single nanoparticle, provided its geometry (size and shape) can be accessed. With the recent development of the far-field spatial modulation spectroscopy (SMS) technique the absorption of a single metal nanoparticle can now be detected and quantitatively measured, permitting its optical characterization. After recalling the principle of this technique, we will describe its coupling with a high sensitivity pump-probe femtosecond setup. This combination permits investigation of the ultrafast response of a single metal nanoparticle whose geometry is optically characterized in-situ. Different results obtained on the optical nonlinear response of a single nanorod and on the electron-phonon coupling in a single nanosphere will be discussed, and compared to ensemble measurement data. Extension of these studies to the investigation of the acoustic vibrational response of a single nano-object will also be illustrated in the case of nanoprisms.

Towards a general rule for n-terminals push-pull devices

Del Nero, Jordan

In this lecture we show that, beyond the particular models, utilizing an hybrid equilibrium/nonequilibrium methodologies it is possible to create a general model for organics push-pull nanoscale devices within sigma, pi or both bonds type in the backbone. It is shown by direct quantum-mechanic calculations under external electric field and a nonequilibrium calculation based on the ballistic Landauer-Bttiker equation that I-V curves are comparable to the equilibrium charge distribution results. These related models were successfully applied and several examples will be done presenting a directional rectification response with differents operational regions. These results could provide novel insights to the emerging and fast growth field of molecular electronics.

Real-time probing of structural dynamics in ferroelectric materials

Elsässer, Thomas

Diffraction of x-rays from crystalline materials allows to determine time averaged equilibrium structures with high precision. Function of physical, chemical, and biological systems is frequently connected with nonequilibrium processes, involving ultrafast changes of electronic and/or nuclear structure. X-ray diffraction with a femtosecond time resolution has developed into an important tool to probe such changes most directly and unravel the mechanisms behind them. In this talk, new results on the interplay of coherent lattice motions and transient electric polarizations in nanolayered ferroelectrics are presented. Femtosecond x-ray diffraction from ferroelectric superlattice structures allows for observing lattice dynamics along different coordinates in real-time, revealing the coupling mechanisms and making polarization switching on ultrafast time scales obvious. As a second application, most recent studies of magnetostriction in a nanolayered system will be discussed.

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Metallic Nanorod arrays for plasmonic and metamaterial applications

Eng, Lukas

Phonon-assisted tunneling in two-electron quantum dot molecules

Grodecka, Anna

Due to their proposed application in various implementations of quantum computation schemes, quantum dot molecules (QDMs) have attracted much interest in theoretical and experimental investigations [1]. Specifically, quantum logical gates realizations based on two-electron spin states in coupled quantum dots (QDs) have been proposed [2]. Many of them employ electron tunneling processes, thus their timescales are of primary importance. Phonon-assisted tunneling has been thoroughly studied only in QDMs doped with one electron [3] but not for the relevant two-electron systems, where the challenge is the simultaneous incorporation of both the phonon and now important Coulomb interaction [4]. In this work, two laterally coupled QDs doped with two electrons are considered. The phonon-assisted electron tunneling between QDs is studied theoretically for the singlet-singlet relaxation channel, i.e. the tunneling from the spatially separated state to the state with two electrons in one QD. The results are compared to a tunneling of a single electron in a QDM, which allows us to indicate the role of the Coulomb interaction in the analyzed processes. Interaction with acoustic phonon modes via deformation potential and piezoelectric coupling is taken into account. It is shown that the piezoelectric mechanism for the considered system is of great

importance and for some ranges of QDM parameters is even the dominant contribution to relaxation in contrast to phonon-induced decoherence processes in a single QD [5,6]. The relaxation rates obtained for GaAs QDs [7] reach much higher values (up to 35/ns) in comparison to other decoherence processes like spin-orbit coupling (0.01/ns).

Therefore, the phonon-assisted tunneling mechanisms cannot be neglected in the process of implementing quantum information processing schemes on QDMs.

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Functional renormalization approach to interacting Bose gases

Hasselmann, Nils

We employ the functional renormalization group to calculate the single-particle spectral density of the two-dimensional Bose gas. Our approach is free of infrared divergences, which plague the usual diagrammatic approaches, and is consistent with the exact Nepomnyashchy relation, which states that the anomalous self-energy vanishes at zero frequency and momentum. We correctly recover asymptotic formulae for the propagators in the limit of small momenta and present results for the damping and dispersion of quasi-particles.

Condensation Kinetics for microcavity polaritons

Haug, Hartmut

A survey of the Boltzmann condensation kinetics is given by comparing the results with experimental findings. The main elements of a quantum kinetics for the condensation are discussed by using a gap-free self-consistent Popov approximation for the spectral functions. The scattering integrals for the excited states and the order parameter are discussed including polariton-phonon and polariton-polariton interactions.

Fermi edge singularities in photoabsorption spectra of mesoscopic systems

Hentschel, Martina

Fermi-edge singularities are among the simplest many-body effects and have been a key interest in condensed matter physics for many years. They have been extensively studied, and are understood, for bulk systems such as metals. In contrast, our focus

here is on small (mesoscopic) systems like quantum dots and graphene. In particular we will address the Fermi-edge singularities in the photoabsorption cross section that are known as the x-ray edge problem. They comprise the phenomena of Anderson orthogonality catastrophe and Mahan's exciton (Mahan-Nozieres-DeDominicis response) and result from the system's many-body response to the sudden, localized perturbation in form of a core hole that is left behind when the x-ray excites a core electron. We show that the mesoscopic regime holds surprises in form of many-body responses that deviate from the macroscopic (bulk, or metallic) case and, moreover, depend on the system geometry. The differences originate in the finite system size, the intrinsic mesoscopic fluctuations, and most importantly, the modifications of the electron dynamics in confined ballistic systems. One of our key findings is that a typically rounded bulk-edge turns into a pronounced peaked edge for a mesoscopic system. A particularly interesting behaviour is seen in graphene where the vanishing density of states at the Dirac point significantly modifies the system's many-body response.

High-field terahertz physics in the non-perturbative regime

Huber, Rupert

Few-cycle multi-terahertz (THz) pulses have evolved into an invaluable probe of low-energy excitations in condensed matter systems. In a next generation of experiments, we now explore THz nonlinear optics in two novel limits: (i) Intense multi-THz transients coherently control the orbital degrees of freedom of optically dark excitons in Cu2O. Internal Rabi flopping allows us to efficiently convert an ensemble of 1s excitons into the 2p state. The results point out a promising route for the preparation of ultracold and dense exciton gases. (ii) Intersubband transitions in semiconductor quantum wells are exploited to demonstrate a sub-cycle switch-on of ultrastrong light-matter coupling to the vacuum field of a THz microcavity. The system sets the stage for a new regime of non-adiabatic quantum electrodynamics.

General analytical insights on surface behaviour of solute particles at interfaces

Ionescu, Remus Amilcar

The surface behaviour of solutes at interfaces continues to be a topic of high interest in recent years. We mention the specific effects of ions at the interfaces of electrolyte solutions and the behaviour of neutrons at the surface of neutron rich nuclei (neutron skin). I will present some analytical results concerning the physical basis of specific ionic effects at surfaces of electrolyte solutions, in particular the effect of permanent or induced dipole moment of ions on their propensity for the interface. Also I will discuss the relevance of this approach to the nuclear matter case.

Control of photon statistics in quantum-dot microcavity lasers

Jahnke, Frank

NEGF-DFT modeling of transport in realistic Silicon nanowires

Jauho, Antti-Pekka

Non-equilibrium ward identity

Kalvova, Andela

The standard Ward Identity connecting the scalar transport vertex correction with one-particle self-energy can be generalized to an arbitrary non-equilibrium process as described by non-equilibrium Green's functions (NGF). The non-perturbative derivation is based on the global U(1) symmetry of the Fermion NGF. The Non-Equilibrium Ward Identity can be related to the renormalized multiplicative composition rule for NGF. For the propagator components of the full NGF, this rule provides a test of non-equilibrium quasi-particle regime. For the G_i component, the rule generalizes the reconstruction equations representing an exact counterpart of the factorization of G_i known as the Generalized Kadanoff-Baym Ansatz. As applications of the Non-Equilibrium Ward Identity, we first demonstrate testing the consistency of approximations on the archetypal example of SCBA for disorder scattering. Second, we present a numerical evaluation of the vertex corrections to the simple multiplicative rules, again for a transient treated in SCBA for disorder scattering. This gives an insight into the reliability of using the NE quasi-particle picture and of the GKBA, two approximations at the heart of deriving quantum transport equations from the full equations of motion for the NGF.

Decoherence due to contacts in ballistic nanostructures

Knezevic, Irena

In quasiballistic nanoscale devices, the process of relaxation towards a steady state cannot be attributed to carrier scattering. Rather, carrier exchange between the active region and the rapidly dephasing contacts governs relaxation. I will present a novel technique for the treatment of quantum transport in quasiballistic semiconductor nanostructures. The approach utilizes a first-principles model interaction between the current-limiting active region and the contacts. With the use of the model interaction and by accounting for the energy relaxation in the contacts due to the electron-electron interaction, irreversible evolution of the active region's many body statistical operator is derived and illustrated on examples of two-terminal nanostructures.

Excitonic and quantum optical correlations in semiconductor nanostructures

Koch, Stephan W.

A microscopic theory is used to consistently model Coulombic and quantum optical correlations in semiconductor nanostructures. The theory is evaluated to analyze entanglement between a photon and quantum-well excitons. It is shown that spectrally

resolved photon-statistics measurements can be used for high-contrast identification of two-photon strong-coupling states known from the famous Jaynes-Cummings ladder.

Spin 1/2 Fermions in the unitary Limit

Kohler, Sigurd H.

This report concerns the energy of a zero-temperature many-body system of spin 1/2 fermions in the unitary limit. In a previous report (nucl-th/0705.0944) this energy was determined to be $\xi = 0.24$ in units of the free gas kinetic energy, appreciably lower than most reports giving $\xi \sim 0.45$. In our calculation the 2-body interaction satisfied exactly the unitary limit i.e. infinite scattering length and effective range $r_0 = 0$. In the present report results with $r_0 > 0$ are shown. A strong dependence on the effective range is found. It is for example found that an increase to $r_0 = 1$ fm increases ξ to ~ 0.4 close to other reports of ξ in the unitary limit. It is concluded that because of the singular character of the unitary limit it is necessary to verify that the interaction actually satisfies unitarity. The calculations done here in a pp-ladder approximation show a resonance in the in-medium interaction close to (and in) the unitary limit. This was already observed in the previous work.

Nonequilibrium superconducting proximity effect in interacting quantum dots

König, Jürgen

We present a real-time diagrammatic theory for transport through interacting quantum dots tunnel coupled to normal and superconducting leads. Our formulation describes both the equilibrium and non-equilibrium superconducting proximity effect in a quantum dot. We apply this theory to a three-terminal transistor geometry, consisting of a single-level quantum dot tunnel coupled to two phase-biased superconducting leads and one voltage-biased normal lead. We compute both the Josephson current between the two superconductors and the Andreev current in the normal lead, and analyze their switching on and off as well as transitions between 0- and π -states as a function of gate and bias voltage. For the limit of large superconducting gaps in the leads, we describe the formation of Andreev bound states within an exact resummation of all orders in the tunnel coupling to the superconducting leads, and discuss their signature in the non-equilibrium Josephson- and Andreev-current and the quantum-dot charge. Finally, we address non-local Andreev effects in geometries with one superconducting and two normal or ferromagnetic leads.

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Effective vortex mass influenced by crystal lattice deformations

Kolaček, Jan

In superconductors penetrated by Abrikosov vortices, the magnetic pressure and the inhomogeneous condensate density induce a deformation of the ionic lattice. We calculate how this deformation corrugates the surface of a semi-infinite sample and estimate how it influences effective vortex mass.

Electron and hole spin dynamics in 2D heterostructures

Korn, Tobias

The spin dynamics in GaAs heterostructures are typically governed by the effective spin-orbit fields, which are modified as the dimensionality is reduced from the bulk to 2D systems. We study the spin dynamics in high-mobility n- and p-modulation-doped systems as well as in systems with embedded paramagnetic impurities by means of time-resolved optical spectroscopy.

Ultrafast coherent dynamics in optically driven BCS systems

Kuhn, Tilmann

Much of our detailed knowledge about semiconductors has been obtained by ultrafast optical measurements. Such methods can be, and in part have been, applied to superconducting materials as well. A superconductor is, in some respect, quite similar to a semiconductor, but it is also distinguished by some unique properties. Both systems exhibit an energy gap, which however in superconductors is much smaller and can typically be changed in a much wider range than in semiconductors, e.g. by varying the temperature or by optically creating quasi-particles. In contrast to semiconductors, the ground state of a superconductor cannot be approximated by a product state in the electron basis. Instead it is made up of a coherent superposition of states with different electron numbers and is a prime example of a state with highly correlated electrons. These similarities and differences make the ultrafast coherent dynamics of superconductors an interesting object of investigation. We have numerically calculated the dynamics of an optically excited superconductor in a mean-field BCS model within the density-matrix formalism. We present simulations of pump-probe measurements with terahertz laser-pulses with a width in the picosecond range. In the probe spectra the energy gap of the superconductor is directly visible as a region of very little absorption followed by a sharp peak at its edge. The gap is decreased by the excitation and can even vanish completely if the pump pulse is sufficiently strong. In addition, two other features well-known from pump-probe spectra in semiconductors can be observed: For sufficiently long pulses a hole-burning effect is seen and in the case when the probe pulse precedes the pump pulse the signals exhibit spectral oscillations. For very short pump pulses a novel regime is reached. In this nonadiabatic regime the modulus of the BCS order parameter performs a fast, damped oscillation in time. In the Bogoliubovian quasi-particle picture, the excited state induced by a short pulse cannot be described by quasiparticle occupations alone and therefore the state changes with time, giving rise to the oscillation. Surprisingly, the gap observed in pump-probe spectra does not shift as a function of the delay time; instead it always reflects the average value of the oscillation. Nevertheless the oscillation may be observed by making use of a coherent control

technique with two short pump pulses followed by a weak probe pulse. Varying the delay time between the two pump pulses produces final states with different gap energies which monitor the oscillation of the order parameter created by the first pump pulse.

Lasing in organic microresonators

Leo, Karl

Thermodynamics of a Trapped Unitary Fermi Gas

Magierski, Piotr

In the last couple of years we have witnessed a tremendous progress in the field of cold fermionic atoms. Ultra cold atomic gases provide a remarkable opportunity to investigate strongly correlated Fermi systems. They are dilute and their interactions can be precisely controlled over an enormous range. In particular, they form unique laboratories where the crossover between the Bose-Einstein condensate and the BCS superfluid can be explored. On the theoretical side, our overall understanding of these remarkable many body systems has improved tremendously even though many questions remain unanswered. During the talk I would like to discuss the properties of dilute and strongly interacting Fermi gas in the so-called unitary regime (when scattering length tends to infinity). I will report on results for the energy, entropy and chemical potential as a function of temperature and give upper bounds on the critical temperature for the onset of superfluidity. The comparison with recent measurements of the entropy and of the critical temperature of a trapped unitary Fermi gas will be presented.

Theory of excitons in single-walled carbon nanotubes

Malic, Ermin

Carbon nanotubes are tiny hollow cylinders constructed by rolling up graphene (a single layer of graphite). They are prototypical one-dimensional structures with diameters in the range of one nanometer and lengths of up to several centimeters. Depending on their microscopic structure and the rolling angle, a variety of metallic and semiconducting nanotubes with different chiralities can be created. We present a microscopic calculation of the excitonic absorption coefficient and Rayleigh scattering cross section for single-walled carbon nanotubes of arbitrary chiral index. Our approach combines the density matrix formalism including the Coulomb and electron-light interaction with the tight-binding approximation. Both the energy renormalization due to the electron-electron coupling and the formation of excitons due to the electron-hole coupling are discussed. We show the diameter and chirality dependence of excitonic effects presenting Kataura plots for optical transition and binding energies. Furthermore, we present results on the excitonic oscillator strength and the influence of the environment in absorption spectra.

Spin-dependent transport through molecular contacts

Mertig, Ingrid

Using density functional theory we have performed theoretical investigations of the electronic properties of a free-standing one-dimensional organometallic vanadium-benzene wire. This system represents the limiting case of multi-decker Vn(C6H6)n+1 clusters which can be synthesized. We predict that the ground state of the wire is a 100

Non-equilibrium polarization and currents in graphene rings

Moskalenko, Andrey

Graphene became a hot topic since the demonstration of its fabrication because of the quasi-relativistic properties of its band structure and its high crystal quality. Mesoscopic effects are of a particular interest as they exhibit features unusual for metallic or semiconductor mesoscopic structures. Recently, mesoscopic graphene rings were fabricated. The properties of the Aharonov-Bohm effect were investigated theoretically and experimentally. We investigate non-equilibrium mesoscopic effects in graphene rings excited by ultrashort asymmetric electromagnetic pulses. Ultrafast generation of charge-polarized and current-carrying states is demonstrated. It is shown that non-equilibrium valley current can be generated in graphene rings threaded by a stationary magnetic flux by application of an appropriate pulse sequence.

Counting statistics of non-Markovian quantum stochastic processes

Novotny, Tomas

We present a recursive method for calculating zero-frequency current cumulants of very high orders for quantum stochastic processes described by non-Markovian generalized master equations (GME) [1,2]. Within the same framework, the finite-frequency noise can also be evaluated. As a specific example, we consider charge transport through two coherently coupled Coulomb blockade quantum dots embedded in a dissipative environment. For high orders, the cumulants show surprising oscillations as functions of the level detuning. Using mathematical properties of derivatives in the complex plane [3] we show that these oscillations are in fact universal and are expected to occur as functions of almost any parameter in a wide class of stochastic processes [4]. We present the first experimental evidence of universal oscillations in electron transport through a single quantum dot [4].

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Tunneling induced level shifts in carbon nanotube Kondo-dots

Paaske, Jens

Coherence length of photons transmitted by nanofiber

Pärs, Martti/Rähn, Mihkel

Photons can be focused into a pinhole with diameter bigger than wavelength without any remarkable loss of the transmitted photons. However, the flow of photons transmitted by a (smaller) subwavelength aperture (SWA) is significantly reduced, which is described by the quantum theory as a reduction of the photon's passage probability through the aperture. One can suppose that the mean frequency of photons passing through SWA cannot remarkably change. But the question arises, whether the coherence length of these photons remains unchanged as well. In order to find out whether the diameter of SWA can actually affect the mean coherence length of transmitted photons, a single-photon interferometer has been built similar to that described in Ref. 1. A single nitrogen-vacancy defect center in diamond is used as a room-temperature source of single photons with suitably short coherence length. Optical fibers with subwavelength tips designed for near-field operation are used as SWAs. Our preliminary experimental results are to be presented.

Laser-field effects on the transport through molecular junctions

Padurariu, Ciprian

In recent years, the tunneling of electrons through a metal-molecule-metal junction has become a topic of intense research [1-3]. The present work examines the regime of weak coupling between the molecule and the metallic leads, employing a quantum master equation approach within second-order perturbation theory in order to derive the equation of motion for the density matrix belonging to the relevant system. The model incorporates excited electronic states of the molecule, coupled by an external laser field. Additionally, the molecular system couples to excitations of electron-hole pairs in the metallic leads [3]. The current flowing through the junction is studied in relation to the strength of these coupling parameters. The goal is to explain the complex dynamics induced by the interplay of the various quantum effects in laser-driven molecular junctions.

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Nonequilibrium quantum dynamics of excitons and spins in quantum dots

Piermarocchi, Carlo

A method to induce and control optically the coupling between spins on two neighboring quantum dots will be discussed. This coupling is robust against decoherence and it can be enhanced by embedding the dots in optical cavities. Optically induced spin coupling can control spin entanglement and realize quantum gates in arrays of dots. Strong dissipation can also be harnessed to generate spin entanglement. This is realized using the quantum Zeno effect, in which a rapid sequence of measurements freezes a system of dots in its initial state.

Emergence of entanglement out of a noisy environment: The case of microcavity polaritons

Portolan, Stefano

The concept of entanglement has played a crucial role in the development of quantum physics. It has gained renewed interest mainly because of the crucial role that such concept plays in quantum information/computation, as a precious resource enabling to perform tasks that are either impossible or very inefficient in the classical realm. Scalable solid-state devices will make use of local electronic states to store quantum correlations. Polaritons on the other hand, as hybrid states of electronic excitations and light, are the most promising solution for generation and control of quantum correlations over longer range. In order to address entanglement in quantum systems, the preferred experimental situations is the few-particle regime. Then, however, noise represents a fundamental limitation, as it tends to lower the degree of non-classical correlations or even completely wash it out. Here we show that microcavity polaritons can be cast in an entangled state in a controlled way. We accurately model the polariton parametric process, producing entanglement, and the time evolution of the competing decoherence processes, using a microscopic time-dependent theory. Our model shows how a tomographic reconstruction, based on two-times correlation functions, can provide a quantitative assessment of the level of entanglement produced under realistic experimental conditions. In particular, we propose an operational method to measure the Entanglement of Formation, out of a dominant time-dependent noise background, without any need for post-processing. Our study provides a suggestive perspective towards hybrid all-optical quantum devices where quantum information can be efficiently generated and controlled within the same structure.

Phonon induced decoherence of two-electron spin states in a double quantum dot

Roszak, Katarzyna

Phonon-induced decoherence of singlet-triplet superpositions in a double quantum dot is studied. We show that the same phonon-induced mechanism that leads to the dephasing of charge states, destroys coherence of two-electron spin states in a system of tunnel-coupled dots. This is due to a two-phonon assisted scattering process involving a virtual transition to the lowest excited states of the double dot. The resulting dephasing rates are compared to the single-phonon assisted transition rates between these lowest energy states to gain understanding of the relevance of the dephasing process.

Phase rigidity and transmission through quantum dots

Rotter, Ingrid

The effective Hamiltonian of an open quantum system is non-Hermitian. Its eigenfunctions are biorthogonal with, in general, non-rigid phases. The phase rigidity varies between 1 (for well isolated resonances) and 0 (for strongly overlapping resonances). The reduction of the phase rigidity is correlated with an enhancement of the transmission. In the regime of overlapping resonances, the transmission does not show single resonance peaks but is plateau-like. Here, the phase rigidity approaches zero and the system becomes transparent.

Ultrafast dynamics of surface plasmon polaritons

Runge, Erich

We discuss the ultra-fast response resulting from the coherent coupling between surface plasmon polaritons (SPP) and quantum well excitons in hybrid metal-semiconductor nanostructures. We compare with recent experimental data on the angle-resolved far-field reflectivity[1], where as a result of the coupling, a significant shift of about 7 meV and an increase in broadening by about 4 meV of the quantum well exciton resonance were observed. Such a strong interaction can, e.g., be used to enhance the luminescence yield of semiconductor quantum structures or to amplify SPP waves. [1] P. Vasa, R. Pomraenke, S. Schwieger, Yu. I. Mazur, Vas. Kunets, P. Srinivasan, E. Johnson, J. E. Kihm, D. S. Kim, E. Runge, G. Salamo, and C. Lienau, Coherent ExcitonSurface-Plasmon-Polariton Interaction in Hybrid Metal-Semiconductor Nanostructures, Phys. Rev. Lett. 101, 116801 (2008)

Modeling of electron transport through single molecules: nonequilibrium vibrons and polarons

Ryndyk, Dmitry

We consider electron transport through single molecules, placed between metallic, semiconductor, or carbon leads, with the focus on the effects of molecular vibrations, the problem being crucial for molecular electronics. On the way to interpretation of modern experiments with single-molecule junctions and STM spectroscopy of single molecules on surfaces, two main theoretical problems are to be solved. First, we formulate an ab initio based interacting many-body model, which includes relevant electron states and interactions: DFT is used to optimize geometry and obtain vibronic parameters; Hartree-Fock based method is more convenient to determine effective electron states and electron-electron interaction. Second, we apply quantum master equation (QME) or nonequilbrium Green function (NGF) method to describe electron transport through a system at finite voltage, taken into account correlation and inelastic effects due to electron-electron and electron-vibron interactions. To this end, we develop the self-consistent transport theory based on the Keldysh formalism for NGFs using a number of complimentary methods, such as equation-of-motion method, diagrammatic method, and functional-derivative method. We investigate some key effects: vibronic instability and excitation of nonequilibrium vibrons in the case of weak electron-vibron

interaction; polaron memory effects and resonant tunneling in the case of strong electron-vibron interaction. Available experimental results are discussed in light of developed theoretical formalism.

Stochastic models for coherent multidimensional spectroscopy : Probing anomalous (aging) spectral diffusion and exciton fluctuations

Sanda, Frantisek

We present two recent advances in the stochastic modelling of 2D spectra.

(i) We applied stochastic model of fluctuating excitons to calculate 2D spectra of simple molecular agreggates (such as dimers). We have treated the effect of fluctuation timescale on exciton transfer expressed in dynamics of some peaks monitoring instantaneous dipolemoments induced by slow fluctuations of excitons. This make some difference against more conventional simulations based on Redfield master equations for the exciton transfer.

(ii) We developed theory of nonlinear response for nonMarkovian fluctuations of transition frequencies with erasure of memory at the points of stochastic jumps (continuous-time-random-walks model) which is capable to treat long time memory effects (anomalous relaxation), including aging processes. Signatures of these memories are found in 2D lineshapes of two state bath jump frequency modulation of a single two level system.

Spatial and spectral control of individual quantum dots

Schmidt, Oliver

Accurate control over spatial position, geometry and lateral arrangement of quantum dots is pursued by many groups world-wide[1]. We use ex-situ and in-situ substrate patterning to create lateral quantum dot molecules [2], quantum rings [3] and highly ordered quantum dot arrays in lateral and vertical directions. Distinct features like anticrossing patterns as well as peak energy oscillations as a function of externally applied magnetic fields are observed for single quantum dot molecules and quantum rings, respectively. Accurate and resolution limited spectral tuning of individual quantum dots is achieved by in-situ laser processing [4], by putting quantum dots into flexible microtube ring resonators [5], and by applying strain with underlying piezoelectric substrates [6]. The techniques we have developed might be helpful to promote a deterministic quantum dot technology fully integrative on a single chip. [1] O. G. Schmidt, ed., Lateral Alignemnt of Epitaxial Quantum Dots (Springer, Berlin, 2007)

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Two-photon photocurrent studies of electron intersubband dynamics in multiple quantum wells

Schneider, Harald

Quantum wells comprising three equidistant subbands, two of which are bound in the well and the third one in the continuum, result in a resonantly enhanced coefficient for two-photon absorption, which is by six orders of magnitude stronger than in usual semiconductors. Exploiting this nonlinearity in two-photon detectors, quadratic autocorrelation of a free-electron laser has recently been demonstrated at room temperature [1]. Temporal resolution of such a two-photon autocorrelator is only limited by the sub-ps intrinsic time constants of the intersubband transition, namely the intersubband relaxation time and the phase relaxation time. Using sub-ps mid-infrared pulses, the approach allows us to determine systematically the dependence of these time constants on structural parameters, and to discriminate between different scattering processes [2].

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Dissipation in driven circuit QED systems

Schön, Gerd

Several recent experiments on quantum state engineering with superconducting circuits realized concepts originally introduced in the field of quantum optics. Motivated by one such experiment we investigate a Josephson qubit coupled to a slow LC oscillator with frequency (MHz) much lower than the qubit's energy splitting (GHz). The qubit is ac-driven to perform Rabi oscillations, and the Rabi frequency is tuned to resonance with the oscillator. The properties of this driven circuit QED system depend strongly on relaxation and decoherence effects in the qubit. We investigate both one-photon and two-photon qubit-oscillator coupling, the latter being dominant at the symmetry point of the qubit. When the qubit driving frequency is blue detuned, we find that the system exhibits lasing behavior (single-atom laser); for red detuning the qubit cools the oscillator. Similar behavior is expected in an accessible range of parameters for a Josephson qubit coupled to a nano -mechanical oscillator. In a different parameter regime, furthering the analogies between superconducting and quantum optical systems, we investigate Sisyphus damping, which is the key element of the Sisyphus cooling protocol, as well as its exact opposite, Sisyphus amplification.

Spindynamics in semiconductor heterostructures

Schüller, Christian

We report about time-resolved optical experiments on the spin dynamics of two-dimensional electron (2DES) and hole systems (2DHS) in GaAs-AlGaAs heterostructures. In high-mobility 2DES we have observed at low temperatures a coherent spin oscillation of electron spins due to the effective magnetic field, caused by spin-orbit interaction. We have found a drastic dependence of the spin dephasing time on the degree of initial spin polarization of the electrons, which can be understood as an effect of the Hartree Fock exchange field. In experiments with inplane magnetic fields, we have detected a strong magnetoanisotropy of spin dephasing for spins aligned in the inplane directions.

Time dependent self interaction correction (TDSIC)

Suraud, Eric

We discuss the self interaction formulation in complement to local density approximation in the framework of density functional theory. We introduce a double set formulation allowing to properly deal with time dependent theories and alos leading to some valuable approximate scheme along the optimized effective potential startegy. We show examples of applications in cluster, molecules and quantum dots.

Work and fluctuation theorems for closed and open quantum nano-systems

Talkner, Peter

Ultrafast dynamics of quantum dots coupled with environment by numerical path integrals

Vagov, Alexei

Path integrals provide a convenient tool to obtain numerical results for the dynamics of the strongly confined nanosize systems such as quantum dots. The method fully explores the relevant memory of the system and thus provides numerically exact results that can later be used to compare with popular approximations in the studies of the dynamics. Results of the method for the dynamics of strongly confined semiconductor quantum dots, coupled to acoustic phonons and driven by external laser pulses, will be presented as an example. The decay time and the frequency of Rabi oscillations in the limit of strong fields and phonon coupling will be obtained and demonstrated to depend notably on the temperature and the applied field. The field dependence is non-monotonic leading to an undamping of Rabi oscillations at high pulse areas.

Size dependent ultrafast electron interactions in metal clusters

Vallée, Fabrice

Ultrafast electron interactions and their modifications by size reduction play key roles in the properties of metal nanoparticles. In this context, optical spectroscopy has been shown to be a very efficient tool for their investigation in nanoparticles embedded in different environment. In particular, increase of the electron-electron coupling and of electron-lattice energy exchanges have been demonstrated when decreasing the size of noble metal particles below 10 nm. These results, obtained in nanoparticles larger than about 3 nm, were modeled in term of surface induced modification of the bulk electron interactions. This approach cannot be extended to the very small size regime, i.e., to a few atom clusters, raising the key question of the transition from a solid-state-like behavior to a molecular one. We will present here extension of the measurements of the electron-lattice energy exchanges to the small size regime, i.e., to noble metal clusters smaller than 2 nm (formed by less than about 250 atoms). Experiments were performed in mass-selected clusters deposited on a substrate, permitting an excellent control of the particle size and of their surface condition. Measurements were performed using a high sensitivity femtosecond pump-probe setup to control the impact of cluster heating on the measured kinetics. The first results show a decrease of the electron-lattice energy exchange rate in the small size regime, in spark contrast with the behavior observed for large particles. This indicates a change in the nature of electron-lattice coupling in these systems. It is ascribed to evolution of the cluster electronic structure, from a quasi-continuous density of states to a discrete one, due to increasing energy separation of the quantized electronic states in small clusters.

Single molecule bridge in transient regime

Velicky, Bedrich

The simplest nanoscopic system, a molecular bridge consisting of a single molecule with one or few electronic or vibronic levels coupled to non-interacting leads [1] can be treated using non-equilibrium Greens functions (NGF) in an elegant manner represented by a time dependent generalization [2,3] of the original Meir-Wingreen approach [4]. In the present work, we concentrate on the transient behavior of the molecular bridge with time variable coupling to the leads. The transient process depends on the initial conditions at a finite time which in turn are formed during the previous history of the system[5]. This is captured by the so-called partitioning in time of the NGF [6]. We explore several general questions, in particular establishing of the steady state, formation of quasiparticle excitations and validity of the non-equilibrium Ward identities which have a direct bearing on the possibility of bringing the general NGF expressions to the quantum transport equations by means of a modified Generalized Kadanoff-Baym ansatz[7].

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Zero-phonon line broadening and satellite peaks in nanowire-based quantum dots

Wacker, Andreas

Decoherence in quantum dots has been of central importance in the past years due to the use of quantum dots as qubits or as single-photon emitters in quantum information schemes. Most studies have focused on self-assembled quantum dots which are embedded in a substrate and thus exposed to three-dimensional bulk phonons [1]. The interaction of single excitons with acoustic phonons has been extensively investigated, revealing the existence of sidebands attached to the central zero-phonon line. Calculations within the standard independent Boson model provide a vanishing broadening of the central peak. Here, we show that the physics of quantum dots embedded in nanowire structures shows distinct differences [2]: (i) The lateral quantization of the phonon spectrum gives rise to the presence of pronounced satellite peaks in the absorption spectrum. These depend strongly on the type of interaction as specifically shown for the deformation potential and piezoelectric scattering mechanism [3]. (ii) The one-dimensional character of the lowest phonon mode provides a finite width of the zero phonon line within the independent Boson model. The calculated broadening is larger than the measured width in bulk-based dots [1], showing the crucial relevance of the dimensionality for the scattering environment. This effect has been very recently observed in a carbon nanotube [4].

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Nonlinear Thz spectroscopy on n-type GaAs

Woerner, Michael

In most THz experiments the THz radiation is used as a linear probe. Using THz radiation for nonlinear excitation requires the ability to generate high enough THz intensities. Our recent development of a simple and reliable method to generate THz pulses with high intensities has paved the way for nonlinear optics in the THz regime. We present various experiments on n-type GaAs which are in strong contrast to the predictions of Drude theory.

Quantum dots coupled to a reservoir of non-equilibrium free carriers

Woggon, Ulrike

The application of quantum dot (QD) lasers and semiconductor optical amplifiers (SOAs) in above 100-Gbit Ethernet networks demands a high frequency response and emission in the optical telecommunication windows at 1.3 to 1.55 mm. A great challenge is the amplification of ultrafast optical pulse trains with pulse separations of 1 picosecond or even below, i.e. of pulse repetition rates around 1 Terahertz. To achieve this, the gain dynamics of powerfully electrically pumped InGaAs-based QD-SOA has to enter a regime of equal time scales for gain recovery and temporal sequences of the input

pulses. Consequently, the understanding of fundamental limits for THz optical pulse train amplification requires a microscopic description by a coupled polarisation- and population dynamics in a thermal non-equilibrium situation going beyond rate-equation based models. We present pump-probe studies of femtosecond pulse trains with up to 1 THz repetition rates and investigate the gain response of a QD-SOA at high electrical injection current and elevated device temperatures. The experimental results are simulated by applying the semiconductor quantum dot Bloch equations including microscopically calculated, temperature-dependent Coulomb scattering rates between quantum dot and 2D-continuum states. While QD-applications like quantum computation require ultralong dephasing times and mechanisms which minimize any type of scattering events, the here discussed QD-application for ultrafast pulse amplification demands the opposite: extreme fast decay of coherence and efficient scattering to destroy polarisation under conditions at which the QD states are coupled to a 2D-reservoir of non-equilibrium charged carriers. Such a situation raises interesting future questions such as the size of the fundamentally shortest time scale for a scattering process, the chance of a control of non-equilibrium population to design initial and final states for a scattering event, and the consequences for quantum dot level design by engineering QD and 2D-carrier system growth parameters.

Ultrafast dynamics of correlated electron systems

Wolf, Martin

Poster

String-vortex solitons in the gauged Heisenberg model

Bogolubsky, Igor

Investigation of field-theoretical models with 2D extended string-like solutions opens new possibilities for theoretical study of nonstationary phenomena in condensed matter physics (e.g. high-temperature superconductivity), biophysics,quantum field theory and cosmology . Such studies should include two main steps: (i) analytical or numerical search for extended 2-dimensional solutions in physically appealing models and (ii) investigation of their nonstationary behaviour: stability, pair and more complicated interactions. In this approach solitons play role of new collective degree of freedom. In our presentation we plan to discuss new features of solitonic strings which have been found recently within the so-called A3M model. This model is the U(1) gauge-invariant extension of the easy-axis Heisenberg antiferromagnet model. This continuous gauge-invariant model posesses Z(2) and local U(1) internal symmetries which result in remarkable properties of its localized solutions. The A3M topological solitons will be compared with Belavin-Polyakov localized solutions in 2D isotropic Heisenberg model and Abrikosov-Nielsen-Olesen defects in the Abelian Higgs model. Nonstationary properties of the A3M solitons will be discussed.

Nanostructure evolution with a combination of Monte-Carlo and phase-field modelling

Gemming, Sybille

The Burton-Cabrera-Frank (BCF) model describes the structural evolution of vicinal surfaces in terms of an incoming particle flux and concentration-dependent desorption and surface diffusion terms. A continuum formulation of the BCF scheme given by a phase-field implementation for the moving-boundary problem yields the long-term evolution of the step structure during a step-flow growth mode. A particle-based Ising-type approach with a Metropolis-Monte-Carlo kinetics additionally provides nucleation processes in a temperature-controlled manner and on a shorter time and length scale. We have integrated both approaches in a hybrid algorithm, which describes adsorption, nucleation, and structure evolution processes at solid-liquid and solid-gas interfaces on both time and length scales. The short term nucleation is resolved by the Monte-Carlo generated dynamics of an anisotropic Ising model, whose interaction parameters stem from first-principles calculations. The long-term microstructure dynamics is calculated by the phase-field method. Several growth modes are distinguished: In addition to step-flow growth the nucleation processes on the terraces can lead to roughening or an epitaxial layer-by-layer growth controlled by temperature and by flux. Observing and controlling hole spin dynamics in 2D hole systems at sub-Kelvin temperatures

Investigation of hydrogen storage in Zr and its alloys

Jain, Ankur

Irradiation effect on structural, chemical composition and electrical properties of Ni3N/Si system

Dhunna, Renu

Annealing effect on structural, magnetic and electrical studies of Fe/Si bilayer system

Lal, Chhagan

A simple model for multiple exciton generation in nanocrystals

Kowalski, Piotr

The possibility of generating more than one electron-hole pair with a single photon absorbed in a semiconductor nanocrystal shows great promise for increasing the efficiency of solar cells. Such a multiple exciton generation process was recently observed in various systems. In this presentation we discuss a model of this process, based on the assumption that the two-pair creation occurs coherently at the time of absorption. We calculate the Coulomb matrix elements between single electron and trion states within a simple uncoupled-band model of the nanocrystal. We show that the mixing between bright excited exciton states and ground state two-pair configurations makes the latter optically active, which opens a path to a direct and instantaneous creation of more than one carrier pair with a single photon absorption process.

Bose condensation for attractive interaction?

Männel, Michael

We investigate an interacting Bose gas using a scheme to eliminate successive collisions. For attractive interaction we find a two-particle bound state. When the binding energy of this bound state becomes twice the chemical potential there is a second order phase transition and a gap appears in the dispersion relation. The gap decreases with increasing density. At the critical point the gap vanishes, the dispersion becomes linear for small momenta and a Bose condensate appears. We interpret the appearance of the gap as a sign of structure formation.

InGaAs QDs dynamics in a population-inverted system and coupling to non-equilibrium reservoirs

Malic, Ermin

Optical properties of metallic single-walled carbon nanotubes

Malic, Ermin

Electron dynamics in molecular wires studied by a density matrix approach

Moevius, Lisa

Recent investigations in the field of molecular elecronics [1-4] are targeted on controlling the current through single molecules by laser fields. In the present work the metal-molecule-metal junction is described using a quantum master equation within second-order perturbation theory due to weak wire-lead coupling [1]. The dynamics of the system can be influenced by applying a laser field, leading to novel effects like coherent destruction of tunneling to effectively suppress the current through the molecular wire. Using a projection operator approach [3] an efficient reduction of dimensionality can be achieved to render effective calculations of longer wires possible.
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Mapping of KPZ growth onto reaction-diffusion particle models

Odor, Geza

We show that a 2+1 dimensional discrete surface growth model exhibiting KPZ class scaling can be mapped onto two dimensional reaction-diffusion model of directed dimers. In case of KPZ height anisotropy the dimers follow driven diffusive motion. We confirm by numerical simulations that the scaling exponents of the dimer model are in agreement with those of the 2+1 d KPZ class. This opens up the possibility of analyzing the KPZ class via reaction-diffusion models and effective simulations.

Single-molecule imaging of terrylene-doped biphenyl single crystals

Pärs, Martti

Over the last two decades the methods of single molecule detection and spectroscopy have played a growing role in material science and biology. The great advantage is that investigations at single molecule level can reveal dynamical and structural features which are obscured or averaged out by using conventional spectroscopic methods. At previews work we have studied fluorescence images of single terylene impurity molecules by using wide-field epifluorescence microscopy. Our home-made room-temperature single molecule imaging (SMI) setup is based on standard microscope. The fluorescence images of single molecules are captured with EMCCD camera. Excitation was carried out by using a CW laser line at 532 nm. The temporal behaviour of fluorescence intensity has been studied by acquiring images sequences of many molecules. The laser excitation induced irreversible photobleaching of single-molecule emitters was studied. The process was inhibited in a nitrogen-enriched atmosphere, thus confirming the role of photochemical reactions between terrylene and oxygen. Detailed spatial analyses of images indicates, that some of terrylene impurity molecules appeared to stay fixed in the host crystal, some of them can be observed to move around over distances of tens of micrometers, probably diffusing along the defects of the crystalline structure. Described technique allows to track single molecules in solids or on surfaces with accuracy better than 100 nm.

Sequence of surface phase transitions at O and CO catalytic reaction on Pd(111)

Petrauskas, Vytautas

The model has been proposed to simulate numerically the reaction $O + CO \rightarrow CO_2$ and occurring phase transitions on Pd(111) surface. With increase of CO coverage the phase transition sequences $(2x2) - O \rightarrow (3x3) - O$ and $(2x2) - O \rightarrow (3x3) - O \rightarrow (2x1) - O$ are obtained for room and lower temperatures respectively. We demonstrate that the reaction rate is the crucial factor determining the occurrence of the (2x1) - O phase and vanishing of the (3x3) - O with decrease of temperature. The reaction at room temperature is found delayed until the (3x3) - O phase occurs. The results strongly support the viewpoint that the reaction proceeds at the perimeter of oxygen islands mostly.

Orthogonality catastrophe in mesoscopic systems (The mesoscopic X-ray edge problem)

Röder, Georg

We study the response of integrable and chaotic mesoscopic systems to a sudden, localized perturbation caused, e.g., by an x-ray exciting a core electron into the conduction band. Anderson orthogonality catastrophe (AOC) refers to the disappearance of the overlap of the many-particle ground states before and after the perturbation is applied in the thermodynamic limit. In contrast, a finite number of particles causes AOC to be incomplete with a broad distribution of AOC overlaps originating from mesoscopic fluctuations, in particular those that occur close to the Fermi energy. We consider two integrable ballistic quantum dots (rectangle and disc with hard walls) subject to a rank-one perturbation and compare the results with those obtained for generic chaotic systems. We find that the distributions of AOC overlaps differ, especially in the presence of a magnetic field. Level degeneracies present in integrable systems lead to additional peaks in the AOC distribution that shift the average overlap to smaller values. Furthermore, we apply these results to study Fermi edge singularities in the photo-absorption spectra of mesoscopic systems and show that their signature can qualitatively deviate from metallic (bulk-like) systems.

Carbon nanotubes as terahertz emitters and detectors

Rosenau da Costa, Marcelo

We propose and justify several schemes, which would utilize the unique electronic properties of carbon-based nanostructures in a range of THz applications. The first scheme is based on the population inversion in quasi-metallic carbon nanotubes (CNTs) induced by an applied voltage. We have shown that in the ballistic transport regime spontaneous emission spectra of quasi-metallic CNTs have a universal frequency and bias voltage dependence with the cut-off frequency controlled by the applied voltage [1]. The second scheme is based on the electronic properties of chiral CNTs, which represent ideal superlattices with a period significantly exceeding inter-atomic distance between two neighboring carbon atoms. An electric field normal to the nanotube axis opens noticeable gaps at the edges of the reduced Brillouin zone [2] resulting in the negative effective-mass region in the CNT energy spectrum. We have studied the Bloch oscillations in long-period CNTs and found the optimal values of the transverse electric field and CNT parameters needed for observation of the negative differential conductance and efficient frequency multiplication in the THz range. Our third CNT-related proposal is based on the Aharonov-Bohm effect in truly metallic (armchair) nanotubes. A magnetic field applied along the nanotube axis opens the band gap in a metallic CNT turning it into a semiconductor. For a typical (10,10) nanotube the gap is in the THz range for experimentally attainable fields of several Tesla. We have shown [3] that applying magnetic field also allows dipole optical transitions between the top valence subband and the lowest conduction subband, which are strictly forbidden in armchair CNTs without the field. In the tight-binding model, the matrix elements of these transitions can be obtained in a simple analytical form. These transitions, which are significantly sharpened by the van Hove singularity, can be used in highly-sensitive detectors of THz radiation. The same system can be used in tunable THz sources based on the four-level scheme, in which optical absorption is proceeded by THz emission across the magnetically induced gap.

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Far-infrared transmission of NbN superconductor film in magnetic field

Šindler, Michal

This poster presents measurements of temperature and magnetic field dependent far-infrared transmission of a thin layer of a thin NbN superconductor layer. For frequencies below the gap peaks in the temperature dependence of transmission were observed. These peaks decrease with magnetic field and vanish at high magnetic fields. Field dependent measurements show a rather complex behavior of transmission for different temperatures. In order to interpret our experimental data, we calculated the transmission of the NbN layer using BCS formula for complex conductivity following Zimmermann and Brandt [1]. For zero magnetic field the experimental and computed data are in a good agreement. A partial disagreement of experiment and calculated results for non-zero magnetic fields is probably due to vortex motion.

Materials modification at Zirconium-Silicon interface using swift heavy ions

Sisodia, Veenu

Multiple electron transfer and transport through a DNA dimer

Tornow, Sabine

We investigate multiple electron transfer in a donor-bridge-acceptor system where the molecular bridge comprises a DNA dimer (AT-AT or GC-GC) strongly coupled to a bosonic bath. The time dependent population probabilities and transfer characteristics of multiple electrons is calculated with the time-dependent renormalization group method at low temperatures and kinetic equations at large temperatures. The related transport properties for a system where donor and acceptor are replaced by left and right leads is discussed in different temperature and coupling regimes.

Corban modified nanostructure of gold nanoparticle

Tripathy, Puspanjali

Tunneling through nanosystems: Combining broadening with many-particle states

Wacker, Andreas

THz sideband generation in GaAs/AlGaAs multi quantum wells

Wagner, Martin

Ac THz electric fields which couple strongly with intraband excitations in semiconductors can lead to spectral sidebands when an interband excitation is present. In this nonlinear mixing process a near-infrared (NIR) laser beam is mixed with a THz beam to generate sidebands around the NIR frequency with a frequency spacing equal to the THz frequency or multiples of it: $\omega = \omega_{NIR} \pm n\omega_{THz}$ (with integer n). In the last years this effect has been investigated in various semiconductor systems (i.e. in bulk GaAs [1] or in multi quantum wells [2, 3]). We investigated the third-order nonlinear mixing process between a near-infrared laser and a free-electron laser in an undoped symmetric AlGaAs/GaAs multi quantum well. The sample is studied in transmission under illumination by FELBE, the free-electron laser (FEL) of the Forschungszentrum Dresden-Rossendorf. Differently from the literature where electronic and heavy-hole intersubband transitions were used, we are covering different hole transitions by tuning the FEL wavelength. We directly compare the n=+2 sideband generation efficiency for a transition between the heavy-hole and light-hole states with the efficiency for the intraexcitonic 1s-2p transition of the heavy-hole. Tuning the FEL to be resonant with the intraexcitonic 1s-2p transition leads to a much larger efficiency up to 0.2%, which is comparable to the best values achieved for an even stronger n=+1 sideband process [2]. [1] M. A. Zudov et al., Phys. Rev. B 64, 121204, 2001

[2] S. G. Carter et al., Appl. Phys. Lett. 84, 840, 2004

[3] S. G. Carter et al., Phys. Rev. B 72, 155309, 2005

Terahertz conductivity of Ge/Si (001) heterostructures with quantum dots

Zhukova, Elena

We performed the first measurments of terahertz spectra of dynamical conductivity of multilayered Ge/Si (001) heterostructures with quantum dots. The structure was characterised with STM to determine geometrical parameters and concentration of Ge dots formed on Si (001) substrate under specified growth temperature. The THz spectra of dynamical conductivity were measured with quasi-optical BWO-spectrometer over a frequency range 200 GHz - 1 THz. We obtained frequency-dependent conductivity of individiual Ge nanostructured layers and are discussing microscopics of charge dynamics within the layers.

Site-selective determination of coordination symmetries by anisotropic anomalous X-ray scattering

Zschornak, Matthias

Based on an experiment of Kirfel and Petcov on rutile (136) P42/mnm, which verified anisotropic anomalous scattering (AAS) by measuring 'Forbidden Reflection near Edge Diffraction' (FRED), we aimed to extend the results with allowed reflections to extract more tensor symmetries of the Ti scattering factor tensor fij by fitting the model of AAS to the experimental data. Furthermore we intended to study possible restrictions for atomic site occupation of unknown structures in an identified space group due to these local symmetry relations exemplary for this model structure. Experiments were carried out at DESY/HASYLAB BL C using a Si (111) double crystal monochromator tuned to an energy of 4985eV. An automated optimization and Y-scan routine for a sample setup with rotating degree of freedom assured AAS measurements at the reflection maxima. The rutile samples investigated were $10 \times 10 \times 10 \times 10$ wafers in (001), (110) and (111) orientation and Y-scans were measured for the reflections 001, 220, 110 and 111. Ti occupies Wyckoff site 2a, its tensor symmetry must follow the local symmetry m.mm leaving 3 complex elements f11, f12, f33. Simulations showed dependencies: 001 to f12, 220 to f11- f33, 110 to f11- f33, 111 to f12. For the 001 reflection intensity real and imaginary part correlate, but the 111 intensity displays asymmetric influence so the ambiguity is separable. The measured data show clear evidence of AAS and the 001 FRED and 111 intensities could be fitted: f'Ti d'12 = -5.44 * 0.5(8), f"Ti d"12 = 3.98 *1.4(2). Since f13 and f23 were refined to zero, the positioning of Ti in the unit cell would

by inverse symmetry arguments only be consistent with respect to site symmetry on Wyckoff sites a, b, e, f, g (out of k).







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