Nonlinear Electron Transport in Nano-Junctions

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Iterative path integral summation approach to nonequilibrium quantum transport

Reinhold Egger

We have developed [1] a numerically exact approach to compute real-time path integral expressions for quantum transport problems out of equilibrium. The scheme is based on a deterministic iterative summation of the path integral (ISPI) for the generating function of the nonequilibrium current. Self-energies due to the leads, being non-local in time, are fully taken into account within a finite memory time, thereby including non-Markovian effects, and numerical results are extrapolated both to vanishing (Trotter) time discretization and to infinite memory time. The method is applied to nonequilibrium transport through an Anderson dot. [1] S. Weiss, J. Eckel, M. Thorwart, R. Egger, preprint arXiv:0802.3374

Non-equilibrium polaronic distributions and transport nonlinearities in suspended junctions.

Denis Feinberg, Alex Zazunov, and Thierry Martin

Transport of electrons through a suspended molecule or carbon nanotube may be strongly coupled to local vibrations. With normal metallic contacts, regimes can occur where the stochastic passage of charges through the junction induces Franck-Condon polaronic steps in the nonlinear I(V) characteristics. We have theoretically examined the role of the asymmetry of the couplings to the two leads, characterized by different contact resistances and capacitances. This may trigger a non-equilibrium distribution of polaronic states, giving rise to a rich behaviour including negative differential conductance features [1]. On the other hand, in a fully coherent transport regime, achieved by forming a Josephson junction with superconducting contacts, we find entangled states of electrons and vibrational modes, and squeezing of the quantum coherent mode fluctuations [2]. [1] A. Zazunov, D. Feinberg and T. Martin, Phys. Rev. B 73, 115405 (2006). [2] A. Zazunov, D. Feinberg, and T. Martin, Phys. Rev. Lett. 97, 196801 (2006).

Singlet-triplet transition in a single molecule transistor

Serge Florens

We have studied low-temperature magneto-transport for a fullerene-based molecular quantum dot obtained via the electromigration technique. Focusing on the even-charge Coulomb diamond, a crossing of singlet and triplet states is observed as a function of the gate voltage. This magnetic transition results in a rich variety of transport regimes, which are analyzed at the light of several Kondo effects. Similarities and differences with previous experiments on different quantum dot systems will be emphasized.

Molecular transport junctions: Inelastic and optical response

Michael Galperin

An intriguing issue in molecular junctions is the role played by nuclear motions in the conduction process. We use the NEGF formalism to describe resonant inelastic electron transport (RIET) and consider optical response of current-carrying molecular junction. Focus of our RIET consideration is strongly correlated transport with molecule being relatively weakly coupled to the leads. In this case we stress necessity for proper "nonequilibrium atomic limit" and discuss a way to introduce it. Optical response of current-carrying junction is discussed within a simple 2-level (HOMO-LUMO) model. Besides coupling to the contacts and molecular vibration, the model takes into account interaction with external (radiation) field and electron-hole excitations in the contacts. We use the approach to study optical response of such junction: absorption, fluorescence, and Raman spectroscopy.

Imaginary-time formulation of steady-state nonequilibrium: nonlinear electron transport in quantum dot systems

Jong Han

Nonlinear transport in nanoscale devices has recently generated a great deal of interest. One of the fundamental challenges in the field is to find reliable theoretical tools which will predict electron transport under finite bias in nano-devices, where strong correlation effects are drastically affected by the nonequilibrium condition. In this talk, by exploiting theoretical similarities between equilibrium and steady-state nonequilibrium, we extend the imaginary-time formalism to the quantum dot transport under finite bias. We numerically implement the formalism through quantum Monte Carlo method. We discuss the evolution of Kondo anomaly and decorrelation effects which manifest in inelastic electron transport such as the Kondo peak splitting due to magnetic field and phonon satellites in molecular devices.

Kondo model with voltage bias and magnetic field - nonequilibrium flow equation approach

Stefan Kehrein

Nonequilibrium Kondo physics in nanostructures driven by an external voltage bias offers interesting insights into the interplay of correlated many-body physics and nonequilibrium. I will discuss how the flow equation approach (method of infinitesimal unitary transformations) permits the calculation of physically relevant quantitites like the local density of states or the dynamical spin susceptibility and show results in different parts of the phase diagram. It will be shown that the current-induced noise plays a similar role to an effective temperature, but with significant quantitative corrections.

Non-Equilibrium Electron Transport through a Double Quantum Dot System and a Three-Electron Orbital System (Poster)

Verena Koerting, S. Schmaus, J. Paaske, and P. Wölfle

We study non-equilibrium transport phenomena in a 4-terminal setup of two quantum dots, coupled by an exchange interaction. Assuming a single electron on each quantum dot, the double quantum dot system is characterized by an interplay between the spin-exchange coupling between the dots and the spin-spin coupling of the dots with the leads, the so-called Kondo interaction. We find that a finite voltage on one quantum dot drives the other quantum dot out of equilibrium. The physics of the Kondo model is calculated to lowest order perturbation theory in the coupling to the leads. Attention has to be paid to the case of very small spin-spin interaction, and the breakdown of a singlet-triplet representation of the double quantum dot system is briefly discussed. Besides the differential conductance we show some preliminary results for the current cross-correlation between the current through the left and right quantum dot and discuss the importance of the transition rates for this quantity. As is well-known from the Kondo e ect at low temperatures logarithmic divergences do not allow for a perturbation expansion. Using two di erent scaling methods out of equilibrium we show that the e ect of a non-equilibrium transfer is enhanced by Kondo correlations. Furthermore we discuss a quantum dot with an orbital structure. Motivated by experiments on InAs nanowires we investigate a Kondo model for three electrons on three levels. The Kondo spin interaction and the orbital potential scattering terms lead to interesting signatures in the differential conductance. We discuss the appearance of negative differential conductance to second order in perturbation theory and additional kinks appearing due to non-equilibrium occupation effects.

Stable two-channel Kondo fixed point of an SU(3) quantum defect in a metal: renormalization group analysis and conductance spikes

Johann Kroha, Michael Arnold, Katinka Ballmann, and Tobias Langenbruch

A physical realization of the two-channel Kondo (2CK) effect is proposed, where a dynamical defect in a metal has a unique ground state and twofold degenerate excited states. In a wide range of parameters the interactions with the electrons renormalize the excited doublet downward below the bare defect ground state, thus stabilizing the 2CK fixed point. In addition to the Kondo temperature T_K the three-state defect exhibits another low-energy scale, associated with ground-to-excited-state transitions, which can be exponentially smaller than T_K. Using the perturbative nonequilibrium renormalization group we demonstrate that this can provide the long-sought explanation of the sharp conductance spikes observed by Ralph and Buhrman in ultrasmall metallic point contacts. The splitting of the conductance spikes in a magnetic field is discussed.

Nonequilibrium Superconducting Proximity Effect in Interacting Quantum Dots

Jürgen König

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.

Nonequilibrium quantum phase transitions

Aditi Mitra and Andrew Millis

An important set of questions in condensed matter relate to the effect of nonequilibrium drives on systems near quantum critical points. In this talk I will present results for the effect of current flow on two systems: one near a ferromagnetic-paramagnetic quantum critical point and the other near a superconductor-metal quantum critical point. For a ferromagnetic system, I will show that current flow has two important effects. One is to induce decoherence which affects the system in ways rather similar to temperature. Second it causes a symmetry breaking which qualitatively has the effect of producing a drift. On the disordered phase and for Ising systems decoherence is the dominant effect, with current induced drift giving only subleading corrections to scaling. On the other hand for models with continuous rotation symmetry, and for broken Galilean invariance, current flow can lead to dynamical instabilities of the ordered phase. For a superconducting order-parameter on the other hand, nonequilibrum effects are even more pronounced as the order-parameter is charged and therefore couples directly to the electric field. For these systems it will be shown that it is the direct-coupling which is the dominant effect on scaling near the critical point, with the effect of current induced decoherence and drift being subdominant.

Fermi liquid and reduced density matrix approaches to an non-equilibrium current through an Anderson impurity

Akira Oguri

In this talk we discuss two aspects of the non-equilibrium Kondo effect in quantum dots and nano-junctions, based on the Anderson impurity model. The first aspect is the low-energy Fermi-liquid properties at small but finite bias voltages V. An exact Ward-identity argument for the Keldysh Green's function shows that, up to terms of order V^2, the voltage dependence of the differential conductance dI/dV and the quasi-particle damping are determined by a set of the renormalized parameters at equilibrium, namely the Kondo temperature T_K and the Wilson ratio R. It also describes a universal scaling behavior between the V^2 term and the T^2 term in the temperature dependence of the conductance. The second aspect is a view seen from a reformulation of the non-equilibrium steady state. It is based on the reduced density matrix (RDM), which is obtained by integrating out one of the two channel degrees of the freedom that can be separated from the dot. The remaining part of the Hilbert space is modelled by a single-channel Anderson model with the RDM that brings the information about the bias voltage V. The RDM describes the mixed states which have an energy window of the range eV, and it shows for large V a close similarity to the high-temperature distribution in the thermal equilibrium. This formulation may be used for constructing a new nonperturbative approach to the non-equilibrium steady state. If time is available, we will also discuss the equilibrium properties of the quantum dots connected to the superconducting (SC) leads, which we studied with the numerical renormalization group (NRG). Furthermore, we can also discuss the competition between the Kondo effect and the Nagaoka ferromagnetism, taking place in the normal triple quantum dots in a triangular configuration.

One-dimensional fermions beyond the Luttinger liquid paradigm

Michael Pustilnik

In this talk I will review recent works on the dynamic correlation functions in one-dimensional systems of interacting fermions. Due to the energy and momentum conservation, the correlation functions exhibit a characteristic threshold behavior. Surprisingly, the conventional harmonic fluid (a.k.a. Luttinger liquid) framework is not sufficient for the description of the threshold singularities in the correlation functions.

The nonequilibrium Kondo model in finite magnetic field: A complete analytic solution in the weak-coupling regime

Herbert Schoeller, Frank Reininghaus, and Thomas Korb

We show how a nonequilibrium perturbative renormalization group (RG) method can be set up to describe the dynamics and the stationary state of a small quantum system coupled to several reservoirs. By using a new cutoff scheme on the imaginary frequency axis we are able to show generically in all orders in the coupling to the reservoirs that the RG flow is cut off by relaxation and dephasing rates. We apply the method to the nonequilibrium anisotropic Kondo model in finite magnetic field and calculate the differential conductance and the magnetic susceptibility analytically in a controlled way up to third order in the renormalized couplings J. We find the well-known logarithmic enhancement of the differential conductance at voltage V equal to the renormalized magnetic field h, but propose further enhancements at V=h/n, n=2, 3, ... in higher-order perturbation theory. A new nonequilibrium effect occurs for the magnetic susceptibility in the regime h << V, where we find a logarithmic enhancement at h=0. Finally, we discuss the difference of the cutoff of the logarithmic enhancements at resonance to the physical relaxation and dephasing rates, and find that the maximum enhancement is proportional to J ln(J).

Single-molecule quantum dots

Herre van der Zant

During the last few years different techniques have become available to study transport through individual molecules. With electromigration, we make nanogaps on an aluminum gate electrode in which single molecules are trapped. Three-terminal measurements on samples with the same molecule (OPV-5, Co4L4 grid molecule, Mn-12, single-metal atom complexes) share common features showing Coulomb blockade and Kondo physics. The junctions form molecular quantum dots and are stable up to temperatures of 200-240 K allowing for temperature-dependent measurements [1]. Of crucial importance is the observation of molecule-specific properties as deduced for example from the interaction between electronic transport and vibrational modes [2] or spin states [3] in the molecule. Other molecule-specific features include a charge-dependent gate and electronic-lead coupling. We have studied in detail [4] transport through a thiol end-capped oligophenylenevinylene molecule with five benzene rings (OPV-5). The measurements show that the spin states, the charging energies and the electronic spectrum are completely renormalized by the presence of the gold electrodes. In case of the doubly charged molecule the data indicate delocalized orbitals with an anti-ferromagnetic ground state and an exchange energy of 1.7 meV. Molecules are provided by Thomas Bjørnholm (OPV-5, single-metal atom complexes), M. Ruben and J.-M. Lehn (Co4L4 grid molecules) and A. Cornia (Mn-12). [1] M. Poot et al., Nano Lett. 6 (2006) 1031. [2] E.A. Osorio et al., Adv. Mater. 19 (2007) 281. [3] H.B. Heersche et al., Rev. Lett. 96 (2006) 206801 (cond-mat/0510732). [4] E.A. Osorio et al., Nano Lett. 7 (2007) 3336.

Electron Pair Resonance in the Coulomb Blockade

Felix von Oppen

Vibration assisted transport through molecular transistors

Maarten Wegewijs

DMRG and quantum impurity models

Andreas Weichselbaum and Jan von Delft

Quantum impurity models are analyzed routinely and reliably at very low energies using the Numerical Renormalization Group (NRG). Its great benefit of energy scale separation, however, comes at the cost of reduced resolution at finite energy. By realizing that the algebraic structure underneath NRG is the same as for the density matrix renormalization group (DMRG), namely matrix product states, several strict NRG contraints such as the rigid discretization scheme can be relaxed due to the variational principle of DMRG. Our recent work in that respect will be discussed.

Universal ac conductance and quantum phase transitions

Gergely Zarand