

## **Teilprojekt B2.02**

# **Single-Electron Effects in Nanostructures**

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## Single-Electron Effects in Nanostructures

### Introduction

In nano-scale devices the energy change associated with the transfer of a single electron charge frequently is significant. Examples are (i) metal islands and tunnel junctions fabricated by lithographic techniques, (ii) quantum dots, created, e.g., by lateral structuring in 2-dimensional electron gases, (iii) molecules, clusters or self-organized grown quantum dots which are coupled to electrodes, as well as (iv) charge traps, such as impurities with atomic dimension. In these systems ‘Coulomb blockade’ effects arise, which make it possible to control and observe the tunneling of single electrons. A rich variety of ‘single-electron’ effects have been observed and studied, both theoretically and experimentally, and, in fact, several applications have been demonstrated by now. The field has remained remarkably active for many years and appears to remain so for some time to come with novel questions arising, e.g., in the context of spin-dependent tunneling, quantum state engineering, and quantum metrology.

Frequently the Coulomb interaction in single-electron devices can be described approximately by an effective capacitance  $C$  and energy scale  $E_C = e^2/2C$ . Modern lithographic techniques allow the controlled fabrication of tunnel junctions with capacitances of the order of  $C = 10^{-15}$  F and below. For these systems the charging energy  $E_C$  is (in temperature units) of the order of 1 Kelvin and higher, and single-electron effects are observable at temperatures below these values. Quantum dots, clusters and charge traps may have an even lower capacitance making single-electron effects observable up to room temperatures. Of particular interest is the single-electron tunneling transistor (SET-transistor), a small island coupled via two low-capacitance tunnel junctions to source and drain electrodes and via a third capacitor to a gate electrode. The gate voltage  $V_g$  allows controlling the current through the transistor. SET-transistors have found technological applications, for instance as ultra-sensitive potential measurement device, as current standard, or primary thermometer in the Kelvin regime.

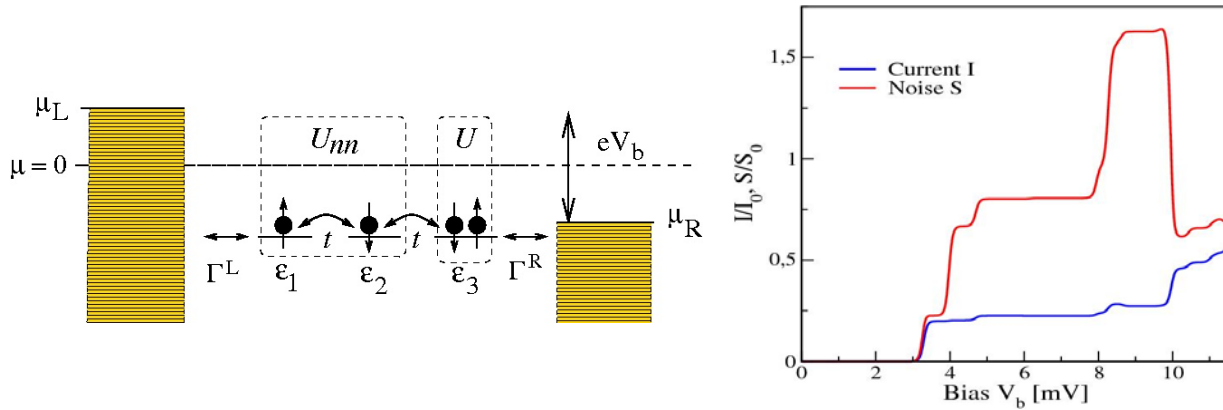
If the tunneling is weak, i.e., the tunneling resistance is high compared to the quantum value  $R_K = h/e^2 = 25.8$  k $\Omega$  only sequential tunneling needs to be considered, and the rates can be calculated by Golden rule arguments. For systems with larger conductance we had developed a systematic description, which allows us to treat coherent and non-equilibrium processes in higher order. During the reporting period we have applied it to a number of physical situations, including:

- shot noise in tunneling through single and multiple quantum dots and molecules, incl. correlation effects,
- spin-dependent tunneling through single-electron tunneling devices,
- non-equilibrium transport through quantum dots with strong coupling to the electrodes. This system displays properties known from Kondo or quantum impurity systems.
- generation and detection of entangled electron states in multi-dot systems, competition of interaction and interference effect, e.g., in Aharonov-Bohm interferometers,
- full counting statistics of single-electron tunneling,
- charge pumping in Josephson junction arrays.

The following pages review several of these topics.

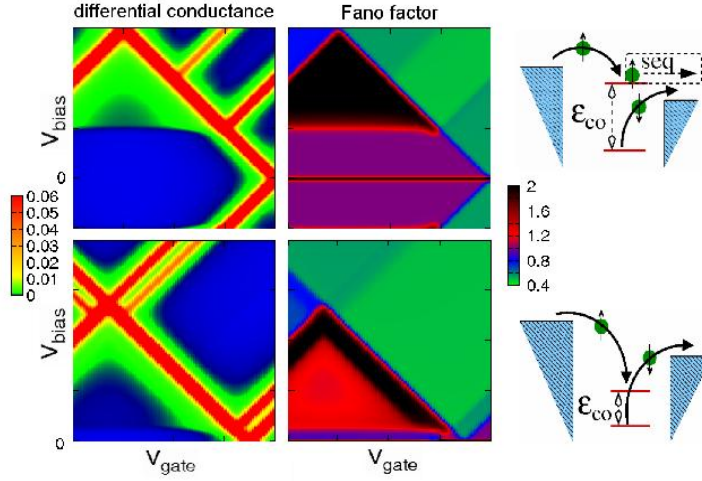
## 1. Shot noise in transport through quantum dots and multi-dot systems

In an earlier funding period we had studied charge transport through nanoscopic objects, e.g., quantum dots or molecules that are weakly coupled to metallic electrodes. The current-voltage characteristics as well as the current noise were calculated within leading and next-to-leading order perturbation expansion in the coupling strengths. Depending on the level positions and the coupling strength to the leads we find regions of negative differential conductance accompanied with super-Poissonian noise, i.e., a noise level above the Poissonian results of uncorrelated tunneling events [1,2]. For non-interacting fermionic systems the Pauli principle would lead to a lower noise level (sub-Poissonian noise). Continuing along these lines we studied in the reporting period charge transport through chains of quantum dots [B2.2:1, B2.2:2]. The dots are fully coherent among each other and weakly coupled to metallic electrodes. If the Coulomb interaction dominates over the interdot hopping the shot noise is strongly enhanced, by a factor of  $\sim 100$ , at biases above the sequential tunneling threshold. This strong effect may allow direct experimental detection of shot noise, e.g., in a chain of quantum dots formed in semiconductor heterostructures. The current is not enhanced in the region of enhanced noise, thus rendering the shot noise super-Poissonian.



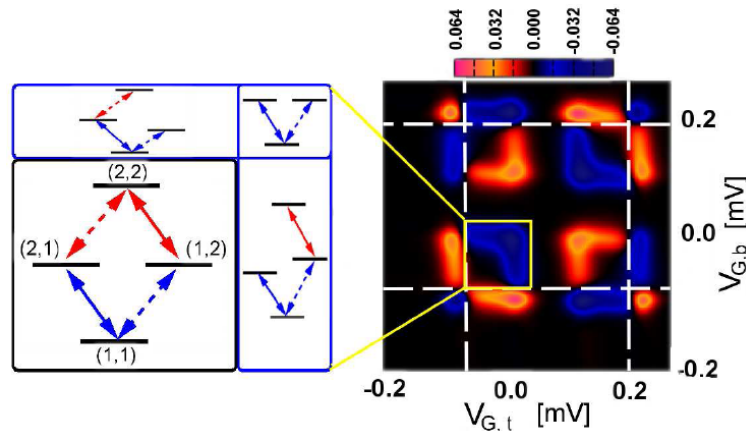
**Fig.1.** *Left:* Transport through three quantum dots between leads with on-site and nearest neighbor interaction. *Right:* Current and shot noise of the three-dot chain.

In multilevel quantum dots coupled to leads we observed that cotunneling assisted sequential tunneling (CAST) processes play a dominant role in the transition region from Coulomb blockade to sequential tunneling. We analyzed for intermediate coupling strength the dependence of the conductance due to CAST processes on the temperature, coupling constant, and gate voltage. Remarkably, the width of the CAST transport feature scales only with temperature, but not with the coupling constant. While the onset of inelastic cotunneling is associated with a super-Poissonian noise, the noise is even stronger above the threshold for CAST processes. [B2.2:18]



**Fig. 2.** *Left panels:* Color-scale plot of the differential conductance vs. gate and bias voltage. The Coulomb diamond edges mark the onset of sequential tunneling. Lines outside the Coulomb diamond correspond to transport via excited states, whereas the horizontal step inside the diamond is due to the onset of inelastic cotunneling. *Right panels:* Fano factor vs. gate and bias voltage. Super-Poissonian Fano factors occur around the inelastic co-tunneling excitation energy and are reduced to sub-Poissonian values outside the Coulomb diamond. *Top and bottom figures:* refer to two choices of the energy levels as indicated in the right hand side of the figure, for a gate voltage close to the center of the Coulomb diamond.

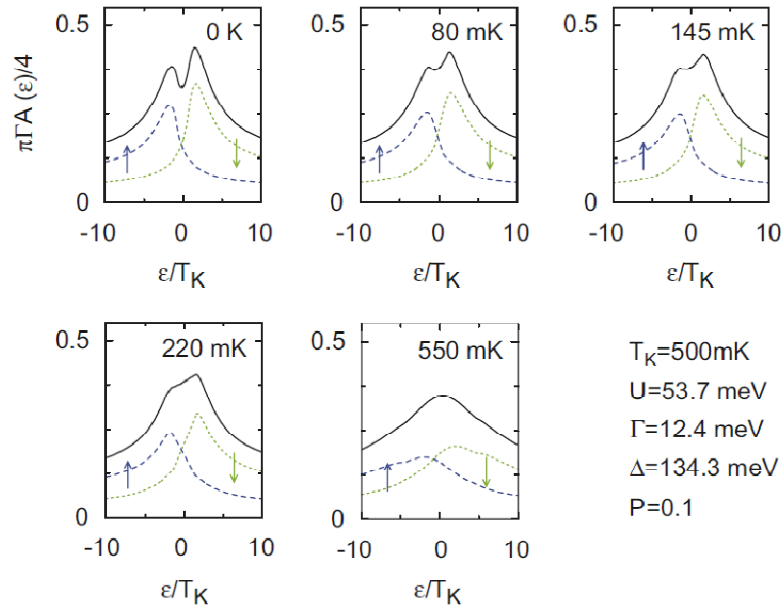
We further investigated cross-correlations in the tunneling currents through two parallel quantum dots coupled to independent electrodes and gates and interacting via an inter-dot Coulomb interaction [3]. The correlations reveal additional information, beyond what can be learned from the current or conductance, about the dynamics of transport processes of the system. We find qualitatively different scenarios for the dependence of the cross-correlations on the two gate voltages. When the temperature is reduced below the inter-dot Coulomb interaction, regions of a given sign change from spherical shapes to angular L-shapes or stripes. Similar shapes have been observed in recent experiments.



**Fig. 3.** *Right:* Cross-correlations versus the two gate voltages  $V_{G,t}$  and  $V_{G,b}$  at low temperature. The cross-correlations develop into L-shapes inside the central region with ground state of one electron on each dot. Dashed lines separate regions of different ground state occupation. *Left:* Sketch of the processes relevant for the lower left negative L – shape. Different combinations of positive and negative processes result in the L-shape of the cross-correlations. From Ref. [3]

## 2. Spin-dependent tunneling in single-electron devices

Both, the investigation of spin dependent electron transport and the study of strong Coulomb interaction effects in transport through nanostructures are by now well-established research areas. The combination of the two different paradigms within one system, however, is still an active research field. A suitable model system for a basic study of the interplay of the two effects is provided by a quantum dot attached to ferromagnetic leads. In earlier work we had studied the Kondo effect in single-electron tunneling through quantum dots, in particular we had investigated how the Kondo effect is modified by the presence of ferromagnetic leads. The real-time diagrammatic technique developed in our group provides a systematic description of the nonequilibrium dynamics of a system with strong local electron correlations. We evaluated the theory in an extension of the "resonant tunneling approximation," introduced earlier, by introducing the self-energy of the off-diagonal component of the reduced propagator in spin space. In this way we developed a charge and spin conserving approximation that accounts not only for Kondo correlations but also for the spin splitting and spin accumulation out of equilibrium. We showed that the Kondo resonances, split by the applied bias voltage, may be spin polarized. A left-right asymmetry in the coupling strength and/or spin polarization of the electrodes significantly affects both the spin accumulation and the weight of the split Kondo resonances out of equilibrium. The effects are observable in the nonlinear differential conductance. [4,5]



**Fig. 4.** Spin-resolved equilibrium spectral function  $A_{\sigma}(\omega, T, V=0)$ . The dashed lines correspond to  $A_{\uparrow}(\omega, T, V=0)$ , the long dashed lines to  $A_{\downarrow}(\omega, T, V=0)$ , and the solid ones to the sum of both. Note that the splitting of the Kondo resonance disappears upon increasing temperature.

During the reporting period we studied the influence of ferromagnetic leads on the Kondo resonance in a quantum dots employing Wilson's numerical renormalization group method, extended to handle leads with a spin asymmetric density of states [B2.2:11]. We identified the effects of (i) a finite spin polarization in the leads (at the Fermi surface), (ii) a Stoner splitting in the bands (governed by the band edges), and (iii) an arbitrary shape of the lead density of states. For a generic lead density of states, the quantum dot favors being occupied by a particular spin species due to exchange interaction with ferromagnetic leads, leading to suppression and splitting of the Kondo resonance.

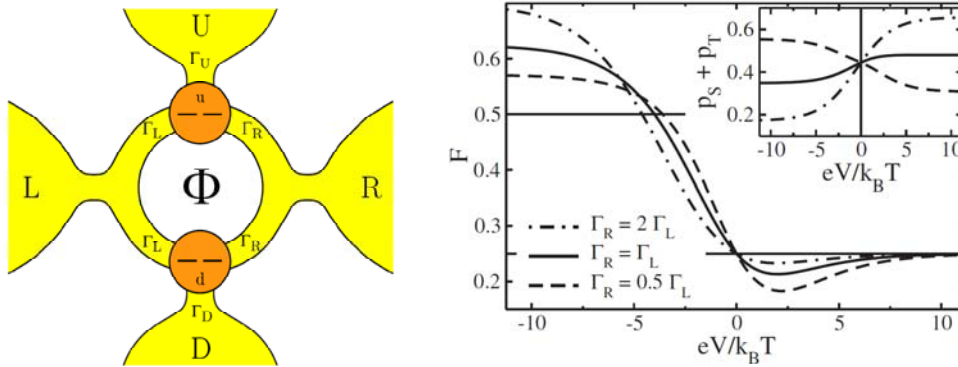
By applying a magnetic field one can compensate this asymmetry and restore the Kondo effect. We studied both the gate voltage dependence (for a fixed band structure in the leads) and the spin polarization dependence (for fixed gate voltage) of this compensation field for various types of bands. Interestingly, we found that the full recovery of the Kondo resonance of a quantum dot in the presence of leads with an energy-dependent density of states is possible not only by an appropriately tuned external magnetic field but also via an appropriately tuned gate voltage. For flat bands, simple formulas for the splitting of the local level as a function of the spin polarization and gate voltage were given.

### **3. Aharonov-Bohm interferometry and spin entanglement in interacting quantum dots.**

The controlled generation and detection of entanglement of quantum states remains one of the fundamental challenges of quantum physics. Experiments with entangled photons have already entered the realm of advanced quantum communication and cryptography. In solid state systems electron spins are considered as prime candidates for the demonstration of such effects. Spin degrees of freedom are only weakly coupled to the environment, which leads to long decoherence times, and coherence lengths well exceeding the micrometer range. Several set-ups involving quantum dots have been proposed to create and detect pairs of spatially separated, spin-entangled electrons. The schemes rely, e.g. on the extraction of Cooper pairs from a superconductor, or the separation of a pair of entangled electrons from a singlet ground state of single or double quantum dots. Evidence of entanglement in these systems can be obtained from noise measurements or coincidence detection.

In Ref. [B2.2:12] we suggested and analyzed a set-up which allows the creation and detection of entanglement of spatially separated electron spins. In this setup two quantum dots are coupled coherently to a joint source electrode on the left and to two independent drain reservoirs at the top and bottom. When a bias voltage is applied, electrons are driven from the source via the dots to the drain electrodes. A nonequilibrium, mixed electronic state is created. For appropriate values of the voltage, due to the strong onsite Coulomb repulsion, a state with two electrons (one on each dot) has a high probability. It turns out to be of the form of a Werner state, with a strong enhancement of the singlet component, although singlet and triplet states are degenerate.

In Ref. [B2.2:19] we extended this work and proposed a detection scheme where pure singlet and triplet states can be distinguished by Aharonov–Bohm (AB) interferometry. For this purpose an additional joint reservoir is coupled to the system closing the AB geometry (Fig. 5). The current to this reservoir is studied in the cotunneling regime. Under certain conditions the entanglement leads to a suppression of the AB oscillations. Hence this part of the set-up serves as a probe of the state of the system and as a detector for entanglement. Exploring the results in a wide parameter range we identify regimes where the double dot has a large probability to be in a singlet state. The predicted behavior provides a proof of concept for the entanglement generation in coherently coupled, nonequilibrium quantum dots.

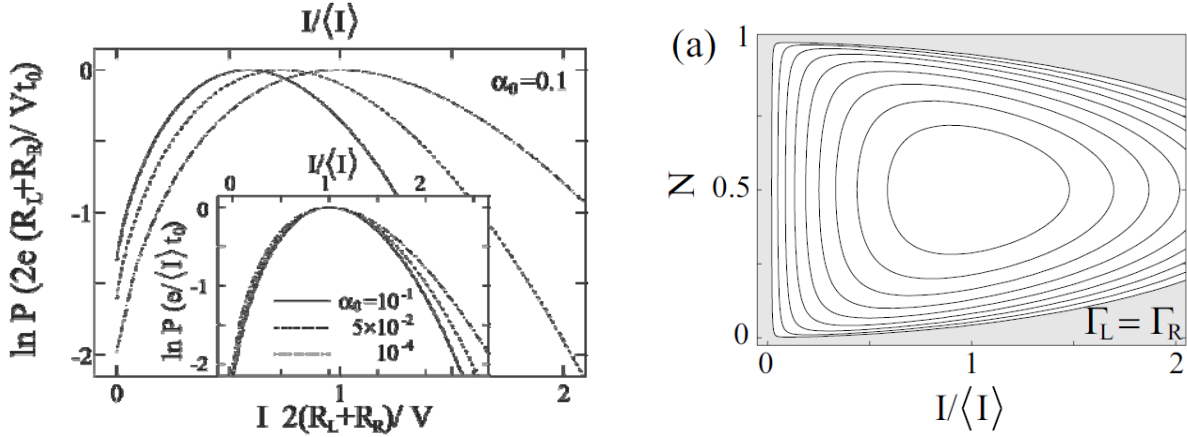


**Fig. 5.** *Left:* Two quantum dots (u and d) coupled to a joint reservoir on the lefthand side (L) and to two separate leads at the top and the bottom (U and D). The second joint reservoir on the right (R) closes the AB ring and is used to probe the state of the system. *Right:* The stationary Werner fidelity  $F$  vs bias voltage for  $\epsilon=0$  and different ratios of the coupling strengths,  $\Gamma_R/\Gamma_L=2, 1, 0.5$ . The inset shows the corresponding stationary overall probabilities  $p_S+p_T$  to find the system doubly occupied.

#### 4. Full counting statistics of single-electron tunneling

Another part of our project is devoted to the study of the Full Counting Statistics (FCS) of charge transfer in mesoscopic conductors. The method of FCS provides a unique tool to study the quantum-mechanical phenomena of current correlations and many-particle entanglement that can be hardly assessed by any other means. The main goal of this method is the evaluation of a statistical probability distribution for the number of electrons traversing the conductor in a given time interval. The first and the second moments of this distribution correspond to the average current and current noise, respectively. In general the  $N$ -th irreducible moment is a measure for correlations between  $N$  particles traversing through the sample.

In Ref. [B2.2:3] we evaluated the current distribution for a single-electron transistor (SET) with intermediate strength tunnel conductance,  $\alpha_0 = h/(4e^2 R) < 1$ , where  $R$  denotes the overall resistance of the transistor. In this situation the quantum fluctuation of charge play a dominant role. They are taken into account by the summation of a certain subclass of diagrams, which correspond to the leading logarithmic approximation in the sense of the renormalization group analysis. In first order in  $\alpha_0$ , our results reproduce the orthodox theory, while in second order they account for non-Markovian cotunneling effects. We have shown that in the non-equilibrium situation quantum fluctuation of charge induce life-time broadening for the charge states of the central island, which suppress the large current fluctuations. The results for the probabilities of the current distribution at the degeneracy point of SET are presented in fig. 6. We find that increasing the interaction strength, controlled by the parameter  $\alpha_0$ , leads to a pronounced suppression of large current fluctuations.



**Fig. 6.** *Left:* Current distribution  $P(I)$  for the symmetric SET at  $T=0$  and  $eV = 0.2 E_c$ , where  $E_c$  is the charging energy, shown at the degeneracy point for a different values of the dimensionless conductance  $\alpha_0$ . Inset shows the same distributions normalized to the average current.

*Right:* Contour plots of the joint probability distribution  $\ln P$  are given. The function has a maximum value  $\ln P(I, N) = 0$  at  $I = \langle I \rangle$  and  $N = \langle N \rangle = (\Gamma_L - \Gamma_R)/2\Gamma$ .

Motivated by recent experiments, we further developed the FCS theory for the joint probability distribution of the current and the electron number inside a quantum dots. We showed that a non-Gaussian exponential distribution appears when there is no dot state close to the lead chemical potentials. The measurement of the joint probability distribution of current and electron number would reveal nontrivial correlations, which reflect the asymmetry of tunnel barriers. We also show that for increasing strength of tunneling, the quantum fluctuations of charge qualitatively change the probability distribution of the electron number [B2.2:10, 19].

## 5. Single-electron tunneling and the fluctuation theorem

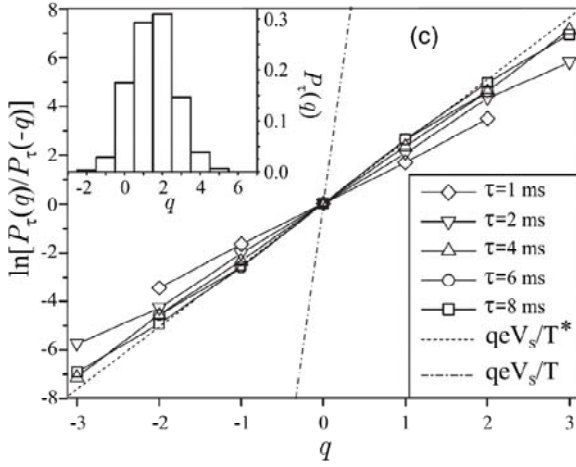
According to the second law of thermodynamics, the entropy of a macroscopic system driven out of equilibrium increases with time until equilibrium is reached. Thus the dynamics of such a system is irreversible. In contrast, for a mesoscopic system performing a random trajectory in phase space and measured during a sufficiently short time, the entropy may either increase or decrease. The “fluctuation theorem” (FT), which relies only on the microreversibility of the underlying equation of motion, states that the probability distribution  $P_\tau(\Delta S)$  for processes increasing or decreasing the entropy by  $\Delta S$  during a time interval  $\tau$  obeys the relation  $P_\tau(\Delta S)/P_\tau(-\Delta S) = \exp(\Delta S)$  [6]. Remarkably, this simple and universal relation remains valid even far from equilibrium. It has been proven for thermally equilibrated systems, Markovian stochastic processes, quantum systems, and mesoscopic conductors. The FT is fundamentally important for transport theory. One of its consequences is the Jarzynski equality, which in turn leads to the 2nd law of thermodynamics. It also leads to the fluctuation-dissipation theorem and Onsager symmetry relations, as well as to their extensions to nonlinear transport.

The FT was first tested in an experiment measuring the distribution of the work done on a colloidal particle placed in a water flow and trapped by an optical tweezer [7]. By monitoring the position fluctuations it is possible to estimate the work done on the particle. For this classical experiment the FT has been confirmed. Only recently experiments were performed with mesoscopic quantum systems [8]. In these experiments the statistics of single-electron tunneling in a double quantum dot



system in a GaAs/GaAlAs heterostructure was probed by an asymmetrically coupled quantum point contact, which allows resolving the direction of the tunneling process.

In Refs. [B2.2:28, B2.2:29] we analyzed these experiments in the frame of the FT. The entropy production is related to the Joule heating,  $\Delta S = qeV_S/T$ , where  $q$  is the number of electron charges  $e$  tunneling across a voltage drop  $V_S$ . Thus the FT simply reduces to  $P_\tau(-q)/P_\tau(q) = \exp(-qeV_S/T)$ . However, the experimental data appeared to violate the FT. After analyzing various potential sources for the discrepancy we concluded that the nonequilibrium shot noise of the quantum point contact (QPC) electrometer, which is used to study the transport, induces strong dot-level fluctuations which significantly influence the tunneling statistics. Taking these modifications into account we find consistency with the FT. We further find that the QPC back-action should only lead to an enhancement of the effective temperature, i.e. the FT relation should be replaced by the following one  $P_\tau(-q)/P_\tau(q) = \exp(-eV_S q/T^*)$ . This relation is indeed confirmed by the experiment with experimentally observed value of  $T^*$  agreeing well with theoretical estimates.



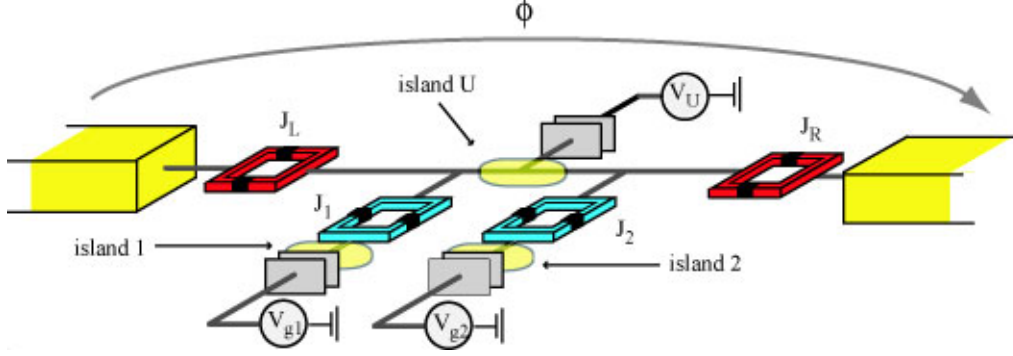
**Fig. 7.** Experimental test of the FT for several time intervals. *Inset:* the measured distribution  $P_\tau(q)$  at  $\tau = 4$  ms.

## 6. Quantum pumps

We have studied charge pumping in Josephson junction systems, i.e., adiabatic transport of charge in the absence of an external bias, induced by a cyclic modulation of the electrostatic potential. In phase-biased Josephson junction arrays in the regime in which the charging energy  $E_C$  is much higher than the Josephson energy  $E_J$ , charge pumping leads to adiabatic transport of single Cooper pairs. There are two reasons to study Cooper pair pumps (CPP): first, the control on the pumped charge in these systems reaches an accuracy that makes them potential candidates for a new metrological current standard. Second, it has been experimentally proven that the charge pumped over a cycle in a CPP is a geometric quantity, which can be directly related to the Berry's phase accumulated by the wave-function of the system.

When the quantum system which undergoes the adiabatic and cyclic evolution is in a degenerate energy eigenspace, the Berry's phase generalizes to a unitary and geometric transformation known as holonomy. We extended the theory of pumping to the case in which the CPP has a degenerate spectrum and related the pumped charge to the non-Abelian holonomy of Wilczek and Zee. We also designed a *non-Abelian superconducting pump*, shown in fig. 8, and discussed some observable effects of the non-Abelian geometric nature of the evolution on pumping [B2.2:15]. If tested experimentally our predictions would lead to the first clear observation of Wilczek- Zee non-Abelian holonomies. The experimental realization of the non-abelian superconducting pump may also have important consequences in the field of quantum computation, paving the way to the realization of holonomic geometric gates. Recently, we extended this work to spin pumping [9].

This work is part of our project in the DFG Priority Program “Semiconductor Spintronics” and is described in the reports of this grant.



**Fig. 8.** Setup of a non-Abelian superconducting pump.

## 7. Dissipation by quasiparticle tunneling and resistive circuits in superconducting electronics

We considered the effect of quasiparticle tunneling on energy relaxation processes in superconducting circuits for different ratios of  $E_J$  and  $E_C$  for both equilibrium and nonequilibrium situations. We conclude that devices with small ratios of  $E_J$  to  $E_C$  are only weakly sensitive to quasiparticle tunneling. The electron temperature has to be significantly enhanced as compared to the base temperature to create a strong influence. To test whether quasiparticle tunneling plays a role as a source of energy decay, direct measurements of the electron temperature should be performed. Additionally we find a phase dependence in the quasiparticle tunneling rates that corresponds to the well known  $\cos(\phi)$ -term in the RCSJ-model. This term has been known since the very first discussion of the Josephson-effect, but so far the experimental validation has proven difficult. At present we are working on a proposal to measure the phase dependence of energy decay rates by putting a SSET in a superconducting ring, and effectively combining the large matrix element of quasiparticle tunneling for large charging energy  $E_C$  with the ability to shift from additive to destructive interference in a controllable fashion.

We further considered charge transport in a superconducting single-electron transistor (SSET) with the gate lead connected resistively to the small island between the Josephson junctions. In the traditional SSET tunneling current between the source and drain are controlled by a gate capacitor. In our alternative setup the gate capacitor is replaced by a large resistor, with resistance larger than the quantum resistance  $R_Q$ . In this situation a net current from the gate into the island is possible, which in certain cases can provide low-noise amplification of the tunneling current. Then, instead of being a field-effect transistor, the device works analogously to the bipolar transistor. This type of low-noise current amplifier has a large field of applications, for example, in quantum metrology.

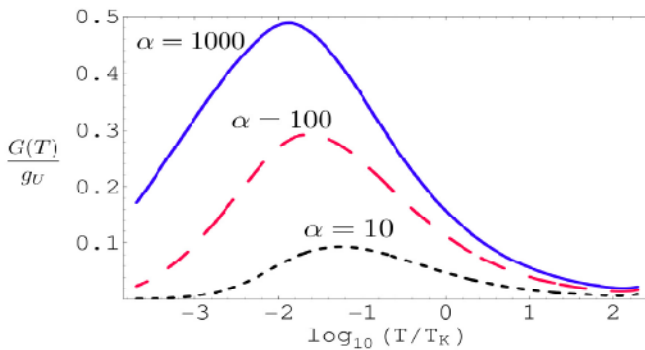
In the past it has been challenging to realize a resistive gate experimentally, as the on-chip resistor has to be large and in the immediate vicinity of the junctions. Also no previous theoretical framework exists for such a situation. At present we are developing the theory to study, together with experimentalists in Helsinki, charge transport in such a system. Novel peak-like features appear in the transport characteristics. These features might be used to provide current and voltage

amplification. In the frame of our theory we are able to explain these features quantitatively as resulting from the interplay of gate current fluctuations, due to Nyquist noise of the resistor, Coulomb blockade of Cooper-pair tunneling across single Josephson junctions, and the simultaneous supercurrent across both Josephson junctions.

## 8. The dynamics and transport properties of spin-1 quantum dot systems

Single-electron transistors (SET) allow probing physical phenomena otherwise inaccessible in bulk materials. Prominent examples are exotic variants of the Kondo effect, including underscreened and overscreened local moments. E.g., in a spin-1/2 SET with additional electron reservoir the overscreened Kondo effect, characterized by non-Fermi liquid behavior can be realized. Spin-1 SETs, which we considered in this project, allow us to probe in a controlled way the physics of the underscreened Kondo effect [B2.2:19]. In general, such transistors, or quantum dots, are described by a two-channel Kondo model with asymmetric coupling constants, so that the spin screening of the dot by the leads is expected to proceed via a two-stage process. When the Kondo temperatures  $T_{K1}$  and  $T_{K2}$  of each channel are widely separated, the dot passes upon cooling through a broad crossover regime  $T_{K2} \ll T \ll T_{K1}$  dominated by underscreened Kondo physics. In contrast to the overscreened Kondo effect, the low-energy excitations of the underscreened model are well defined and the impurity scattering of electrons is elastic. However, the phase scattering shift has a non-analytic energy dependence near the Fermi surface. In a bulk system this non-analyticity gives rise to singular thermodynamic behavior. In a SET the singular Fermi liquid behavior manifests itself in experimentally accessible transport properties, such as, for instance, the differential conductance.

We determined the temperature and voltage dependences of the differential conductance with results shown in fig. 9. At low temperatures, destructive interference between resonant scattering in both channels leads to a suppression of the conductance of the dot. We developed a microscopic model to describe the growth, and ultimate suppression, of the conductance in the two channel Kondo model as it is screened successively by its two channels. Our analysis is based on a large- $N$  approximation in which the localized spin degrees of freedom are described in the frame of the Schwinger boson formalism. The temperature dependence of the differential conductance for different ratios of two Kondo temperatures is demonstrated in the figure. As expected, the closer the two Kondo temperatures are to each other, the faster the differential conductance get suppressed.



**Fig. 9.** Differential conductance versus temperature for different ratio of the two Kondo temperatures.

## 9. Impurities and Bose-Einstein condensates

We considered an atomic quantum dot confined between two weakly coupled Bose-Einstein condensates, where the dot serves as an additional tunneling channel. It is shown that this embedded atomic quantum dot is a pseudospin subject to an external torque, and therefore equivalent to a

quantum top. We demonstrate in a numerical analysis of the time-dependent coupled evolution equations that this microscopic quantum top is very sensitive to any deviation from linear oscillatory behavior of the condensates. For sufficiently strong dot-condensate coupling, the atomic quantum dot can induce or modify the tunneling between the macroscopic condensates in the two wells [B2.2:7].

We studied an atomic quantum dot representing a single hyperfine “impurity” atom which is coherently coupled to two well-separated Bose-Einstein condensates, in the limit when the coupling between the dot and the condensates dominates the intercondensate tunneling coupling. It is demonstrated that the quantum dot by itself can induce large-amplitude Josephson-like oscillations of the particle imbalance between the condensates, which display a two-frequency behavior. For noninteracting condensates, we provide an approximate solution to the coupled nonlinear equations of motion which allows us to obtain these two frequencies analytically [B2.2:16].

**For references labeled as [B2.2:...] see the list of publications of the subproject.**

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