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TT 8.29 Fr 14:00 Poster TU C

Electronic and Optoelectronic Properties of Single-Molecule Junctions — •Joachim Reichert[1], Cao Qi[1], Harald Fuchs[1], Ivan Stich[2], and Dominik Marx[3] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität Münster, D - 48149 Münster — [2]Center for Computational Material Science, Slovak University of Technology, Ilkovicova 3, 812 19 Bratislava — [3]Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D - 44780 Bochum

Recent developments and advances in atomic-scale imaging and manipulation techniques enables access to a new field of single molecule experiments. Electronic transport measurements through single organic molecules which are immobilized by self assembling techniques between two metallic electrodes (e.g. mechanically controlled breakjunction [1]) as well as tunnelling experiments through molecular films with STM have proven the ability of organic molecules to act as functional parts in nanoscale-devices. Especially scanning near-field optical microscopy (SNOM) with its ability to apply an optical field to a molecular system in a controlled manner enlarges the range of experimental available properties in metal-anchored molecular junctions. With a combination of these techniques we want to study the electronic/optoelectronic properties of single molecules covalently linked between a metallic substrate and a SNOM-tip to improve the understanding of electronic transport through single molecules.

[1] J. Reichert, R. Ochs, D. Beckmann, H.B. Weber, M. Mayor, H. v. Löhneysen, Phys.Rev.Lett. 88, 176804 (2002). [2] H.-U. Danzebrink, U. C. Fischer, NATO ASI Series 242, 255, 303 (1993).

TT 8.30 Fr 14:00 Poster TU C

Discrete low-bias conductance fluctuations in molecular break-junctions — •Jan U. Würfel, Mark Elbing, Marcel Mayor, and Heiko B. Weber — Institut für Nanotechnologie, FZ Karlsruhe

We investigate the electronic transport properties of gold-molecule-gold junctions using the mechanically-controllable break-junction (MCBJ) technique. We have shown in former studies that under certain conditions single-molecule contacts could be achieved [1]. Here, we study the longterm stability (up to days) of stable and reproducible contacts, which show discrete transitions in the conductance at low bias ($\sim$ 10 mV). Some of the conductance values could be identified as integer multiples of a fixed value. This may suggest an integer number of molecules contributing. The findings are discussed.

[1] Phys. Rev. Lett., **88**, 176804 (2002)

TT 8.31 Fr 14:00 Poster TU C

A perturbative expansion of shot noise in quantum dots and molecules — •Matthias Hettler[1], Jasmin Aghassi[1,2], Axel Thielmann[1], Jürgen König[3], and Gerd Schön[1,2] — [1]Forschungszentrum Karlsruhe, Institut für Nanotechnologie,76021 Karlsruhe, Germany — [2]Institut für Theoretische Festkörperphysik , Universität Karlsruhe, 76128 Karlsruhe, Germany — [3]Institut für Theoretische Physik III, Ruhr-Universität Bochum, 44780 Bochum, Germany

We study current and shot noise in perturbation theory in the coupling of a mesoscopic object (e.g. quantum dot or molecule) to metallic electrodes. We explicitly account for the electronic interactions and the resulting many-body states of the molecule/quantum dots, and allow for relaxation of the excited states. We present in some detail the diagrammatic technique that allows for the computation of the noise to second order in the molecule-electrode coupling. In particular, we discuss the influence of co-tunneling processes as well as the effect of intermolecular (interdot) couplings and relaxation on the shot noise. Furthermore, we find the Fano factor to be very sensitive to the tunnel-coupling strength, which may serve as a spectroscopic tool for the various coupling strengths.

TT 8.32 Fr 14:00 Poster TU C

Nanoscale electrodes on cleaved edge semiconductor surfaces for molecular electronics applications — •Sebastian Strobel[1], Sebastian Luber[1], Dieter Schuh[1], Werner Wegscheider[2], and Marc Tornow[1] — [1]Walter Schottky Institut, TU München, 85748 Garching, Germany — [2]Institut für Angewandte und Experimentelle Physik, U Regensburg, 93040 Regensburg, Germany

Current efforts in molecular electronics target at novel concepts for future nano-electronics thereby aiming at a fundamental understanding of charge transfer mechanism in (bio-) molecular "wires" such as DNA. Starting point is the preparation of suitable nanogap - electrodes that serve as electrical contacts to the molecules.

We present a novel strategy based on a semiconductor heterostructure grown by molecular beam epitaxy that consists of a AlGaAs layer into which a thin layer of GaAs (5 - 20 nm) is embedded. After cleaving the structure an atomically flat plane is obtained. Subsequent selective etching of the GaAs layer perpendicular to that plane and evaporation of a few nanometer thick metal film yields the nano-gap electrodes.

We successfully bridged nano-gap electrodes with single, 30 nm diameter colloidal Au nano-particles by AC electric trapping. The resulting drop in resistance of up to seven orders of magnitude verified the electrical functionality of our devices. First measurements on electrodes functionalized with organic self-assembled monolayers will be presented.

TT 8.33 Fr 14:00 Poster TU C

Multiphoton photofieldemission in electromigrated nanogaps — •S. Dantscher[1], D. Wolpert[1], W. Pfeiffer[1], J. U. Würfel[2], and H. B. Weber[2] — [1]Physikalisches Institut, Universität Würzburg, Am Hubland, 97074 Würzburg — [2]FZ Karlsruhe, Institut für Nanotechnologie, PO-Box 3640, 76021 Karlsruhe

The combination of nanocontacts and laser excitation offers the possibility of studying photoinduced nonequilibrium transport phenomena and therefore also electron dynamics on the nanometer scale. Using the method of electromigration, contacts with electrode distances in the range of several nanometers can be produced. For relatively large gaps no tunnel current is detectable, i.e. with a moderate applied DC bias, that avoids field emission, these junctions carry no significant current.

We have investigated photocurrents in such contacts under illumination with ultrashort femtosecond laserpulses. The use of a microscope objective as focusing element provides focal radii down to $2\mu m$ resulting in maximum intensities during the pulses of $10^{10} W/cm^2$. Under these conditions and with bias voltages in the range of $\pm$ 5V photo induced currents are detected. The intensity dependences exhibit power laws with exponents up to 3, indicating that multiphoton excitation is responsible for the detected current. Moreover the multiphoton order depends on the actual junction parameters, such as the applied bias. This suggests that the photocurrent flows in the nanogap. The observed bias dependence is attributed to photofieldemission, i.e. the multiphoton photocurrent is influenced by the static field distribution in the gap. In addition, also dynamic field effects might affect the signals.

TT 8.34 Fr 14:00 Poster TU C

Molecular conductance at finite voltage: bias driven evolution of Kohn-Sham-orbitals — •Max Koentopp, Ferdinand Evers, Florian Weigend, Mark Elbing, Rolf Ochs, Marcel Mayor, and Heiko Weber — Institut für Nanotechnologie, Forschungszentrum Karlsruhe, 76021 Karlsruhe, Germany

Ground state density functional theory calculations yield the exact electron density if the exact exchange-correlation functional is employed.

The evolution of the equilibrium density with parametric changes in the Hamiltonian, e.g. realized by a change in the electrostatic potential, can provide crucial information about transport properties, like the Coulomb blockade.

To test our ideas, we perform model calculations using TURBOMOLE for a diode molecule, which exhibits a structure of a double quantum dot and has been investigated experimentally [1]. In particular, we investigate the origin of the characteristic peak structure in the differential conductance. Our results are consistent with the interpretation that the stepwise increase of the conductance occurs when the number of occupied levels of one of the dots, that have an energy above the lowest unoccupied level of the other dot, increases by one.

[1] M. Elbing, R. Ochs, M. Mayor, H. Weber, M. Koentopp, F. Evers, F. Weigend, Proc. Nat. Acad. Sci. USA, submitted.

TT 8.35 Fr 14:00 Poster TU C

Manipulating a molecule's conformation with gates: a molecular switch — •Andreas Arnold, Max Koentopp, Ferdinand Evers, and Oliver Rubner — Institut für Nanotechnologie, Forschungszentrum Karlsruhe, 76021 Karlsruhe, Germany

Molecules can undergo a conformational change when being charged. For molecules connected to external leads their excess charge becomes a parameter that can be tuned by means of a gate. Therefore, the mole-

cular conformation can be controlled at will, which may proove useful for potential applications, e. g. a molecular switch. We present a calculation based on density functional theory using TURBOMOLE for the model system bipyridine. Our calculation shows, that the equilibrium angle between the two benzene rings can indeed be controlled by the gate voltage. In particular, adding an excess charge of 2 electrons to the molecule takes the system from a strongly tilted, low conductance state over into an almost planar, high conductance configuration.

TT 8.36 Fr 14:00 Poster TU C

Perfekte Quanteninformationsbertragung in Spinketten — •Peter Karbach und Joachim Stolze — Institut für Physik, Universität Dortmund, 44221 Dortmund

Gekoppelte Spins 1/2 werden in der Quanteninformationsverarbeitung viel diskutiert, in letzter Zeit zunehmend auch als Mittel zum *Transport* von Quanteninformation. Hierbei spielen eindimensionale Systeme (Spinketten) naturgemäß eine besonders wichtige Rolle. Die kürzlich gefundene *perfekte* Abbildung eines Zustands zwischen dem ersten und letzten Spin einer speziellen inhomogenen XX-Kette (Christandl et al., PRL **92**, 187902 (2004)) kann verallgemeinert werden auf die „Spiegelung“ eines Zustands zwischen den beiden Hälften der Kette (Albanese et al. quant-ph/0405029). Wir zeigen, wie die beiden einzigen bisher bekannten Ketten mit perfekter Spiegelung eines Zustands nahezu beliebig verallgemeinert werden können. Hierzu muss nur das Einteilchen-Energiespektrum der Spinkette in der Darstellung wechselwirkungsfreier spinloser Fermionen gewisse Eigenschaften besitzen. Wir diskutieren Beispiele perfekt spiegelnder Spinketten und demonstrieren deren Eigenschaften; z.B. sind alle Autokorrelationen dieser Systeme für beliebige Temperaturen strikt periodisch.

TT 8.37 Fr 14:00 Poster TU C

Long Josephson junctions as vortex qubits — •A. Kemp, A. N. Price und A. V. Ustinov — Physikalisches Institut III, Universität Erlangen-Nürnberg, Erwin-Rommel-Str 1., 91058 Erlangen, Germany

We have investigated the properties of Josephson vortices in annular Josephson junctions of circumference comparable to the Josephson penetration depth, at millikelvin temperatures. The fluctuation-induced activation of these vortices exhibits a systematic magnetic field and temperature dependence. We evaluate the height of the potential barrier between two spatially separated vortex states in long heart-shaped junctions. Reproducibility of the initial vortex state is guaranteed through the use of current injectors. Such injected fluxons are manipulated by means of homogeneous magnetic fields produced by microstrips carrying rectangular pulses. Low temperature microwave transmission characteristics show that such microstrips offer the possibility to control the barrier height of a vortex qubit on sub-nanosecond timescales.

TT 8.38 Fr 14:00 Poster TU C

Driven two-level system in a photonic crystal — •Geesche Boedecker and Carsten Henkel — Institut für Physik, Universität Potsdam, Am Neuen Palais 10, 14469 Potsdam

We discuss a specific system-reservoir model with strong coupling and long-range temporal memory in the bath. The model can be physically realized with a coherently driven two-level system embedded in a photonic crystal. The problem differs from the usual spin-boson setting in several respects: the bath is essentially at zero temperature, its spectral density is zero in some finite frequency interval (photonic bandgap), and the two-level system is only coupled to near-resonant bath modes (rotating wave approximation). Its emission spectrum has been characterized only in the weak coupling limit in the quantum optics literature. We discuss here numerically exact simulation schemes for this non-Markovian problem and compare them to approximations based on the path integral formulation.

TT 8.39 Fr 14:00 Poster TU C

Bi- and tripartite entanglement in a flux-qubit triangle — •Johannes Ferber and Frank Wilhelm — LMU München, Department für Physik, and CeNS

We are investigating a system of three superconducting flux qubits, inductively coupled by a surrounding loop or via shared lines.

We derive the possible coupling strength between the qubits and determine the energy level structure. We show, that for a proper and physical choice of parameters, the system shows strong three-qubit entanglement, quantified by the 3-tangle of the system [1].

Systems consisting of three qubits provide the possibility of examining quantum nonlocality using GHZ-states in a potentially more convenient way than the two-qubit Bell inequality. Based on our results, we discuss the feasibility of such a GHZ-experiment using flux qubits. Moreover, we outline applications of three-bit interactions to the acceleration of quantum algorithms.

[1] V. Coffmann, J. Kundu, and W. K. Wooters, Phys. Rev. **A 61**, 052306 (2000).

TT 8.40 Fr 14:00 Poster TU C

Continuous measurement of two spin qubits in quantum dots — •Holger Schaefers and Walter T. Strunz — Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg, Germany

We investigate two electron spin qubits in quantum dots. The spins are measured by separate currents through the dots. Our approach is based on quantum trajectories , widely used in quantum optics, here adapted to describe conditional quantum dot dynamics in a fermionic environment. We use the quantum trajectory approach to simulate the quantum dynamics conditioned on the continuous measurement outcome, here the electron currents through the dots. We investigate counting statistics of the currents with respect to signatures of entanglement of the spins.

TT 8.41 Fr 14:00 Poster TU C

Fabrication of superconducting qubit stuctures — •Georg Wild, Tobias Heimbeck, Heribert Knoglinger, Karl Madek, Matteo Mariantoni, Christian Probst, Achim Marx, and Rudolf Gross — Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany

Solid state based quantum bits (qubits) promise to be producible using present day micro- and nanofabrication technologies thus allowing scalability up to systems comprising a large number of qubits. Superconducting qubits are advantageous because of the superconducting energy gap. Superconducting qubits based on Josephson junctions where the Josephson coupling energy is larger than the charging energy are usually called flux qubits. We are fabricating flux qubits with different designs based on Al/Al_2O_3 tunnel junctions. Measurements on various test structures (Josephson junctions, SQUIDs, qubits) help to analyze and further optimize the system parameters and to compare the different qubit variants. Flux qubits require an external magnetic field bias generating half a flux quantum in the ring defining the qubit to reach the degeneracy point. To shift this degeneracy point to zero field a π-shift element has to be inserted into the ring. We have started to develop a process to fabricate π-shifters based on superconductor/ferromagnet/superconductor Josephson junctions where a thin ferromagnetic NiPd layer is embedded between two Nb layers. This work was supported by the Sonderforschungsbereich 631 of the Deutsche Forschungsgemeinschaft.

TT 8.42 Fr 14:00 Poster TU C

Low temperature setup for characterization of superconducting qubits — •Karl Madek, Tobias Heimbeck, Heribert Knoglinger, Matteo Mariantoni, Christian Probst, Georg Wild, Achim Marx, and Rudolf Gross — Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany

In recent years interest in quantum computing has been continously growing. Because of the superconducting energy gap superconducting devices are promising candidates for quantum bits suggesting sufficiently large decoherence times. In order to experimentally investigate superconducting qubits well shielded low temperature measurement setups are required. We have established a dilution unit with several layers of mumetal and cryoperm shields and several stages of low pass filters at different temperatures in the biasing lines. A semirigid coaxial cable with thermally anchored attenuators is used for microwave spectroscopy on superconducting devices. Furthermore, the whole setup is placed in a shielded room. Measurements of the escape rate of Josephson junctions out of the zero voltage state using a current ramping technique serve to evaluate the quality of the shielding. The observation of a crossover from the quantum tunneling regime to the thermal regime shows the negligibility of noise. This work was supported by the Sonderforschungsbereich 631 of the Deutsche Forschungsgemeinschaft.