

son tunnel junctions with a critical current density around 500 A/cm². We have also developed a design for reading out such qubits using inductive coupling. Results reflecting actual progress in this experiment will be presented.

[1] I. Chiorescu et al., *Science* **299**, 1869 (2003)

[2] S.P. Yukon, *Physica C* **368**, 320 (2002)

[3] J.I. Cirac and P. Zoller, *Phys. Rev. Lett.* **74**, 4091 (1995)

TT 26.23 Wed 14:30 P1

Long Josephson junction filters for qubit control — ●H. H. EGLMEIER¹, A. KEMP¹, V.S. KAPLUNENKO², and A. V. USTINOV¹ — ¹University of Erlangen-Nuremberg — ²Stanford linear accelerator, metrological measurement

Josephson junctions have been demonstrated to perform as macroscopic quantum systems with a well-controlled Hamiltonian. Most superconducting qubits require magnetic flux control for their operation. One choice is to use rapid single flux quantum (RSFQ) logic for qubit control and interfacing with room temperature electronics.

Decoherence due to 1/f noise in the RSFQ circuitry leads to the need for efficient low-frequency isolation between the control circuitry and the qubit. We present characterization measurements and simulations of a novel low-pass filter based on a long Josephson junction.

An input signal fed into the long junction is transmitted only if its frequency exceeds the plasma frequency of the junction, otherwise it is attenuated as an exponentially vanishing (evanescent) wave. For qubit control one can use low frequency signals which are only transmitted as multiples of the flux quantum. The transmission properties of the filter in the GHz range are currently investigated experimentally.

TT 26.24 Wed 14:30 P1

Preparation and readout of bistable vortex states in a long annular Josephson junction containing a lithographic microshort. — ●ALEXANDER KEMP, ASTRIA PRICE, and ALEXEY V. USTINOV — Physikalisches Institut III, Universitaet Erlangen-Nuernberg, Erlangen D-91058, Germany

We demonstrate classical state preparation and readout for a novel type of vortex qubit, in which a short section of the insulating barrier of a long annular Josephson junction is made slightly wider. This section of the junction acts like a microshort, where the height of the potential barrier so created can be tuned during experiment by varying the strength of an applied in-plane magnetic field. We develop a model for the double well potential, based on the one-dimensional sine-Gordon equation, in which the change in vortex rest mass energy due to the wider section of the junction is explicitly considered, and find the magnetic field dependence of the barrier height. Good agreement with measured vortex depinning currents from each well is obtained. The vortex was prepared in a given well by applying a series of "shaker" bias current pulses to the junction.

TT 26.25 Wed 14:30 P1

Frequency dependence of full counting statistics in AC-biased mesoscopic conductors — ●DMITRY BAGRETS¹ and FABIO PISTOLESI² — ¹Institut für Theoretische Festkörperphysik, Universität Karlsruhe, D-76128, Karlsruhe, Germany — ²Laboratoire de Physique et Modélisation des Milieux Condensés, CNRS-UJF B.P. 166, F-38042 Grenoble, France

We develop a theory to obtain the current noise and the full counting statistics of charge transfer for AC biased mesoscopic conductors. We illustrate the theory by considering two specific examples: a diffusive wire and a chaotic quantum dot. We find that all cumulants of current fluctuations depend on the frequency Ω of the external AC field on the scale of the inverse diffusion time through the structure. This dependence stems from the multiple photon absorption processes and disappears when the AC voltage amplitude V is much smaller than $\hbar\Omega/e$ (e being the electron charge). The detection of the frequency dependence of the second cumulant, the current noise, is within reach of present experimental technology.

TT 26.26 Wed 14:30 P1

Full Counting Statistics of an Aharonov-Bohm Interferometer with an embedded Quantum Dot — ●DANIEL URBAN and JÜRGEN KÖNIG — Ruhr-Universität Bochum, 44780 Bochum, Germany

The electron's wave nature becomes apparent in Aharonov-Bohm interferometers, where constructive and destructive interference between two electron paths can be observed. The visibility of the Aharonov-Bohm

signal provides information on the coherence of transport channels.

Correlations of electron transport are reflected in shot noise and higher moments of the current distribution. These reveal information not contained in the average current. All moments can be conveniently extracted from the Cumulant Generating Function, whose calculation is the aim of Full Counting Statistics (FCS).

Originally developed for situations without interaction FCS has recently been extended to strongly interacting systems such as quantum dots. Treating the coupling to the leads perturbatively, it was found that non-Markovian effects cannot be neglected [1]. We expand this scheme to describe a quantum dot embedded in an Aharonov-Bohm geometry.

[1] A. Braggio, J. König, and R. Fazio, cond-mat/0507527, submitted to *Phys. Rev. Lett.*

TT 26.27 Wed 14:30 P1

Revealing entanglement of spin qubits with counting statistics — ●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 propose a simple experiment and give a sufficient criterion for revealing entanglement with the help of counting statistics.

TT 26.28 Wed 14:30 P1

Molecular conductance from ab initio calculations: self energies and absorbing boundary conditions — ●ANDREAS ARNOLD¹ and FERDINAND EVERS² — ¹Institut für Theorie der kondensierten Materie, Universität Karlsruhe, 76128 Karlsruhe, Germany — ²Institut für Nanotechnologie, Forschungszentrum Karlsruhe, 76021 Karlsruhe, Germany

Calculating an exact self energy for ab initio transport calculations relevant to *Molecular Electronics* can be troublesome. Errors or insufficient approximations made at this step are a frequent reason why many molecular transport studies become inconclusive. We propose a simple and efficient approximation scheme, that follows from interpreting the self energy as an absorbing boundary condition of an effective Schrödinger equation. Our approximation is controlled by a small parameter, which essentially is the inverse number of electrode atoms, that are kept in the ab initio calculation.

The method is illustrated using a tight binding wire as a toy model, for which an analytical solution is available, against which we can check our numerical results. Also more realistic applications for transport calculations based on the density functional theory have been performed. They yield results in very good agreement with the conventional way to set up the electronic self energy.

TT 26.29 Wed 14:30 P1

Structure and conductance histogram of atomic-sized Au contacts — ●MARKUS DREHER¹, FABIAN PAULY², JAN HEURICH², CARLOS CUEVAS^{2,3}, ELKE SCHEER¹, and PETER NIELABA¹ — ¹Physics Department, University of Konstanz, 78457 Konstanz, Germany — ²Institut für Theoretische Festkörperphysik, University of Karlsruhe, 76128 Karlsruhe, Germany — ³Forschungszentrum Karlsruhe, Institut für Nanotechnologie, 76021 Karlsruhe

Many experiments have shown that the conductance histograms of metallic atomic-sized contacts exhibit a peak structure, which is characteristic for the corresponding material. The origin of these peaks still remains as an open problem. In order to shed some light on this issue, we present a theoretical analysis of the conductance histograms of Au atomic contacts. We have combined classical molecular dynamics simulations of the breaking of nanocontacts with conductance calculations based on a tight-binding model. This combination gives us access to crucial information such as contact geometries, forces, minimum cross section, total conductance and transmission coefficients of the individual conduction channels.

The ensemble of our results suggests that the low temperature Au conductance histograms are a consequence of a subtle interplay between mechanical and electrical properties of these nanocontacts. At variance with other suggestions in the literature, our results indicate that the Au conductance histograms are not a simple consequence of conductance

quantization or of existence of exceptionally stable radii.

TT 26.30 Wed 14:30 P1

Absence of fractional conductance quantization in ferromagnetic atomic contacts — ●MICHAEL HÄFNER¹, JUAN-CARLOS CUEVAS^{1,2,3}, JANNE VILJAS¹, DIEGO FRUSTAGLIA³, and FABIAN PAULY¹ — ¹Institut für Theoretische Festkörperphysik, Universität Karlsruhe, 76128 Karlsruhe, Germany — ²Departamento de Física Teórica de la Materia Condensada C-V, Universidad Autónoma de Madrid, 28049 Madrid, Spain — ³Quantum Transport and Information, Scuola Normale Superiore, 56126 Pisa, Italy

In this work we present a theoretical analysis of the current through atomic contacts of ferromagnetic materials (Co and Ni). Several experimental groups have recently reported the observation of half-integer conductance quantization in nanowires of these materials. This suggests that the current in these contacts is completely spin polarized and all the contributing channels are perfectly transmissive. In order to analyze these surprising observations, we have performed conductance calculations of Ni and Co atomic junctions based on a tight-binding model. Contrary to these experiments, we find that the conductance is in general neither quantized nor spin polarized. We show that the transport is mainly dominated by both the s and d bands close to the Fermi energy. These bands give rise to several conduction channels that are partially open. Typically, both spin bands give a significant contribution to the transport suggesting that the fractional conductance quantization should not appear in ferromagnetic atomic contacts.

TT 26.31 Wed 14:30 P1

Influence of vibrations on electronic transport through DNA — ●BENJAMIN SCHMIDT^{1,2}, MATTHIAS HETTLER², GERD SCHÖN^{1,2}, E.B. STARIKOV², and WOLFGANG WENZEL² — ¹Institut für Theoretische Festkörperphysik, Universität Karlsruhe, 76128 Karlsruhe, Germany — ²Institut für Nanotechnologie, Forschungszentrum Karlsruhe, 76021 Karlsruhe, Germany

Conductance measurements on DNA 'wires' display various types of behavior ranging from insulating over semi-conducting to quasi-metallic, depending on the measurement setup and the measured DNA molecule. The variance of the experimental results as well as ab-initio calculations suggest that the environment and vibrational modes of DNA have a dominating influence on the transport properties of DNA wires. In this work we study transport through simple models of homogeneous DNA wires (poly-DNA) using standard Green function technique and Landauer-Buettiker formalism. In particular, we address the influence of specific DNA vibrational modes (with parameters determined by ab-initio methods) on transport in the presence of an environment described by a general bosonic bath. We can describe the crossover from semi-conducting to quasi-metallic behavior in dependence of temperature and the electronic coupling to the vibrational modes and bath.

TT 26.32 Wed 14:30 P1

Influence of Adsorbates on the Structure and Electronic Properties of Molecular-size Junctions — ●SÖREN WOHLTHAT¹, FABIAN PAULY¹, JANNE VILJAS¹, JUAN-CARLOS CUEVAS^{2,1,3}, and GERD SCHÖN^{1,3} — ¹Institut für Theoretische Festkörperphysik, Universität Karlsruhe, D-76128 Karlsruhe — ²Departamento de Física Teórica de la Materia Condensada C-V, Universidad Autónoma de Madrid, E-28049 Madrid, Spain — ³Forschungszentrum Karlsruhe, Institut für Nanotechnologie, 76021 Karlsruhe

During the last few years, the conduction properties of molecular-size contacts between two metallic leads have attracted a great deal of attention. Motivated by recent experiments concerning the effect of hydrogen [1] and oxygen [2] on metallic nanocontacts, we investigate theoretically the influence of adsorbates on this type of junctions. We analyse the stability of different geometries and determine their electronic transport properties. The calculations are based on density functional theory (DFT) using the quantum chemistry package TURBOMOLE. The electronic transport properties are obtained by non-equilibrium Green's function (NEGF) techniques. Our simulations show that adsorbates have a significant influence on the properties of our molecular-size junctions and that they could serve as design tools for future atomic and molecular circuits.

[1] R.H.M. Smit et al., Nature 419, 906, (2002).

[2] W.H.A. Thijssen et al., cond-mat/0509376.

TT 26.33 Wed 14:30 P1

First-principles study of single row Al and Pt wires — ●THOMAS GNIELKA^{1,2}, KLAUS-PETER BOHNEN¹, and ROLF HEID¹ — ¹Forschungszentrum Karlsruhe, Institut für Festkörperphysik, D-76021 Karlsruhe — ²Universität Karlsruhe, Fakultät für Physik, D-76128 Karlsruhe

Over the past several years there has been a great deal of interest in the physical properties of atomic wires. Although there have been some studies of the structural and electronic properties of nanowires so far lattice dynamics of these systems has been hardly studied. This is in strong contrast to the importance of lattice dynamics for structural stability (Peierls transition) and superconductivity. Thus we have investigated the lattice dynamics, the atomic and electronic structures and the relation between them for single-row Al and Pt wires using density-functional theory. The calculations reveal that the wires transform from planar zigzag structure to linear and further to dimerized wires during elongation. Phonon dispersions have been calculated and anomalies nicely correlate with Fermi surface nesting effects. Dimerization effects as seen for Pt wires on Ge(100) seem to be qualitatively in agreement with these findings, however the substrate influence has still to be studied. Preliminary results seem to indicate the importance of substrate effects.

TT 26.34 Wed 14:30 P1

Transport properties of carbon nanotubes synthesized by chemical vapor deposition — ●T. PIETSCH, I. MÖNCH, J. SCHUMANN, K. BIEDERMANN, H. VINZELBERG, and B. BÜCHNER — IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany

The electrical properties of multiwalled carbon nanotubes (MWCNT) synthesized by chemical vapor deposition (CVD) depend on the used CVD method. In this work we investigate MWCNT with outer diameters from 30 to 60 nm and length over 6 μm grown by a thermal-catalytic CVD method. TEM images show that the concentric layers of the nanotubes are not perfect. The MWCNT devices for the transport measurement with low ohmic contacts were prepared by using an ac-electrophoresis deposition either on Ti-microfinger structures followed by a HV annealing at 800°C or on oxidized silicon wafers with prestructured leads, electron beam lithography, oxygen plasma treatment and evaporated Cr/Au contacts on the nanotubes. The contact resistance are for the Ti contacts about 50 k Ω and for the Cr/Au contacts smaller than 1 k Ω . The average intrinsic room temperature resistance of the MWCNT measured in four-point configuration is 1500 $\mu\Omega\text{cm}$ and comparable to that of natural graphite of 1350 $\mu\Omega\text{cm}$. At room temperature the current-voltage characteristics are linear but at low temperatures not linear. The temperature coefficient of the zero-bias resistance in the temperature range between 300K and 4.2K is negative. Positive magnetoresistances at 4.2K of about 2 % at 8T were measured. The results show that - caused by the defect structure of the MWCNT walls - the conduction is diffusive.

TT 26.35 Wed 14:30 P1

Transport through molecules — ●BERND BRIECHLE, SIMON VERLEGER, and ARTUR ERBE — Universität Konstanz, Fachbereich Physik, 78457 Konstanz

The aim of our studies is the characterisation of electronic transport through a single or a few molecules. It is important that the coupling of the molecules to the electrodes is mechanically and electronically stable throughout the experiment. As a first step two different structures allowing for the change of the mechanical coupling will be analysed to find an optimal configuration. On the one hand a mechanically controllable break-junction (MCB) technique will be studied, on the other a shadow evaporation technique based on a silicon structure will be tested. Transport through the molecules can be investigated at different temperatures. Additionally the integration of a gate electrode for detailed characterisation of the charge transport is in preparation.

TT 26.36 Wed 14:30 P1

Hofstadter butterfly of carbon nanotubes — ●NORBERT NEMEC and GIANAURELIO CUNIBERTI — Institut für theoretische Physik, Universität Regensburg, 93040 Regensburg

The electronic spectrum of a two dimensional square lattice in a perpendicular magnetic field, known as Hofstadter butterfly, was discovered in Regensburg thirty years ago [1]. We have calculated the Hofstadter butterfly for carbon nanotubes (CNTs) in the tight-binding approximation. For the case of single wall CNTs, it is straightforward to imple-